

## Oxidation Dynamics of Methionine with Singlet Oxygen:

### Effects of Methionine Ionization and Microsolvation

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#### Cartesian coordinates for all the structures in Figure 1, optimized at B3LYP/6-311++G(d,p)

##### [Met - H]<sup>-</sup>\_1

C1 -2.426315 0.606942 -0.040173  
C2 -1.302707 -0.379512 0.465707  
C3 0.042901 0.024575 -0.166378  
C4 1.214428 -0.743039 0.438216  
S5 2.862810 -0.436553 -0.328022  
C6 3.107292 1.329056 0.073884  
O7 -3.275206 0.104883 -0.818257  
O8 -2.327688 1.782639 0.377644  
N9 -1.601112 -1.798885 0.173701  
H10 -1.223209 -0.242333 1.550825  
H11 -2.287585 -1.750399 -0.585083  
H12 -2.120669 -2.187041 0.955834  
H13 0.161133 1.101567 -0.026394  
H14 -0.001159 -0.169964 -1.243846  
H15 1.049842 -1.815969 0.317865  
H16 1.305260 -0.538479 1.510759  
H17 4.102429 1.602453 -0.281702  
H18 3.059544 1.491577 1.153249  
H19 2.366803 1.957324 -0.421693

##### [Met - H]<sup>-</sup>\_2

C1 1.859224 0.801124 -0.181312  
C2 1.496292 -0.727012 -0.281165  
C3 0.030157 -0.946816 0.155879  
C4 -0.987337 -0.336421 -0.807940  
S5 -2.735601 -0.377216 -0.217912  
C6 -2.688758 0.973442 1.012627  
O7 2.467001 1.142863 0.863337

O8 1.468437 1.516048 -1.136311  
N9 2.372160 -1.582862 0.548873  
H10 1.596173 -1.034715 -1.328241  
H11 2.637692 -0.981207 1.332886  
H12 3.243189 -1.719448 0.041762  
H13 -0.089013 -0.516439 1.157015  
H14 -0.145963 -2.023153 0.252591  
H15 -1.006071 -0.894112 -1.748951  
H16 -0.723176 0.693934 -1.050869  
H17 -3.701450 1.088596 1.403649  
H18 -2.373913 1.907281 0.543615  
H19 -2.013928 0.737564 1.836291

##### [Met - H]<sup>-</sup>\_3

C1 2.270310 -0.446548 -0.042995  
C2 1.345735 0.636632 0.642928  
C3 -0.071509 0.080014 0.896773  
C4 -0.765644 -0.333069 -0.398254  
S5 -2.540119 -0.802222 -0.222759  
C6 -3.299742 0.841639 0.018994  
O7 2.833515 -0.088717 -1.107848  
O8 2.334753 -1.541764 0.557105  
N9 1.294896 1.887035 -0.144774  
H10 1.791837 0.822569 1.628463  
H11 1.916950 1.710288 -0.938708  
H12 1.704691 2.649887 0.383265  
H13 -0.659646 0.853953 1.405108  
H14 0.004800 -0.784359 1.560012  
H15 -0.285103 -1.220104 -0.816016  
H16 -0.704053 0.465311 -1.140822  
H17 -4.378767 0.690008 0.088109  
H18 -3.084673 1.496111 -0.828559

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H19 -2.949442 1.314475 0.937975

[Met - H]<sub>4</sub>

C1 -2.104955 -0.564970 -0.084805  
 C2 -1.049613 0.575302 -0.339889  
 C3 0.009306 0.563835 0.782899  
 C4 0.956858 -0.639004 0.761810  
 S5 2.285016 -0.577060 -0.514696  
 C6 3.344266 0.748700 0.162487  
 O7 -3.218226 -0.187166 0.357091  
 O8 -1.705589 -1.733193 -0.314744  
 N9 -1.667021 1.918624 -0.407865  
 H10 -0.541188 0.368075 -1.286372  
 H11 -2.542321 1.815908 0.113106  
 H12 -1.965970 2.079905 -1.365918  
 H13 -0.513806 0.565263 1.749009  
 H14 0.565825 1.506190 0.737410  
 H15 0.385475 -1.539399 0.523689  
 H16 1.451297 -0.776513 1.729131  
 H17 4.205036 0.843172 -0.502562  
 H18 3.699835 0.494209 1.164865  
 H19 2.820060 1.705468 0.194046

[Met - H](H<sub>2</sub>O)<sub>1</sub>

C1 1.918551 0.124102 0.210611  
 C2 0.592830 0.901540 0.510970  
 C3 -0.587899 0.135825 -0.118178  
 C4 -1.935682 0.696513 0.326039  
 S5 -3.418340 -0.057171 -0.462674  
 C6 -3.321916 -1.766393 0.176445  
 O7 2.688767 0.647163 -0.636214  
 O8 2.064923 -0.958943 0.829762  
 N9 0.607328 2.298701 0.033917  
 H10 0.460233 0.897858 1.598787  
 H11 1.266225 2.298795 -0.747672  
 H12 1.057846 2.875482 0.738761  
 H13 -0.488001 -0.915495 0.161643  
 H14 -0.508208 0.198452 -1.209102  
 H15 -1.994616 1.756280 0.069839  
 H16 -2.055767 0.610748 1.411480  
 H17 -4.214249 -2.287456 -0.174788  
 H18 -3.315265 -1.772640 1.268887  
 H19 -2.438311 -2.284516 -0.196830  
 O20 4.571265 -1.529970 -0.416694  
 H21 3.812782 -1.687233 0.177001  
 H22 4.264523 -0.681984 -0.782788

[Met - H](H<sub>2</sub>O)<sub>2</sub>

C1 -2.343196 -0.051610 -0.360263  
 C2 -1.173100 -0.681688 0.473366

C3 0.160240 -0.447747 -0.264714  
 C4 1.362113 -0.831345 0.593645  
 S5 3.006256 -0.664307 -0.217796  
 C6 3.103159 1.150118 -0.422576  
 O7 -3.113596 -0.846868 -0.933858  
 O8 -2.374571 1.212727 -0.384386  
 N9 -1.364400 -2.122050 0.740382  
 H10 -1.129259 -0.145844 1.428382  
 H11 -1.977046 -2.443645 -0.012607  
 H12 -1.925291 -2.223732 1.581441  
 H13 0.212089 0.605657 -0.547284  
 H14 0.163670 -1.041787 -1.185438  
 H15 1.294673 -1.883642 0.876601  
 H16 1.386293 -0.238258 1.513544  
 H17 4.095973 1.371519 -0.818658  
 H18 2.978938 1.654729 0.537407  
 H19 2.349370 1.516094 -1.119340  
 O20 -0.774847 3.050792 0.717125  
 H21 -1.211812 3.841111 0.389427  
 H22 -1.338078 2.311486 0.350795

[Met - H](H<sub>2</sub>O)<sub>3</sub>

C1 -1.945535 -0.559355 -0.085849  
 C2 -0.571800 -1.078503 0.467230  
 C3 0.569188 -0.267265 -0.177813  
 C4 1.917712 -0.558153 0.474291  
 S5 3.377365 0.255874 -0.298212  
 C6 3.000177 2.016710 0.012296  
 O7 -2.549413 -1.310574 -0.877273  
 O8 -2.275027 0.588853 0.323670  
 N9 -0.362160 -2.522597 0.240180  
 H10 -0.563513 -0.880783 1.545210  
 H11 -0.945618 -2.740844 -0.571132  
 H12 -0.794558 -3.035763 1.003106  
 H13 0.312851 0.791394 -0.094664  
 H14 0.619130 -0.514895 -1.243934  
 H15 2.132180 -1.626894 0.410759  
 H16 1.905940 -0.284529 1.534939  
 H17 3.856586 2.592290 -0.343366  
 H18 2.867502 2.203250 1.080610  
 H19 2.108587 2.336521 -0.527510  
 O20 -4.328020 2.332434 -0.002803  
 H21 -3.920353 2.937199 0.622861  
 H22 -3.680225 1.580940 -0.016430

[Met - H](H<sub>2</sub>O)<sub>4</sub>

C1 -1.723210 1.090802 -0.036713  
 C2 -0.778848 -0.089737 0.404623  
 C3 0.622207 0.115619 -0.199207  
 C4 1.664978 -0.804595 0.429912

S5 3.351105 -0.721973 -0.305041  
 C6 3.834521 0.987315 0.125287  
 O7 -2.782809 0.770853 -0.652215  
 O8 -1.329807 2.233309 0.265033  
 N9 -1.255241 -1.450549 0.106481  
 H10 -0.689790 -0.004889 1.495367  
 H11 -1.553385 -1.461414 -0.867241  
 H12 -2.116505 -1.619002 0.620070  
 H13 0.885727 1.165461 -0.060553  
 H14 0.576800 -0.072156 -1.279148  
 H15 1.362130 -1.846870 0.313699  
 H16 1.759525 -0.608504 1.503233  
 H17 4.862220 1.122853 -0.216376  
 H18 3.797376 1.140856 1.206394  
 H19 3.195757 1.719821 -0.368619  
 O20 -4.575611 -1.087310 0.045351  
 H21 -3.885546 -0.441608 -0.270276  
 H22 -5.237379 -0.520392 0.449980

[Met - H](H<sub>2</sub>O)<sub>2\_1</sub>

C1 -1.399992 0.399499 -0.313259  
 C2 -0.004335 0.996815 -0.677224  
 C3 1.086553 0.218408 0.085597  
 C4 2.489697 0.584120 -0.390880  
 S5 3.876653 -0.179401 0.545587  
 C6 3.630826 -1.947876 0.156841  
 O7 -2.125251 1.086621 0.441370  
 O8 -1.640607 -0.737210 -0.805822  
 N9 0.113921 2.440275 -0.400735  
 H10 0.145103 0.830321 -1.749734  
 H11 -0.496729 2.614096 0.399148  
 H12 -0.323182 2.952010 -1.162034  
 H13 0.892619 -0.848008 -0.050199  
 H14 0.995132 0.437956 1.155020  
 H15 2.643876 1.659762 -0.286082  
 H16 2.620600 0.332490 -1.448835  
 H17 4.462332 -2.489970 0.610393  
 H18 3.646665 -2.114852 -0.922698  
 H19 2.695113 -2.323497 0.571511  
 O20 -4.690785 0.134084 1.307432  
 H21 -4.625590 -0.722486 0.856446  
 H22 -3.836191 0.547727 1.071017  
 O23 -3.924249 -2.114669 -0.477719  
 H24 -4.354029 -1.922503 -1.315652  
 H25 -3.058988 -1.620964 -0.541083

[Met - H](H<sub>2</sub>O)<sub>2\_2</sub>

C1 -1.842390 -0.398733 0.076066  
 C2 -0.509646 -0.931773 0.685144  
 C3 0.666886 -0.492720 -0.210538

C4 2.016596 -0.757032 0.451687  
 S5 3.491027 -0.330868 -0.561992  
 C6 3.331527 1.488690 -0.647341  
 O7 -2.591764 -1.231684 -0.477570  
 O8 -2.037519 0.850697 0.177856  
 N9 -0.492428 -2.394353 0.869907  
 H10 -0.386930 -0.453697 1.663023  
 H11 -1.089929 -2.769989 0.132235  
 H12 -0.984630 -2.618497 1.730094  
 H13 0.551485 0.570885 -0.428729  
 H14 0.611170 -1.035095 -1.160853  
 H15 2.122439 -1.821302 0.669758  
 H16 2.095088 -0.212307 1.397782  
 H17 4.228571 1.861617 -1.144802  
 H18 3.271262 1.918055 0.354365  
 H19 2.454268 1.788967 -1.220023  
 O20 -4.568576 0.758145 -1.191898  
 H21 -3.827371 1.186963 -0.728579  
 H22 -4.225164 -0.151308 -1.167827  
 O23 -0.451381 2.727234 1.308307  
 H24 -1.010743 3.504046 1.226700  
 H25 -1.002879 2.000290 0.915702

[Met - H](H<sub>2</sub>O)<sub>2\_3</sub>

C1 -1.477278 0.454739 0.150131  
 C2 -0.321382 -0.564127 0.427971  
 C3 0.996205 -0.023040 -0.158028  
 C4 2.213092 -0.797665 0.342028  
 S5 3.822832 -0.317038 -0.407235  
 C6 4.000371 1.392052 0.215238  
 O7 -2.488291 0.029120 -0.485626  
 O8 -1.299757 1.612730 0.586963  
 N9 -0.544804 -1.941303 -0.032335  
 H10 -0.215738 -0.595318 1.519858  
 H11 -0.832672 -1.902540 -1.007972  
 H12 -1.352864 -2.330454 0.446637  
 H13 1.065017 1.033144 0.107122  
 H14 0.951781 -0.083809 -1.252323  
 H15 2.103038 -1.858021 0.107923  
 H16 2.309619 -0.710166 1.429352  
 H17 4.973841 1.752570 -0.121468  
 H18 3.973827 1.411934 1.307207  
 H19 3.223085 2.045691 -0.181244  
 O20 -3.831484 -2.253248 0.056795  
 H21 -4.565803 -1.900322 0.566343  
 H22 -3.325125 -1.444932 -0.211695  
 O23 -3.807183 2.626642 -0.322700  
 H24 -3.774209 1.707886 -0.635147  
 H25 -2.937808 2.642351 0.120014

[Met - H](H<sub>2</sub>O)<sub>2</sub>\_4

C1 2.050967 -0.094595 0.247462  
 C2 0.668741 0.495125 0.698677  
 C3 -0.467017 -0.219977 -0.054827  
 C4 -1.841984 0.033798 0.560872  
 S5 -3.255690 -0.745662 -0.324035  
 C6 -2.877408 -2.519013 -0.095362  
 O7 2.818151 0.699788 -0.356278  
 O8 2.239995 -1.301533 0.525428  
 N9 0.616268 1.965538 0.499246  
 H10 0.567369 0.268319 1.765718  
 H11 1.429142 2.154359 -0.098967  
 H12 0.831299 2.427515 1.378430  
 H13 -0.233691 -1.286656 -0.046616  
 H14 -0.464734 0.110049 -1.099657  
 H15 -2.083240 1.098835 0.554198  
 H16 -1.869084 -0.308377 1.601018  
 H17 -3.711530 -3.076934 -0.524315  
 H18 -2.795699 -2.765190 0.965826  
 H19 -1.958780 -2.804686 -0.608216  
 O20 -1.563226 3.481250 -0.497155  
 H21 -1.692167 3.190085 -1.404252  
 H22 -0.808272 2.928557 -0.165253  
 O23 4.852159 -1.351628 -0.647621  
 H24 4.072421 -1.710486 -0.184460  
 H25 4.517701 -0.448617 -0.779537

MetH<sup>+</sup>(H<sub>2</sub>O)<sub>1</sub>

C1 -2.063875 -0.942587 0.239992  
 C2 -0.792376 -0.312789 -0.331621  
 C3 0.384271 -1.307433 -0.330102  
 C4 1.647736 -0.819796 -1.053581  
 S5 2.531673 0.605603 -0.286057  
 C6 3.406212 -0.212567 1.099055  
 O7 -2.510479 -0.635056 1.316511  
 O8 -2.567636 -1.857909 -0.582321  
 N9 -0.506453 0.897625 0.516387  
 H10 -3.355016 -2.261283 -0.179637  
 H11 -0.990496 0.035697 -1.347375  
 H12 -0.792306 0.696372 1.482178  
 H13 0.517650 1.111271 0.472478  
 H14 -1.056518 1.725918 0.200028  
 H15 0.031147 -2.210296 -0.835840  
 H16 0.612828 -1.600570 0.700167  
 H17 1.408926 -0.492942 -2.068673  
 H18 2.358684 -1.642715 -1.143964  
 H19 3.959479 0.570868 1.616526  
 H20 4.112170 -0.943638 0.705759  
 H21 2.719257 -0.686364 1.800157  
 O22 -2.073843 3.027491 -0.387191

H23 -1.800966 3.801363 -0.894055  
 H24 -2.962575 3.218127 -0.064007

MetH<sup>+</sup>(H<sub>2</sub>O)<sub>2</sub>

C1 -1.761955 0.308921 -0.151920  
 C2 -0.338227 0.157968 -0.711247  
 C3 0.444993 -0.940596 0.028340  
 C4 1.848012 -1.229236 -0.522437  
 S5 3.093381 0.116170 -0.301617  
 C6 3.540188 -0.084280 1.462701  
 O7 -2.056858 1.272198 0.525317  
 O8 -2.527472 -0.699351 -0.475041  
 N9 0.312295 1.513382 -0.532819  
 H10 -3.446299 -0.607114 -0.077696  
 H11 -0.380602 -0.057920 -1.780088  
 H12 -0.160018 1.969085 0.265421  
 H13 1.346628 1.390579 -0.369767  
 H14 0.172045 2.115424 -1.346476  
 H15 -0.154679 -1.850956 -0.057564  
 H16 0.488868 -0.701692 1.096357  
 H17 1.814671 -1.413779 -1.599046  
 H18 2.249209 -2.131399 -0.058000  
 H19 4.271498 0.693229 1.682433  
 H20 4.003737 -1.059053 1.612400  
 H21 2.682449 0.034809 2.124446  
 O22 -4.922138 -0.491505 0.571204  
 H23 -5.221574 0.282449 1.060860  
 H24 -5.692410 -1.043451 0.397879

MetH<sup>+</sup>(H<sub>2</sub>O)<sub>3</sub>

C1 2.264480 -0.527055 0.048184  
 C2 0.794475 -0.655272 0.448941  
 C3 -0.127682 -0.964202 -0.746522  
 C4 -1.531983 -1.449940 -0.358034  
 S5 -2.586145 -0.264358 0.581508  
 C6 -3.159982 0.849305 -0.753962  
 O7 2.883861 0.505104 0.106602  
 O8 2.746040 -1.697692 -0.363837  
 N9 0.385735 0.630021 1.117432  
 H10 3.678583 -1.596376 -0.618117  
 H11 0.711321 -1.452850 1.192313  
 H12 0.651710 1.467084 0.542090  
 H13 -0.657224 0.609767 1.226428  
 H14 0.827009 0.739282 2.032482  
 H15 0.353455 -1.756838 -1.325227  
 H16 -0.178000 -0.087147 -1.399551  
 H17 -1.465966 -2.334091 0.280778  
 H18 -2.079320 -1.745188 -1.254765  
 H19 -3.811159 1.583605 -0.280054  
 H20 -3.740174 0.280618 -1.480401

H21 -2.336783 1.366388 -1.247348  
 O22 1.156914 2.789168 -0.429552  
 H23 0.882611 3.703385 -0.563096  
 H24 2.111728 2.752280 -0.569022

MetH<sup>+</sup>(H<sub>2</sub>O)<sub>2</sub>\_1

C1 -1.734715 -0.122104 0.102673  
 C2 -0.313309 0.150319 -0.408821  
 C3 0.500365 -1.151961 -0.512586  
 C4 1.895474 -1.007572 -1.135112  
 S5 3.141420 -0.082605 -0.136348  
 C6 3.601203 -1.333875 1.117275  
 O7 -2.070558 0.210780 1.220377  
 O8 -2.466161 -0.751398 -0.784266  
 N9 0.297875 1.126019 0.563008  
 H10 -3.378676 -0.951339 -0.423583  
 H11 -0.367717 0.641044 -1.382267  
 H12 -0.150535 0.972589 1.477113  
 H13 1.329099 0.972631 0.616990  
 H14 0.106110 2.110560 0.285223  
 H15 -0.085664 -1.829907 -1.139081  
 H16 0.563306 -1.622926 0.474109  
 H17 1.842707 -0.475595 -2.088353  
 H18 2.309175 -1.995247 -1.345627  
 H19 4.355193 -0.868028 1.751491  
 H20 4.040035 -2.202098 0.625840  
 H21 2.754143 -1.634180 1.733817  
 O22 -4.872235 -1.278159 0.162736  
 H23 -5.131192 -1.071441 1.067323  
 H24 -5.596454 -1.765327 -0.244308  
 O25 -0.313730 3.737557 -0.277075  
 H26 -1.126199 4.207215 -0.054880  
 H27 0.276170 4.392528 -0.668031

MetH<sup>+</sup>(H<sub>2</sub>O)<sub>2</sub>\_2

C1 1.747784 -0.094646 0.327965  
 C2 0.278745 -0.427970 0.614640  
 C3 -0.475679 -0.926432 -0.631355  
 C4 -1.822417 -1.603903 -0.340220  
 S5 -3.125693 -0.563619 0.446029  
 C6 -3.703088 0.433702 -0.976931  
 O7 2.178939 1.037580 0.390495  
 O8 2.427848 -1.174858 0.023097  
 N9 -0.378066 0.807069 1.174104  
 H10 3.386721 -0.963735 -0.173618  
 H11 0.247976 -1.193853 1.394116  
 H12 -0.208468 1.639032 0.559561  
 H13 -1.407191 0.625784 1.224652  
 H14 -0.017214 1.038219 2.101203  
 H15 0.170494 -1.661288 -1.118271

H16 -0.593616 -0.099278 -1.338540  
 H17 -1.685695 -2.442990 0.346465  
 H18 -2.235840 -2.012839 -1.263865  
 H19 -4.505102 1.068046 -0.599841  
 H20 -4.106290 -0.223996 -1.746785  
 H21 -2.914478 1.062487 -1.390908  
 O22 0.208417 2.925251 -0.510563  
 H23 -0.109447 3.806488 -0.735400  
 H24 1.174177 2.948824 -0.528602  
 O25 4.965772 -0.696392 -0.532790  
 H26 5.420950 0.126881 -0.325166  
 H27 5.640691 -1.366510 -0.686706

MetH<sup>+</sup>(H<sub>2</sub>O)<sub>2</sub>\_3

C1 1.934738 0.995314 0.152888  
 C2 0.580886 0.601968 -0.434435  
 C3 -0.583300 1.401994 0.183635  
 C4 -1.899432 1.326368 -0.604390  
 S5 -2.693451 -0.330579 -0.743102  
 C6 -3.432986 -0.511960 0.921683  
 O7 2.609319 0.268601 0.839541  
 O8 2.259755 2.241179 -0.194360  
 N9 0.402515 -0.873285 -0.234171  
 H10 3.116481 2.473344 0.200282  
 H11 0.618853 0.782319 -1.512065  
 H12 0.569294 -1.142928 0.759197  
 H13 -0.582330 -1.108657 -0.476607  
 H14 1.057150 -1.412426 -0.833811  
 H15 -0.274811 2.450242 0.213859  
 H16 -0.725639 1.088303 1.222714  
 H17 -1.743617 1.649327 -1.636758  
 H18 -2.628773 2.008991 -0.164504  
 H19 -3.945072 -1.474029 0.926626  
 H20 -4.165347 0.278046 1.087796  
 H21 -2.681554 -0.503412 1.711645  
 O22 0.896828 -1.441164 2.470985  
 H23 0.672014 -2.102408 3.134641  
 H24 1.791681 -1.135348 2.665123  
 O25 2.270171 -2.121461 -1.946208  
 H26 3.187061 -2.279149 -1.692561  
 H27 2.124208 -2.629292 -2.752694

MetH<sup>+</sup>(H<sub>2</sub>O)<sub>2</sub>\_4

C1 -0.408971 2.430948 -0.085358  
 C2 -0.033316 1.001879 0.308261  
 C3 1.463253 0.892882 0.658500  
 C4 1.901357 -0.464970 1.225082  
 S5 1.863623 -1.889082 0.054559  
 C6 3.373388 -1.582688 -0.933313  
 O7 -0.660731 2.747295 -1.220871

O8 -0.391465 3.249174 0.964303  
N9 -0.415800 0.131720 -0.855635  
H10 -0.604453 4.151907 0.674369  
H11 -0.642804 0.695430 1.160736  
H12 -0.297962 0.671972 -1.720859  
H13 0.191978 -0.715157 -0.871986  
H14 -1.430320 -0.153549 -0.794295  
H15 1.662853 1.656853 1.415046  
H16 2.064157 1.161245 -0.216852  
H17 1.258545 -0.762448 2.057356  
H18 2.915775 -0.386924 1.619972  
H19 3.429685 -2.389785 -1.663493  
H20 4.250684 -1.627764 -0.288224  
H21 3.338322 -0.629192 -1.460168  
O22 -4.026592 -2.788582 0.543311  
H23 -4.536295 -2.839319 1.359405  
H24 -4.191449 -3.611102 0.069304  
O25 -3.036302 -0.488282 -0.549368  
H26 -3.411337 -1.312375 -0.168092  
H27 -3.758295 -0.031662 -0.993746