

## Supporting Information

### Elucidating Potential Energy Surfaces for Singlet O<sub>2</sub> Reactions with Protonated, Deprotonated and Di-deprotonated Cystine Using A Combination of Approximately Spin Projected Density Functional Theory and Guided-Ion-Beam Mass Spectrometry

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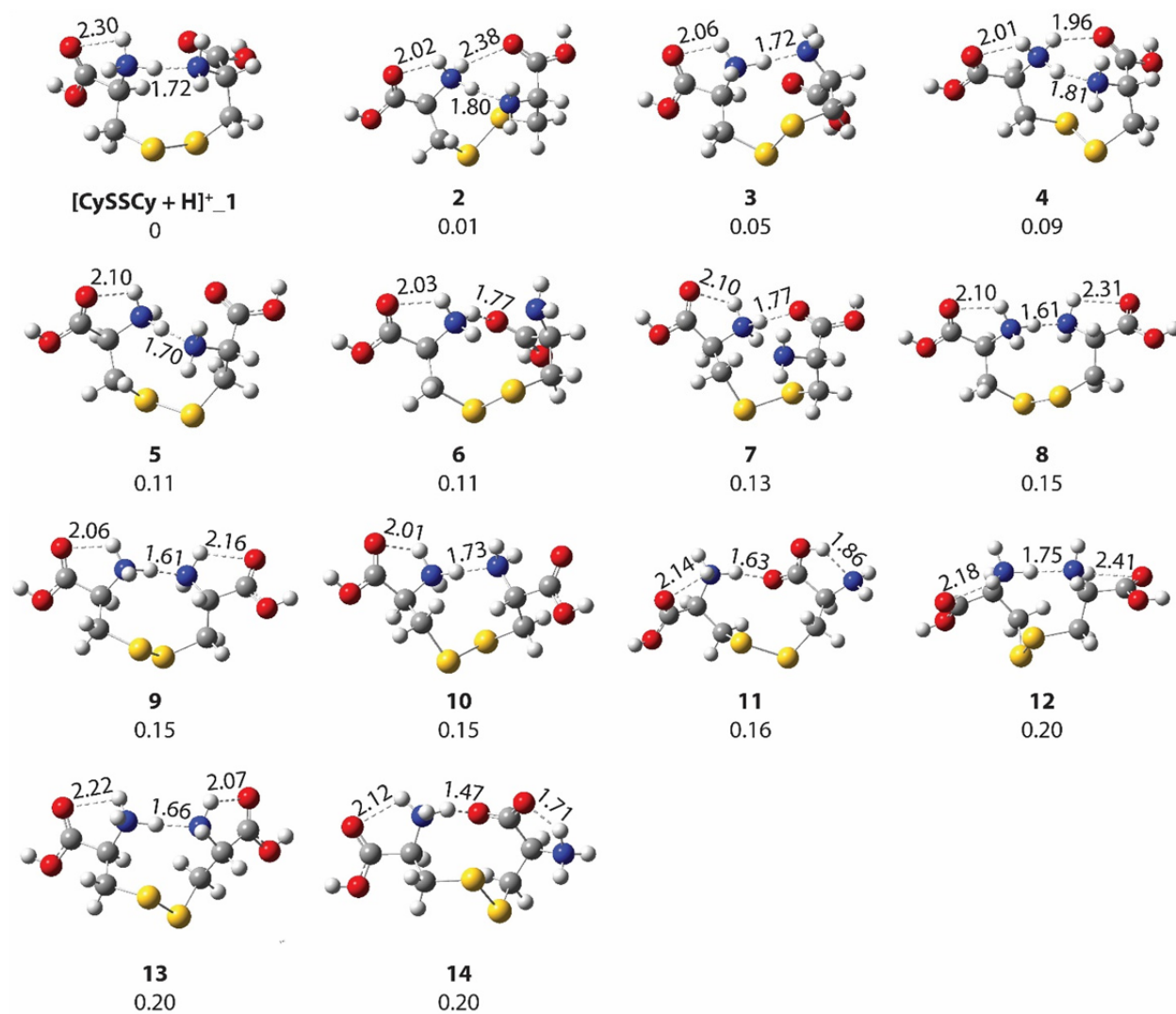
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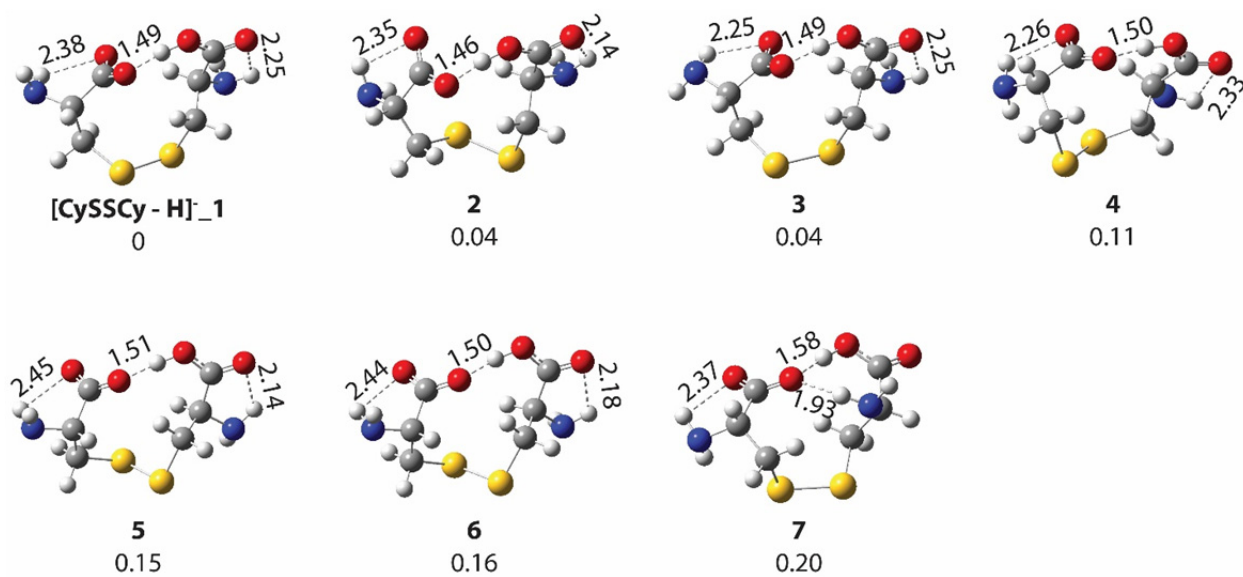
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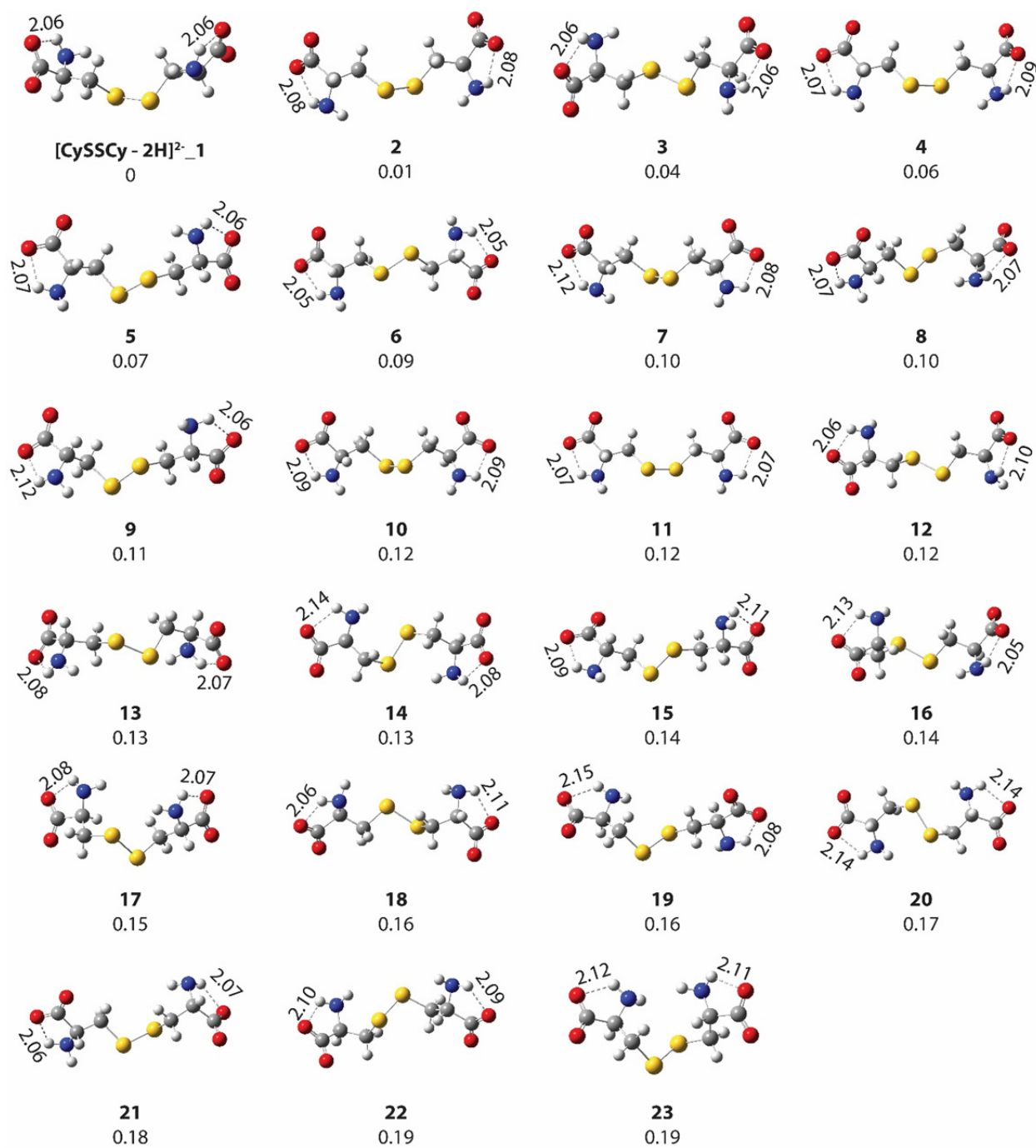
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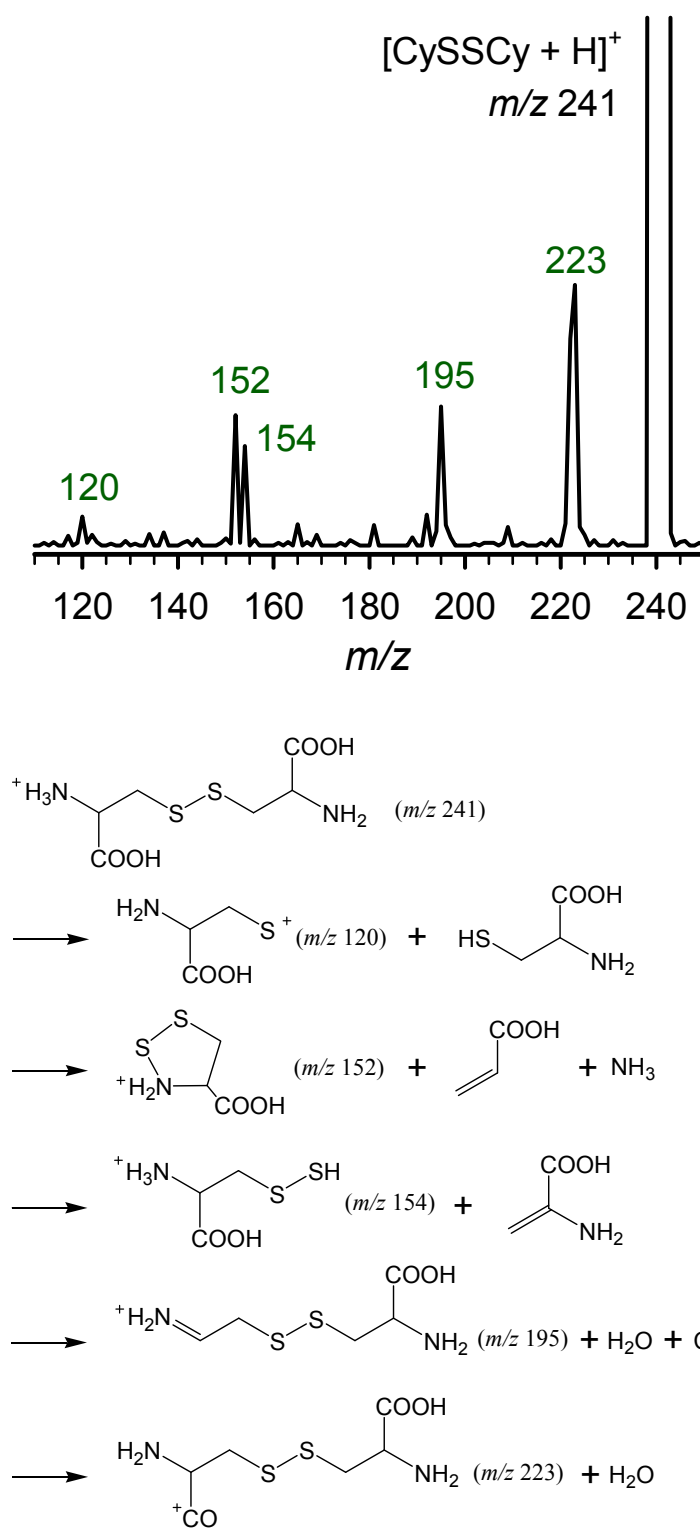
**Fig. S1** Stable tautomers/rotamers of [CySSCy + H]<sup>+</sup>. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p).



**Fig. S2** Stable tautomers/rotamers of [CySSCy - H]<sup>-1</sup>. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p).



**Fig. S3** Stable tautomers/rotamers of  $[\text{CySSCy} - 2\text{H}]^{2-}$ . Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p).



**Fig. S4** (Top) Product ion mass spectrum for  $[\text{CySSCy} + \text{H}]^+ + {}^1\text{O}_2$  obtained at  $E_{col} = 1.0$  eV; and (bottom) fragmentation scheme.

**Cartesian coordinates and energies  
for protonated CySSCy in Fig. S1,  
optimized at B3LYP/6-311++G(d,p)**

**[CySSCy + H]<sup>+</sup>\_1**

C1 -1.851929 -1.635987 -0.316734  
 O2 -0.757288 -2.134155 -0.192638  
 O3 -2.705254 -1.926142 -1.300022  
 H4 -2.307658 -2.588440 -1.888638  
 C5 -2.437790 -0.589221 0.628776  
 H6 -3.448168 -0.931192 0.887998  
 N7 -1.582791 -0.490358 1.827509  
 H8 0.113335 -0.498576 1.514509  
 H9 -1.852623 0.326220 2.371120  
 H10 -1.744959 -1.298739 2.425350  
 C11 -2.626318 0.768874 -0.069268  
 S12 -1.245074 1.502508 -1.041512  
 H13 -3.404188 0.664596 -0.829165  
 H14 -2.981957 1.508519 0.650541  
 S15 0.065425 2.302013 0.418967  
 C16 1.650617 1.455532 0.011805  
 C17 1.633489 -0.071496 0.053438  
 H18 1.977642 1.766861 -0.978938  
 H19 2.359008 1.872170 0.735842  
 H20 0.923464 -0.448657 -0.685848  
 N21 1.178763 -0.600223 1.377393  
 H22 1.669645 -0.138913 2.146307  
 H23 1.414454 -1.595942 1.429354  
 C24 2.998351 -0.699426 -0.239211  
 O25 3.512660 -1.505837 0.492146  
 O26 3.503614 -0.253494 -1.388070  
 H27 4.356209 -0.688804 -1.556178

Zero-point correction= 0.214960 (Hartree/Particle)  
 Thermal correction to Energy= 0.230751  
 Thermal correction to Enthalpy= 0.231695  
 Thermal correction to Gibbs Free Energy= 0.170699  
 Sum of electronic and zero-point Energies= -1443.105900  
 Sum of electronic and thermal Energies= -1443.090110  
 Sum of electronic and thermal Enthalpies= -1443.089166  
 Sum of electronic and thermal Free Energies= -1443.150162

**[CySSCy + H]<sup>+</sup>\_2**

C1 -2.677128 -1.246575 -0.147442  
 O2 -1.873495 -2.020628 -0.613554  
 O3 -3.934140 -1.117690 -0.574681  
 H4 -4.090584 -1.734235 -1.308905  
 C5 -2.378531 -0.272369 0.991723  
 H6 -3.235996 -0.307820 1.675487  
 N7 -1.126738 -0.684599 1.654110  
 H8 -1.255500 -1.595993 2.090495  
 H9 0.168846 -0.982246 0.440265  
 H10 -0.922929 -0.036595 2.412090  
 C11 -2.298665 1.174184 0.470960  
 S12 -1.070381 1.480419 -0.879777  
 H13 -3.263716 1.454253 0.045596  
 H14 -2.080308 1.864812 1.287261

S15 0.599349 2.356597 0.025709  
 C16 1.730345 1.004583 0.578327  
 C17 1.961045 -0.143796 -0.409431  
 H18 2.671442 1.539789 0.719942  
 H19 1.420203 0.611874 1.548179  
 H20 2.046026 0.247673 -1.425823  
 N21 0.841096 -1.144014 -0.370699  
 H22 0.247950 -1.114296 -1.201574  
 H23 1.251439 -2.085528 -0.280846  
 C24 3.244597 -0.934023 -0.105421  
 O25 3.240513 -2.122921 0.090533  
 O26 4.314321 -0.147336 -0.108997  
 H27 5.111547 -0.677090 0.060341

Zero-point correction= 0.215194 (Hartree/Particle)  
 Thermal correction to Energy= 0.230803  
 Thermal correction to Enthalpy= 0.231747  
 Thermal correction to Gibbs Free Energy= 0.171082  
 Sum of electronic and zero-point Energies= -1443.105280  
 Sum of electronic and thermal Energies= -1443.089670  
 Sum of electronic and thermal Enthalpies= -1443.088726  
 Sum of electronic and thermal Free Energies= -1443.149391

**[CySSCy + H]<sup>+</sup>\_3**

C1 1.721878 -1.394623 0.857854  
 O2 0.642926 -1.923257 0.990241  
 O3 2.559966 -1.123771 1.859887  
 H4 2.158140 -1.401840 2.698712  
 C5 2.329961 -1.014139 -0.490774  
 H6 3.282257 -1.560920 -0.536465  
 N7 1.411811 -1.438929 -1.561002  
 H8 -0.175570 -0.795964 -1.382484  
 H9 1.821257 -1.220557 -2.467119  
 H10 1.299210 -2.450619 -1.529265  
 C11 2.716355 0.470915 -0.598804  
 S12 1.408210 1.739390 -0.876910  
 H13 3.302874 0.756384 0.273261  
 H14 3.354607 0.615872 -1.476216  
 S15 0.321283 1.765191 0.940977  
 C16 -1.398672 1.352599 0.435754  
 C17 -1.698094 -0.084336 0.004388  
 H18 -1.965235 1.561390 1.345753  
 H19 -1.735308 2.068701 -0.319030  
 H20 -1.222960 -0.794491 0.685081  
 N21 -1.176082 -0.390186 -1.371412  
 H22 -1.158767 0.451690 -1.950768  
 H23 -1.835039 -1.048830 -1.810813  
 C24 -3.197236 -0.415621 -0.028716  
 O25 -3.716294 -0.957633 -0.972176  
 O26 -3.805664 -0.070759 1.100962  
 H27 -4.740087 -0.335719 1.061661

Zero-point correction= 0.215140 (Hartree/Particle)  
 Thermal correction to Energy= 0.230653  
 Thermal correction to Enthalpy= 0.231598  
 Thermal correction to Gibbs Free Energy= 0.171910  
 Sum of electronic and zero-point Energies= -1443.103781  
 Sum of electronic and thermal Energies= -1443.088268

Sum of electronic and thermal Enthalpies= -1443.087323  
 Sum of electronic and thermal Free Energies= -1443.147011

#### [CySSCy + H]<sup>+</sup>\_4

C1 -2.153322 -1.406880 -0.526200  
 O2 -1.229684 -2.140431 -0.805944  
 O3 -3.185563 -1.186997 -1.340521  
 H4 -3.064832 -1.697657 -2.157572  
 C5 -2.349953 -0.698246 0.818182  
 H6 -3.248488 -1.178175 1.231523  
 N7 -1.184117 -0.916015 1.692662  
 H8 -1.181539 -0.219318 2.433766  
 H9 -1.257214 -1.824179 2.145805  
 C10 -2.727331 0.788778 0.678572  
 S11 -1.392431 2.053682 0.596790  
 H12 -3.399447 0.917650 -0.166945  
 H13 -3.266697 1.110672 1.575057  
 S14 -0.175853 1.497787 -1.031528  
 C15 1.451136 1.178413 -0.203076  
 C16 2.012430 -0.226475 -0.452392  
 H17 2.157476 1.901216 -0.609356  
 H18 1.335827 1.376710 0.863863  
 H19 2.048004 -0.423906 -1.526265  
 N20 1.198775 -1.305221 0.196904  
 H21 1.843268 -1.889886 0.749416  
 H22 0.411073 -0.966814 0.828799  
 C23 3.441221 -0.382449 0.092250  
 O24 3.734901 -1.225293 0.902611  
 O25 4.269852 0.504500 -0.445433  
 H26 5.165758 0.372121 -0.092017  
 H27 0.685607 -1.886369 -0.476914

Zero-point correction= 0.214848 (Hartree/Particle)  
 Thermal correction to Energy= 0.230642  
 Thermal correction to Enthalpy= 0.231586  
 Thermal correction to Gibbs Free Energy= 0.170430  
 Sum of electronic and zero-point Energies= -1443.102649  
 Sum of electronic and thermal Energies= -1443.086855  
 Sum of electronic and thermal Enthalpies= -1443.085911  
 Sum of electronic and thermal Free Energies= -1443.147066

#### [CySSCy + H]<sup>+</sup>\_5

C1 3.191270 -1.040964 0.120971  
 O2 3.038157 -2.177034 0.491490  
 O3 4.304054 -0.324184 0.242156  
 H4 4.993464 -0.861423 0.667779  
 C5 2.083656 -0.246502 -0.586035  
 H6 2.409072 -0.087679 -1.617581  
 N7 0.877274 -1.134447 -0.608881  
 H8 1.181409 -2.109955 -0.497575  
 H9 0.178919 -0.931448 0.195252  
 H10 0.339218 -1.059376 -1.472287  
 C11 1.810134 1.110812 0.078340  
 S12 0.538834 2.125541 -0.808004  
 H13 1.508496 0.998465 1.119898  
 H14 2.733426 1.689255 0.058808

S15 -1.090146 2.307529 0.505125  
 C16 -2.262969 1.006423 -0.071971  
 C17 -2.309991 -0.305813 0.768210  
 H18 -3.249698 1.470944 -0.061484  
 H19 -2.005257 0.805578 -1.111724  
 H20 -3.093068 -0.214818 1.524785  
 N21 -1.003413 -0.627586 1.375803  
 H22 -0.740239 0.140527 1.990940  
 H23 -1.094135 -1.454722 1.963767  
 C24 -2.682442 -1.432307 -0.193503  
 O25 -1.870014 -2.055620 -0.839197  
 O26 -4.001481 -1.599077 -0.274823  
 H27 -4.201331 -2.282813 -0.936048

Zero-point correction= 0.214990 (Hartree/Particle)  
 Thermal correction to Energy= 0.230702  
 Thermal correction to Enthalpy= 0.231646  
 Thermal correction to Gibbs Free Energy= 0.170337  
 Sum of electronic and zero-point Energies= -1443.101953  
 Sum of electronic and thermal Energies= -1443.086241  
 Sum of electronic and thermal Enthalpies= -1443.085297  
 Sum of electronic and thermal Free Energies= -1443.146606

#### [CySSCy + H]<sup>+</sup>\_6

C1 1.977738 -1.270313 0.842002  
 O2 0.899698 -1.827336 0.932585  
 O3 2.766274 -1.036663 1.885161  
 H4 2.338118 -1.355960 2.696411  
 C5 2.605305 -0.781532 -0.460722  
 H6 3.655926 -1.102621 -0.409237  
 N7 1.879904 -1.346147 -1.596528  
 H8 2.022092 -2.351691 -1.646284  
 H9 2.239172 -0.962323 -2.466181  
 C10 2.675509 0.759400 -0.530686  
 S11 1.167573 1.726574 -0.965973  
 H12 3.102955 1.162770 0.386612  
 H13 3.352127 1.038543 -1.344008  
 S14 0.064867 1.857816 0.852108  
 C15 -1.604681 1.303052 0.312933  
 C16 -1.842199 -0.208075 0.241170  
 H17 -2.270765 1.716626 1.072268  
 H18 -1.853230 1.790146 -0.632630  
 H19 -1.594962 -0.665932 1.200905  
 N20 -0.995662 -0.880337 -0.801630  
 H21 -0.275475 -1.483914 -0.351940  
 H22 -1.612756 -1.430752 -1.416691  
 C23 -3.298654 -0.559136 -0.094664  
 O24 -3.596557 -1.241110 -1.042515  
 O25 -4.142875 -0.030382 0.783762  
 H26 -5.053949 -0.280138 0.554278  
 H27 -0.448422 -0.216055 -1.366692

Zero-point correction= 0.215083 (Hartree/Particle)  
 Thermal correction to Energy= 0.230879  
 Thermal correction to Enthalpy= 0.231823  
 Thermal correction to Gibbs Free Energy= 0.171117  
 Sum of electronic and zero-point Energies= -1443.101852  
 Sum of electronic and thermal Energies= -1443.086056

Sum of electronic and thermal Enthalpies= -1443.085112  
 Sum of electronic and thermal Free Energies= -1443.145818

**[CySSCy + H]<sup>+</sup>\_7**

C1 -2.229501 -1.487708 0.054383  
 O2 -1.158013 -1.946115 -0.295308  
 O3 -3.392443 -1.944758 -0.399797  
 H4 -3.235163 -2.663199 -1.034735  
 C5 -2.419738 -0.325000 1.021840  
 H6 -3.386916 -0.490234 1.516150  
 N7 -1.294773 -0.268808 1.951249  
 H8 -1.249164 -1.114672 2.513054  
 H9 -1.426145 0.503841 2.598721  
 C10 -2.574304 0.999544 0.242682  
 S11 -1.309657 1.410132 -1.037353  
 H12 -3.508520 0.983449 -0.324035  
 H13 -2.628450 1.833218 0.945177  
 S14 0.304537 2.319009 -0.050557  
 C15 1.364231 0.949827 0.570498  
 C16 2.098307 0.133868 -0.492870  
 H17 2.109127 1.467467 1.178712  
 H18 0.759293 0.308808 1.217442  
 H19 2.549264 0.796243 -1.237440  
 N20 1.173069 -0.802696 -1.228387  
 H21 0.701192 -0.332917 -2.003540  
 H22 1.723116 -1.603812 -1.568196  
 C23 3.223395 -0.756394 0.057882  
 O24 3.343054 -1.911296 -0.263821  
 O25 4.031013 -0.083990 0.869646  
 H26 4.755786 -0.662780 1.160856  
 H27 0.407183 -1.186699 -0.627895

Zero-point correction= 0.214936 (Hartree/Particle)  
 Thermal correction to Energy= 0.230897  
 Thermal correction to Enthalpy= 0.231841  
 Thermal correction to Gibbs Free Energy= 0.170402  
 Sum of electronic and zero-point Energies= -1443.101460  
 Sum of electronic and thermal Energies= -1443.085499  
 Sum of electronic and thermal Enthalpies= -1443.084555  
 Sum of electronic and thermal Free Energies= -1443.145994

**[CySSCy + H]<sup>+</sup>\_8**

C1 -3.638692 -0.983374 -0.157071  
 O2 -3.819324 -1.881173 -0.936071  
 O3 -4.603349 -0.328674 0.500747  
 H4 -5.466100 -0.699991 0.252876  
 C5 -2.237883 -0.479863 0.238676  
 H6 -2.112835 -0.759372 1.291507  
 N7 -1.207475 -1.178227 -0.555104  
 H8 -1.536316 -2.128481 -0.735276  
 H9 -1.145871 -0.746687 -1.476860  
 C10 -2.132544 1.043907 0.121569  
 S11 -0.633437 1.846059 0.843010  
 H12 -2.226351 1.370997 -0.916426  
 H13 -2.951214 1.501132 0.678347  
 S14 0.714430 1.969010 -0.798926

C15 2.220807 1.111746 -0.186533  
 C16 2.216198 -0.416525 -0.244715  
 H17 3.007970 1.479588 -0.847354  
 H18 2.454931 1.468768 0.819480  
 H19 1.961586 -0.743348 -1.257075  
 N20 1.203915 -1.014816 0.682485  
 H21 0.227322 -1.142354 0.178321  
 H22 1.576889 -1.906865 1.033420  
 C23 3.571076 -1.052683 0.106200  
 O24 3.672089 -1.953628 0.898990  
 O25 4.563076 -0.507102 -0.589185  
 H26 5.399807 -0.951939 -0.371714  
 H27 1.045506 -0.405877 1.489140

Zero-point correction= 0.214367 (Hartree/Particle)  
 Thermal correction to Energy= 0.230078  
 Thermal correction to Enthalpy= 0.231022  
 Thermal correction to Gibbs Free Energy= 0.169779  
 Sum of electronic and zero-point Energies= -1443.100480  
 Sum of electronic and thermal Energies= -1443.084770  
 Sum of electronic and thermal Enthalpies= -1443.083826  
 Sum of electronic and thermal Free Energies= -1443.145068

**[CySSCy + H]<sup>+</sup>\_9**

C1 -3.489471 -0.918809 0.131549  
 O2 -3.772781 -2.036998 -0.211041  
 O3 -4.340062 -0.043149 0.677298  
 H4 -5.216508 -0.455428 0.751903  
 C5 -2.067979 -0.345615 0.029244  
 H6 -1.736701 -0.194614 1.063751  
 N7 -1.176924 -1.335028 -0.612249  
 H8 -1.654021 -2.240085 -0.593354  
 H9 -1.059838 -1.108889 -1.598584  
 C10 -2.066179 1.021162 -0.661494  
 S11 -0.428142 1.821091 -0.963631  
 H12 -2.479628 0.952827 -1.673430  
 H13 -2.689744 1.711077 -0.096560  
 S14 0.452877 1.843718 0.966268  
 C15 2.098129 1.080089 0.628359  
 H16 2.688390 1.751633 0.007033  
 H17 2.569576 1.041830 1.615779  
 H18 1.662846 -0.194880 -1.041273  
 N19 1.199290 -1.274926 0.694240  
 H20 0.227850 -1.372799 0.168243  
 H21 1.697060 -2.175823 0.734914  
 C22 3.458842 -0.940533 -0.155838  
 O23 3.687903 -2.058322 0.232354  
 O24 4.324675 -0.126801 -0.749783  
 H25 5.185504 -0.570635 -0.834864  
 C26 2.072245 -0.299735 -0.032304  
 H27 1.021476 -0.968664 1.652595

Zero-point correction= 0.214457 (Hartree/Particle)  
 Thermal correction to Energy= 0.230073  
 Thermal correction to Enthalpy= 0.231017  
 Thermal correction to Gibbs Free Energy= 0.170079  
 Sum of electronic and zero-point Energies= -1443.100273  
 Sum of electronic and thermal Energies= -1443.084657



Sum of electronic and thermal Enthalpies= -1443.083713  
 Sum of electronic and thermal Free Energies= -1443.144651

**[CySSCy + H]<sup>+</sup>\_10**

C1 3.308791 -1.061889 -0.444113  
 O2 3.669927 -2.116704 0.005265  
 O3 4.023326 -0.294856 -1.279327  
 H4 4.874891 -0.727289 -1.456455  
 C5 1.943120 -0.427167 -0.131822  
 H6 1.450402 -0.261887 -1.094809  
 N7 1.110683 -1.342484 0.671761  
 H8 1.135062 -2.263170 0.232836  
 H9 1.570898 -1.493711 1.570402  
 C10 2.141822 0.937809 0.542235  
 S11 0.606397 1.801461 1.082410  
 H12 2.712943 0.840106 1.472108  
 H13 2.695573 1.597516 -0.123440  
 S14 -0.491815 2.093670 -0.675468  
 C15 -1.470523 0.549423 -0.937926  
 C16 -2.332481 0.079305 0.237179  
 H17 -2.135009 0.830543 -1.757694  
 H18 -0.834775 -0.263173 -1.292906  
 H19 -2.850804 0.934130 0.678872  
 N20 -1.523400 -0.593412 1.315857  
 H21 -1.376980 0.030125 2.110222  
 H22 -2.045513 -1.432771 1.611213  
 C23 -3.403226 -0.945635 -0.176097  
 O24 -3.517397 -2.012572 0.373002  
 O25 -4.161758 -0.490462 -1.164673  
 H26 -4.847894 -1.144365 -1.381357  
 H27 -0.530891 -0.891203 0.995740

Zero-point correction= 0.214757 (Hartree/Particle)  
 Thermal correction to Energy= 0.230524  
 Thermal correction to Enthalpy= 0.231468  
 Thermal correction to Gibbs Free Energy= 0.169596  
 Sum of electronic and zero-point Energies= -1443.100372  
 Sum of electronic and thermal Energies= -1443.084605  
 Sum of electronic and thermal Enthalpies= -1443.083661  
 Sum of electronic and thermal Free Energies= -1443.145533

**[CySSCy + H]<sup>+</sup>\_11**

C1 2.036920 -1.231921 0.273280  
 O2 0.992967 -1.245777 0.909232  
 O3 2.368087 -2.202606 -0.546832  
 H4 3.280602 -1.968099 -0.868159  
 C5 3.022700 -0.059532 0.326196  
 H6 3.119763 0.249908 1.369978  
 N7 4.288930 -0.529282 -0.258930  
 H8 -1.884086 -2.684581 0.462829  
 H9 4.738805 0.164962 -0.845499  
 H10 4.956947 -0.818047 0.448652  
 C11 2.480007 1.126667 -0.506852  
 S12 1.108483 2.146994 0.173474  
 H13 3.282388 1.866669 -0.585499  
 H14 2.225575 0.816715 -1.522323

S15 -0.674890 1.295295 -0.538061  
 C16 -1.424520 0.592655 1.009179  
 C17 -2.300784 -0.639054 0.737724  
 H18 -2.055436 1.352107 1.470023  
 H19 -0.616407 0.329126 1.688688  
 H20 -2.720399 -0.967264 1.691283  
 N21 -1.508198 -1.784156 0.160328  
 H22 -1.599156 -1.755862 -0.864106  
 H23 -0.486741 -1.724709 0.434195  
 C24 -3.451156 -0.374716 -0.240824  
 O25 -3.507257 -0.895286 -1.325774  
 O26 -4.327613 0.483403 0.267245  
 H27 -5.032943 0.654046 -0.379643

Zero-point correction= 0.214779 (Hartree/Particle)  
 Thermal correction to Energy= 0.230608  
 Thermal correction to Enthalpy= 0.231553  
 Thermal correction to Gibbs Free Energy= 0.170162  
 Sum of electronic and zero-point Energies= -1443.100155  
 Sum of electronic and thermal Energies= -1443.084326  
 Sum of electronic and thermal Enthalpies= -1443.083381  
 Sum of electronic and thermal Free Energies= -1443.144772

**[CySSCy + H]<sup>+</sup>\_12**

C1 -3.387663 -0.521161 -0.317382  
 O2 -3.419189 -0.389455 -1.512642  
 O3 -4.354919 -0.210484 0.538559  
 H4 -5.107194 0.173896 0.057627  
 C5 -2.169812 -1.096450 0.416486  
 H6 -2.485038 -1.979944 0.977694  
 N7 -1.201064 -1.553052 -0.642192  
 H8 -1.416749 -2.504620 -0.944877  
 H9 -1.313744 -0.944909 -1.464188  
 H10 -0.168638 -1.496680 -0.329840  
 C11 -1.529351 -0.110245 1.401631  
 S12 -1.182979 1.593889 0.801912  
 H13 -2.238829 0.055292 2.216251  
 H14 -0.632541 -0.553360 1.837248  
 S15 0.115878 1.385322 -0.831666  
 C16 1.777203 1.067442 -0.081620  
 C17 2.351060 -0.313844 -0.444215  
 H18 2.442882 1.841395 -0.464108  
 H19 1.691854 1.197242 0.998972  
 H20 2.404433 -0.398945 -1.532457  
 N21 1.533330 -1.430364 0.074954  
 H22 1.921024 -2.298735 -0.294113  
 H23 1.710328 -1.500918 1.079173  
 C24 3.782794 -0.401787 0.109132  
 O25 4.080037 -1.061310 1.070644  
 O26 4.629006 0.359215 -0.595677  
 H27 5.515110 0.299366 -0.201918

Zero-point correction= 0.214918 (Hartree/Particle)  
 Thermal correction to Energy= 0.230685  
 Thermal correction to Enthalpy= 0.231629  
 Thermal correction to Gibbs Free Energy= 0.170257  
 Sum of electronic and zero-point Energies= -1443.098686  
 Sum of electronic and thermal Energies= -1443.082920

Sum of electronic and thermal Enthalpies= -1443.081976  
 Sum of electronic and thermal Free Energies= -1443.143348

**[CySSCy + H]<sup>+</sup>\_13**

C1 -3.384093 -0.981422 -0.171161  
 O2 -3.468751 -2.113629 0.230742  
 O3 -4.206231 -0.423533 -1.064258  
 H4 -4.884935 -1.069764 -1.319443  
 C5 -2.304364 0.003615 0.305874  
 H6 -2.832414 0.835047 0.783098  
 N7 -1.447532 -0.705779 1.289881  
 H8 -1.908457 -1.597439 1.493104  
 H9 -1.426543 -0.179134 2.159201  
 C10 -1.514435 0.551037 -0.890992  
 S11 -0.566333 2.118547 -0.647494  
 H12 -0.875267 -0.229882 -1.308460  
 H13 -2.210964 0.855461 -1.676147  
 S14 0.668766 1.885846 1.029737  
 C15 2.174321 1.065976 0.363003  
 C16 1.946277 -0.375888 -0.101807  
 H17 2.574647 1.647799 -0.465768  
 H18 2.897951 1.106641 1.184377  
 H19 1.305222 -0.367892 -0.986742  
 N20 1.246275 -1.197606 0.940271  
 H21 0.163768 -0.993407 1.005195  
 H22 1.417814 -2.190595 0.744468  
 C23 3.229805 -1.125380 -0.481889  
 O24 3.480219 -2.226977 -0.065070  
 O25 3.975647 -0.416422 -1.323100  
 H26 4.766878 -0.925889 -1.567843  
 H27 1.650026 -1.020688 1.863315

Zero-point correction= 0.214237 (Hartree/Particle)  
 Thermal correction to Energy= 0.229945  
 Thermal correction to Enthalpy= 0.230889  
 Thermal correction to Gibbs Free Energy= 0.169029  
 Sum of electronic and zero-point Energies= -1443.098378  
 Sum of electronic and thermal Energies= -1443.082670  
 Sum of electronic and thermal Enthalpies= -1443.081725  
 Sum of electronic and thermal Free Energies= -1443.143585

**[CySSCy + H]<sup>+</sup>\_14**

C1 1.733951 1.535218 -0.122529  
 O2 2.203596 1.927749 0.953360  
 O3 0.639252 1.808478 -0.680187  
 H4 -0.595856 1.797916 0.114028  
 C5 2.630907 0.525872 -0.916344  
 H6 3.074360 1.062151 -1.758127  
 N7 3.737543 0.176568 0.047605  
 H8 3.560158 0.903401 0.807418  
 H9 3.598205 -0.762095 0.440235  
 H10 4.677688 0.251207 -0.339115  
 C11 1.863903 -0.682935 -1.444729  
 S12 1.358184 -1.969304 -0.213898  
 H13 1.001914 -0.307398 -1.991394  
 H14 2.470071 -1.275697 -2.137383

S15 0.255007 -1.057600 1.324795  
 C16 -1.504033 -1.044622 0.776040  
 C17 -1.930888 0.159089 -0.076779  
 H18 -1.727327 -1.966271 0.240906  
 H19 -2.063248 -1.065873 1.717742  
 H20 -1.424520 0.121617 -1.043808  
 N21 -1.563509 1.475979 0.536322  
 H22 -2.306168 2.153611 0.324569  
 H23 -1.482220 1.422838 1.552700  
 C24 -3.439524 0.185778 -0.354738  
 O25 -4.120290 1.157995 -0.155090  
 O26 -3.863095 -0.972928 -0.856343  
 H27 -4.813948 -0.913540 -1.049066  
 Zero-point correction= 0.214186 (Hartree/Particle)  
 Thermal correction to Energy= 0.229485  
 Thermal correction to Enthalpy= 0.230429  
 Thermal correction to Gibbs Free Energy= 0.170936  
 Sum of electronic and zero-point Energies= -1443.097944  
 Sum of electronic and thermal Energies= -1443.082646  
 Sum of electronic and thermal Enthalpies= -1443.081702  
 Sum of electronic and thermal Free Energies= -1443.141194

**Cartesian coordinates and energies  
for deprotonated CySSCy in Fig. S2,  
optimized at B3LYP/6-311++G(d,p)**

**[CySSCy - H]<sup>-</sup>\_1**

C1 -1.084475 -1.483261 0.058322  
 O2 -0.765705 -1.733223 1.235284  
 O3 -0.353092 -1.593524 -0.977597  
 H4 1.127384 -1.756701 -0.888737  
 C5 -2.520232 -0.949234 -0.178100  
 H6 -2.753119 -1.011425 -1.243406  
 N7 -3.530904 -1.725932 0.571405  
 H8 -3.126339 -1.911044 1.489256  
 C9 -2.648360 0.511525 0.284629  
 S10 -1.798699 1.792562 -0.740389  
 H11 -3.704830 0.791123 0.250561  
 H12 -2.297114 0.617744 1.313169  
 S13 0.010115 2.231024 0.230795  
 C14 1.262493 1.110458 -0.557065  
 C15 1.911056 0.163615 0.465061  
 H16 0.747885 0.566066 -1.346664  
 H17 2.025746 1.758998 -0.994518  
 H18 1.120706 -0.388394 0.978700  
 N19 2.681384 0.937101 1.444701  
 H20 2.670768 0.458398 2.338837  
 H21 3.652524 0.946492 1.137846  
 C22 2.793036 -0.862371 -0.291558  
 O23 4.009873 -0.775435 -0.270342  
 O24 2.164740 -1.801971 -0.964134  
 H25 -3.627243 -2.637985 0.132308

Zero-point correction= 0.186891 (Hartree/Particle)  
 Thermal correction to Energy= 0.202495  
 Thermal correction to Enthalpy= 0.203439  
 Thermal correction to Gibbs Free Energy= 0.143586  
 Sum of electronic and zero-point Energies= -1442.239958  
 Sum of electronic and thermal Energies= -1442.224353  
 Sum of electronic and thermal Enthalpies= -1442.223409  
 Sum of electronic and thermal Free Energies= -1442.283262

**[CySSCy - H]<sup>-</sup>\_2**

C1 -1.386009 -1.620797 -0.110770  
 O2 -1.345060 -2.356742 0.881386  
 O3 -0.493780 -1.482375 -1.016646  
 H4 0.908811 -1.826999 -0.771791  
 C5 -2.668830 -0.761505 -0.344617  
 H6 -3.174500 -1.217594 -1.207898  
 N7 -3.617687 -0.777101 0.778483  
 H8 -3.594840 -1.722675 1.156307  
 H9 -3.224676 -0.216539 1.533118  
 C10 -2.341578 0.671188 -0.768102  
 S11 -1.370904 1.586420 0.533460  
 H12 -1.728605 0.662087 -1.665395  
 H13 -3.260829 1.232996 -0.947254  
 S14 0.267965 2.413161 -0.472963  
 C15 1.407188 0.994761 -0.800454

C16 1.846224 0.182106 0.429809  
 H17 0.928607 0.353701 -1.537581  
 H18 2.275988 1.488426 -1.247796  
 H19 0.941814 -0.169729 0.933504  
 N20 2.664910 0.984707 1.340002  
 H21 2.331373 0.893201 2.291669  
 H22 3.612938 0.615353 1.308047  
 C23 2.622233 -1.070569 -0.063795  
 O24 3.824011 -1.160518 0.130664  
 O25 1.942957 -1.989099 -0.707242

Zero-point correction= 0.186268 (Hartree/Particle)  
 Thermal correction to Energy= 0.202044  
 Thermal correction to Enthalpy= 0.202988  
 Thermal correction to Gibbs Free Energy= 0.142083  
 Sum of electronic and zero-point Energies= -1442.238721  
 Sum of electronic and thermal Energies= -1442.222945  
 Sum of electronic and thermal Enthalpies= -1442.222001  
 Sum of electronic and thermal Free Energies= -1442.282905

**[CySSCy - H]<sup>-</sup>\_3**

C1 -1.090231 -1.515848 0.017298  
 O2 -0.777441 -1.827809 1.180094  
 O3 -0.350024 -1.543129 -1.014733  
 H4 1.125950 -1.728021 -0.923884  
 C5 -2.525271 -0.970295 -0.198926  
 H6 -2.758285 -1.016596 -1.265150  
 N7 -3.455879 -1.825965 0.551714  
 H8 -2.997853 -2.073249 1.427185  
 H9 -4.318430 -1.334801 0.768614  
 C10 -2.620252 0.494371 0.285099  
 S11 -1.787436 1.795583 -0.738012  
 H12 -3.672687 0.801972 0.279372  
 H13 -2.245193 0.579032 1.307221  
 S14 0.012457 2.241621 0.244077  
 C15 1.273136 1.129426 -0.540666  
 C16 1.899107 0.159516 0.473560  
 H17 0.769447 0.602947 -1.349152  
 H18 2.046808 1.782855 -0.951760  
 H19 1.098407 -0.398563 0.963576  
 N20 2.657363 0.908995 1.480771  
 H21 2.634443 0.409170 2.363091  
 H22 3.632556 0.922412 1.186977  
 C23 2.787637 -0.855698 -0.290605  
 O24 4.004327 -0.772868 -0.250805  
 O25 2.164309 -1.777752 -0.990191

Zero-point correction= 0.186672 (Hartree/Particle)  
 Thermal correction to Energy= 0.202231  
 Thermal correction to Enthalpy= 0.203175  
 Thermal correction to Gibbs Free Energy= 0.143389  
 Sum of electronic and zero-point Energies= -1442.238408  
 Sum of electronic and thermal Energies= -1442.222849  
 Sum of electronic and thermal Enthalpies= -1442.221905  
 Sum of electronic and thermal Free Energies= -1442.281691

**[CySSCy - H]<sup>-</sup>\_4**

C1 0.850047 1.641553 0.259578  
 O2 0.514889 1.922912 1.418639  
 O3 0.128923 1.702541 -0.792122  
 H4 -1.371042 1.661206 -0.837112  
 C5 2.337292 1.224357 0.005517  
 H6 2.786248 2.140664 -0.409881  
 N7 3.087220 0.869824 1.212527  
 H8 2.626343 1.356464 1.980430  
 H9 2.942046 -0.118557 1.403087  
 C10 2.491167 0.200402 -1.117900  
 S11 2.104765 -1.596125 -0.795425  
 H12 1.883138 0.522364 -1.959712  
 H13 3.539722 0.131663 -1.426507  
 S14 0.480647 -1.725093 0.525869  
 C15 -0.995013 -1.175799 -0.453583  
 C16 -1.922386 -0.355579 0.460977  
 H17 -0.621497 -0.570241 -1.275587  
 H18 -1.518279 -2.053766 -0.838309  
 H19 -1.305255 0.345319 1.028763  
 N20 -2.614764 -1.241246 1.400679  
 H21 -2.877747 -0.715351 2.227743  
 H22 -3.487862 -1.537531 0.968436  
 C23 -2.895791 0.477241 -0.410201  
 O24 -4.067057 0.159284 -0.522694  
 O25 -2.384442 1.528282 -1.017228

Zero-point correction= 0.187071 (Hartree/Particle)  
 Thermal correction to Energy= 0.202607  
 Thermal correction to Enthalpy= 0.203552  
 Thermal correction to Gibbs Free Energy= 0.143957  
 Sum of electronic and zero-point Energies= -1442.235799  
 Sum of electronic and thermal Energies= -1442.220262  
 Sum of electronic and thermal Enthalpies= -1442.219318  
 Sum of electronic and thermal Free Energies= -1442.278913

**[CySSCy - H]<sup>-</sup>\_5**

C1 -1.621311 -1.453514 0.188176  
 O2 -2.078217 -1.934586 1.234743  
 O3 -0.534748 -1.742411 -0.410464  
 H4 0.927846 -2.020924 -0.170978  
 C5 -2.480642 -0.369136 -0.525659  
 H6 -2.039453 -0.158647 -1.502140  
 N7 -3.877242 -0.805816 -0.737271  
 H8 -4.159869 -1.287715 0.115911  
 H9 -3.889007 -1.512844 -1.467578  
 C10 -2.550742 0.931634 0.282204  
 S11 -0.979684 1.647772 0.928654  
 H12 -3.081848 1.694935 -0.288384  
 H13 -3.101655 0.744987 1.210410  
 S14 0.208739 2.153136 -0.723267  
 C15 1.257472 0.650515 -1.016646  
 C16 2.065442 0.214395 0.216111  
 H17 0.608276 -0.145620 -1.371214  
 H18 1.941497 0.980035 -1.803671  
 H19 1.348239 0.067225 1.033652

N20 3.089867 1.207491 0.550475  
 H21 2.814613 1.767557 1.346873  
 H22 3.957732 0.722232 0.757842  
 C23 2.728989 -1.166945 -0.001825  
 O24 3.940789 -1.286958 0.034887  
 O25 1.937818 -2.200942 -0.195854

Zero-point correction= 0.186623 (Hartree/Particle)  
 Thermal correction to Energy= 0.202427  
 Thermal correction to Enthalpy= 0.203371  
 Thermal correction to Gibbs Free Energy= 0.142054  
 Sum of electronic and zero-point Energies= -1442.234606  
 Sum of electronic and thermal Energies= -1442.218802  
 Sum of electronic and thermal Enthalpies= -1442.217858  
 Sum of electronic and thermal Free Energies= -1442.279175

**[CySSCy - H]<sup>-</sup>\_6**

C1 -1.602358 -1.453479 0.198783  
 O2 -2.070936 -1.950645 1.232732  
 O3 -0.492434 -1.707240 -0.371836  
 H4 0.943892 -2.049600 -0.109986  
 C5 -2.468897 -0.389116 -0.534657  
 H6 -2.022846 -0.188661 -1.510967  
 N7 -3.860487 -0.840491 -0.746607  
 H8 -4.139929 -1.319057 0.109576  
 C9 -2.552537 0.923034 0.253745  
 S10 -0.992473 1.661550 0.901976  
 H11 -3.085595 1.673380 -0.332019  
 H12 -3.110137 0.746869 1.180193  
 S13 0.202047 2.161473 -0.743561  
 C14 1.304046 0.691969 -1.004527  
 C15 2.026601 0.198725 0.261625  
 H16 0.707316 -0.105553 -1.440580  
 H17 2.033582 1.065509 -1.729977  
 H18 1.257303 0.015983 1.016298  
 N19 2.988253 1.187081 0.753835  
 H20 2.959338 1.230409 1.765794  
 H21 3.919502 0.866636 0.496699  
 C22 2.718858 -1.160227 -0.031743  
 O23 3.932275 -1.222131 -0.134569  
 O24 1.956036 -2.225306 -0.153608  
 H25 -3.863787 -1.553255 -1.471392

Zero-point correction= 0.186575 (Hartree/Particle)  
 Thermal correction to Energy= 0.202547  
 Thermal correction to Enthalpy= 0.203492  
 Thermal correction to Gibbs Free Energy= 0.141024  
 Sum of electronic and zero-point Energies= -1442.234598  
 Sum of electronic and thermal Energies= -1442.218625  
 Sum of electronic and thermal Enthalpies= -1442.217681  
 Sum of electronic and thermal Free Energies= -1442.280149

**[CySSCy - H]<sup>-</sup>\_7**

C1 1.231145 -1.697945 -0.020375  
 O2 1.454602 -2.413482 -1.000868  
 O3 0.113607 -1.538495 0.585031  
 H4 -1.346401 -1.755717 0.021797  
 C5 2.430597 -0.922449 0.617827

H6 2.608938 -1.420600 1.582082  
N7 3.678582 -1.007183 -0.153955  
H8 3.729667 -1.958132 -0.513919  
H9 3.561403 -0.447373 -0.997312  
C10 2.116034 0.534119 0.973005  
S11 1.782554 1.608524 -0.513901  
H12 1.236664 0.601017 1.608937  
H13 2.972448 0.976314 1.486926  
S14 -0.137975 2.391564 -0.210489  
C15 -1.262041 1.013563 -0.729433  
C16 -2.281711 0.571593 0.340780  
H17 -1.804312 1.342671 -1.618269  
H18 -0.609736 0.190149 -1.009235  
H19 -3.061883 1.332961 0.419244  
N20 -1.690950 0.392041 1.664799  
H21 -2.400750 0.074875 2.316862  
H22 -0.950501 -0.309216 1.625297  
C23 -3.012618 -0.686062 -0.203704  
O24 -2.324348 -1.817788 -0.264142  
O25 -4.180193 -0.630145 -0.542106

Zero-point correction= 0.187615 (Hartree/Particle)  
Thermal correction to Energy= 0.203103  
Thermal correction to Enthalpy= 0.204047  
Thermal correction to Gibbs Free Energy= 0.143928  
Sum of electronic and zero-point Energies= -1442.232661  
Sum of electronic and thermal Energies= -1442.217173  
Sum of electronic and thermal Enthalpies= -1442.216228  
Sum of electronic and thermal Free Energies= -1442.276348

**Cartesian coordinates and energies  
for di-deprotonated CySSCy in Fig. S3,  
optimized at B3LYP/6-311++G(d,p)**

**[CySSCy - 2H]<sup>2-</sup>\_1**

C1 4.392728 0.699043 -0.415419  
O2 4.714482 1.828552 0.026551  
O3 4.759708 0.121654 -1.461653  
C4 3.362651 -0.120210 0.476961  
H5 3.769440 -1.136702 0.539612  
N6 3.262234 0.463520 1.822441  
H7 3.642290 1.407377 1.731806  
H8 2.296043 0.523744 2.128332  
C9 2.029599 -0.192683 -0.279087  
S10 0.882138 -1.388991 0.572354  
H11 1.547140 0.786902 -0.309262  
H12 2.203259 -0.555251 -1.290987  
S13 -0.882263 -1.386003 -0.579403  
C14 -2.030261 -0.195118 0.278858  
C15 -3.362529 -0.117181 -0.478110  
H16 -2.205104 -0.564354 1.288141  
H17 -1.547556 0.784102 0.316085  
H18 -3.769689 -1.133072 -0.547740  
N19 -3.260465 0.475192 -1.819652  
H20 -3.639469 1.418893 -1.723277  
H21 -2.293995 0.536150 -2.124518  
C22 -4.393071 0.696737 0.418571  
O23 -4.713538 1.829427 -0.016098  
O24 -4.761583 0.112568 1.460503

Zero-point correction= 0.172972 (Hartree/Particle)  
Thermal correction to Energy= 0.189291  
Thermal correction to Enthalpy= 0.190235  
Thermal correction to Gibbs Free Energy= 0.124661  
Sum of electronic and zero-point Energies= -1441.616015  
Sum of electronic and thermal Energies= -1441.599695  
Sum of electronic and thermal Enthalpies= -1441.598751  
Sum of electronic and thermal Free Energies= -1441.664325

**[CySSCy - 2H]<sup>2-</sup>\_2**

C1 4.448016 0.999478 0.002408  
O2 5.171549 0.712618 0.987593  
O3 4.372810 2.065174 -0.644866  
C4 3.466189 -0.153600 -0.479552  
H5 3.471979 -0.118849 -1.574852  
N6 3.948361 -1.459560 -0.013656  
H7 4.523360 -1.256712 0.805214  
H8 3.172653 -2.057483 0.255896  
C9 2.052630 0.206099 0.008015  
S10 0.814154 -1.015229 -0.667368  
H11 1.995387 0.154522 1.097163  
H12 1.783090 1.204908 -0.333378  
S13 -0.814154 -1.015229 0.667368  
C14 -2.052630 0.206099 -0.008014  
C15 -3.466189 -0.153600 0.479552  
H16 -1.783090 1.204907 0.333379

H17 -1.995387 0.154523 -1.097162  
H18 -3.471979 -0.118849 1.574852  
N19 -3.948361 -1.459560 0.013656  
H20 -4.523361 -1.256711 -0.805213  
C21 -4.448016 0.999478 -0.002408  
O22 -5.171550 0.712618 -0.987593  
O23 -4.372810 2.065174 0.644865  
H24 -3.172653 -2.057483 -0.255897

Zero-point correction= 0.173145 (Hartree/Particle)  
Thermal correction to Energy= 0.189325  
Thermal correction to Enthalpy= 0.190269  
Thermal correction to Gibbs Free Energy= 0.125140  
Sum of electronic and zero-point Energies= -1441.615600  
Sum of electronic and thermal Energies= -1441.599421  
Sum of electronic and thermal Enthalpies= -1441.598476  
Sum of electronic and thermal Free Energies= -1441.663605

**[CySSCy - 2H]<sup>2-</sup>\_3**

C1 -4.490911 -0.294107 0.704130  
O2 -4.837613 0.331785 1.735312  
O3 -4.862187 -1.415748 0.294867  
C4 -3.420075 0.436176 -0.215908  
H5 -3.790720 0.328978 -1.242482  
N6 -3.320970 1.860642 0.134364  
H7 -3.722153 1.932775 1.070903  
H8 -2.353245 2.166545 0.163532  
C9 -2.094867 -0.330781 -0.110853  
S10 -0.899101 0.292893 -1.397488  
H11 -1.642843 -0.195544 0.874163  
H12 -2.268742 -1.389156 -0.298635  
S13 0.862453 -0.825261 -1.109540  
C14 1.989404 0.247043 -0.087400  
C15 3.349084 -0.440815 0.036163  
H16 2.105479 1.203091 -0.593095  
H17 1.545839 0.381484 0.899592  
H18 3.659733 -0.751925 -0.976064  
N19 3.305892 -1.577826 0.966639  
H20 3.118027 -2.450686 0.485933  
H21 4.233033 -1.615184 1.390454  
C22 4.495517 0.575763 0.471966  
O23 5.377540 0.083437 1.218947  
O24 4.427084 1.721541 -0.018807

Zero-point correction= 0.172788 (Hartree/Particle)  
Thermal correction to Energy= 0.189102  
Thermal correction to Enthalpy= 0.190046  
Thermal correction to Gibbs Free Energy= 0.124426  
Sum of electronic and zero-point Energies= -1441.614490  
Sum of electronic and thermal Energies= -1441.598176  
Sum of electronic and thermal Enthalpies= -1441.597232  
Sum of electronic and thermal Free Energies= -1441.662852

**[CySSCy - 2H]<sup>2-</sup>\_4**

C1 4.481919 0.978862 0.066822  
O2 5.130141 0.732141 1.113772  
O3 4.472553 2.011931 -0.635828

C4 3.515025 -0.181669 -0.424371  
 H5 3.584259 -0.192633 -1.517912  
 N6 3.954244 -1.472279 0.120950  
 H7 4.468833 -1.242979 0.972256  
 H8 3.155579 -2.055582 0.353426  
 C9 2.079206 0.209857 -0.033744  
 S10 0.867360 -1.030358 -0.725053  
 H11 1.960892 0.205330 1.051611  
 H12 1.839054 1.195533 -0.430887  
 S13 -0.815625 -0.995596 0.537015  
 C14 -2.049448 0.169337 -0.235328  
 C15 -3.432888 -0.140718 0.336032  
 H16 -1.769636 1.195248 -0.007341  
 H17 -2.039512 -0.005606 -1.311320  
 H18 -3.347599 -0.157923 1.437428  
 N19 -3.964417 -1.405289 -0.190668  
 H20 -3.688077 -2.194981 0.381917  
 H21 -4.978385 -1.300936 -0.174552  
 C22 -4.476426 1.033025 0.073930  
 O23 -5.660656 0.649505 -0.100109  
 O24 -4.022823 2.193999 0.127413

Zero-point correction= 0.172889 (Hartree/Particle)  
 Thermal correction to Energy= 0.189126  
 Thermal correction to Enthalpy= 0.190070  
 Thermal correction to Gibbs Free Energy= 0.124643  
 Sum of electronic and zero-point Energies= -1441.613742  
 Sum of electronic and thermal Energies= -1441.597506  
 Sum of electronic and thermal Enthalpies= -1441.596562  
 Sum of electronic and thermal Free Energies= -1441.661988

### [CySSCy - 2H]<sup>2-</sup>\_5

C1 4.553576 0.229662 -0.434487  
 O2 4.969186 1.376689 -0.729104  
 O3 4.972109 -0.886306 -0.812960  
 C4 3.312868 0.180383 0.558694  
 H5 3.569044 -0.573550 1.312890  
 N6 3.109780 1.485981 1.203916  
 H7 3.629151 2.150683 0.627852  
 H8 2.129092 1.748848 1.205399  
 C9 2.095856 -0.330561 -0.222007  
 S10 0.691628 -0.709493 0.943875  
 H11 1.753745 0.417886 -0.940614  
 H12 2.355821 -1.252652 -0.739651  
 S13 -0.818903 -1.495845 -0.295761  
 C14 -1.985924 -0.085773 -0.664841  
 C15 -3.249781 -0.104588 0.187342  
 H16 -1.443040 0.849878 -0.547988  
 H17 -2.246744 -0.219056 -1.717744  
 H18 -2.947582 0.054161 1.235363  
 N19 -3.983065 -1.369137 0.018665  
 H20 -3.692029 -2.053983 0.707759  
 H21 -4.964447 -1.132305 0.163126  
 C22 -4.207343 1.115894 -0.138818  
 O23 -5.436007 0.875143 -0.014506  
 O24 -3.643929 2.190411 -0.437127

Zero-point correction= 0.172824 (Hartree/Particle)  
 Thermal correction to Energy= 0.189099  
 Thermal correction to Enthalpy= 0.190043  
 Thermal correction to Gibbs Free Energy= 0.123465  
 Sum of electronic and zero-point Energies= -1441.613596  
 Sum of electronic and thermal Energies= -1441.597321  
 Sum of electronic and thermal Enthalpies= -1441.596377  
 Sum of electronic and thermal Free Energies= -1441.662955

### [CySSCy - 2H]<sup>2-</sup>\_6

C1 -4.593275 0.495141 -0.500924  
 O2 -5.511273 -0.131253 -1.087798  
 O3 -4.506266 1.715625 -0.253034  
 C4 -3.421130 -0.419617 0.069687  
 H5 -3.673772 -0.513186 1.139874  
 N6 -3.428467 -1.725012 -0.607047  
 H7 -4.377972 -1.839380 -0.961839  
 C8 -2.056890 0.264198 -0.024744  
 S9 -0.877329 -0.581103 1.141617  
 H10 -1.665089 0.184014 -1.039045  
 H11 -2.145603 1.306364 0.274061  
 S12 0.877333 0.581137 1.141613  
 C13 2.056883 -0.264167 -0.024755  
 C14 3.421141 0.419608 0.069695  
 H15 2.145568 -1.306340 0.274033  
 H16 1.665089 -0.183959 -1.039057  
 H17 3.673787 0.513143 1.139884  
 N18 3.428515 1.725023 -0.607003  
 H19 3.212377 2.481223 0.033126  
 H20 4.378019 1.839364 -0.961807  
 C21 4.593257 -0.495171 -0.500941  
 O22 5.511264 0.131210 -1.087816  
 O23 4.506220 -1.715657 -0.253069  
 H24 -3.212287 -2.481223 0.033056

Zero-point correction= 0.172718 (Hartree/Particle)  
 Thermal correction to Energy= 0.188994  
 Thermal correction to Enthalpy= 0.189938  
 Thermal correction to Gibbs Free Energy= 0.124674  
 Sum of electronic and zero-point Energies= -1441.612648  
 Sum of electronic and thermal Energies= -1441.596371  
 Sum of electronic and thermal Enthalpies= -1441.595427  
 Sum of electronic and thermal Free Energies= -1441.660692

### [CySSCy - 2H]<sup>2-</sup>\_7

C1 -4.317072 0.817788 0.248283  
 O2 -5.200206 0.637827 -0.629714  
 O3 -4.212279 1.742758 1.082458  
 C4 -3.150777 -0.252893 0.263374  
 H5 -2.828974 -0.373863 1.301423  
 N6 -3.642537 -1.530502 -0.263637  
 H7 -4.377560 -1.289922 -0.929059  
 H8 -2.897483 -2.032047 -0.739694  
 C9 -1.984241 0.354698 -0.535740  
 S10 -0.547044 -0.768174 -0.897236  
 H11 -2.327679 0.619079 -1.542849  
 H12 -1.607363 1.254585 -0.048747

S13 0.557395 -0.886078 0.890803  
 C14 1.946772 0.334708 0.668394  
 C15 3.148124 -0.204836 -0.097898  
 H16 1.552060 1.234174 0.200828  
 H17 2.237297 0.567836 1.697075  
 H18 2.808145 -0.447048 -1.118419  
 N19 3.728293 -1.374827 0.578218  
 H20 3.284188 -2.233140 0.270498  
 H21 4.712640 -1.380122 0.313642  
 C22 4.269173 0.895777 -0.311681  
 O23 5.445072 0.450837 -0.359065  
 O24 3.868281 2.070371 -0.457709

Zero-point correction= 0.172950 (Hartree/Particle)  
 Thermal correction to Energy= 0.189045  
 Thermal correction to Enthalpy= 0.189989  
 Thermal correction to Gibbs Free Energy= 0.125324  
 Sum of electronic and zero-point Energies= -1441.612142  
 Sum of electronic and thermal Energies= -1441.596048  
 Sum of electronic and thermal Enthalpies= -1441.595103  
 Sum of electronic and thermal Free Energies= -1441.659769

#### [CySSCy - 2H]<sup>2-</sup>\_8

C1 4.485765 0.686488 -0.030117  
 O2 4.741206 1.557307 0.836499  
 O3 5.058653 0.468954 -1.123351  
 C4 3.264468 -0.277538 0.284278  
 H5 3.639198 -1.292235 0.102464  
 N6 2.833690 -0.147699 1.682014  
 H7 3.246194 0.726239 2.011063  
 H8 1.823592 -0.082626 1.755551  
 C9 2.168230 -0.006445 -0.748696  
 S10 0.856402 -1.316439 -0.928770  
 H11 1.669765 0.949355 -0.569381  
 H12 2.627040 0.014976 -1.740715  
 S13 -0.640290 -0.917745 0.498133  
 C14 -1.963412 0.014838 -0.425126  
 C15 -3.250646 0.000973 0.398004  
 H16 -1.636599 1.038995 -0.589961  
 H17 -2.120484 -0.496107 -1.375420  
 H18 -3.007772 0.362676 1.412963  
 N19 -3.863609 -1.334640 0.425386  
 H20 -3.512548 -1.892257 1.196027  
 H21 -4.863058 -1.171176 0.542469  
 C22 -4.311833 1.065559 -0.127392  
 O23 -5.511818 0.720528 0.016556  
 O24 -3.846679 2.135990 -0.568751

Zero-point correction= 0.172785 (Hartree/Particle)  
 Thermal correction to Energy= 0.189048  
 Thermal correction to Enthalpy= 0.189992  
 Thermal correction to Gibbs Free Energy= 0.124670  
 Sum of electronic and zero-point Energies= -1441.612248  
 Sum of electronic and thermal Energies= -1441.595985  
 Sum of electronic and thermal Enthalpies= -1441.595041  
 Sum of electronic and thermal Free Energies= -1441.660363

#### [CySSCy - 2H]<sup>2-</sup>\_9

C1 -4.290647 0.977441 -0.342754  
 O2 -5.307730 0.322506 -0.689703  
 O3 -4.026739 2.183420 -0.536924  
 C4 -3.168426 0.140184 0.396940  
 H5 -2.684895 0.801391 1.121251  
 N6 -3.776215 -1.002969 1.085902  
 H7 -4.602179 -1.248420 0.539555  
 H8 -3.133127 -1.789791 1.110903  
 C9 -2.131182 -0.241868 -0.675102  
 S10 -0.835721 -1.481411 -0.182812  
 H11 -2.634507 -0.756338 -1.502295  
 H12 -1.632877 0.645200 -1.066973  
 S13 0.633831 -0.436632 0.904866  
 C14 2.011539 -0.171837 -0.320047  
 C15 3.279652 0.247694 0.422256  
 H16 2.186650 -1.111901 -0.838776  
 H17 1.711737 0.606631 -1.022569  
 H18 3.434373 -0.467891 1.247506  
 N19 3.200191 1.632313 0.908501  
 H20 2.855553 1.677948 1.861170  
 H21 4.156165 1.986482 0.875825  
 C22 4.581504 0.060563 -0.476203  
 O23 5.475066 0.924393 -0.293330  
 O24 4.598263 -0.946955 -1.213769

Zero-point correction= 0.172899 (Hartree/Particle)  
 Thermal correction to Energy= 0.189085  
 Thermal correction to Enthalpy= 0.190029  
 Thermal correction to Gibbs Free Energy= 0.124927  
 Sum of electronic and zero-point Energies= -1441.612030  
 Sum of electronic and thermal Energies= -1441.595844  
 Sum of electronic and thermal Enthalpies= -1441.594899  
 Sum of electronic and thermal Free Energies= -1441.660002

#### [CySSCy - 2H]<sup>2-</sup>\_10

C1 4.318992 0.831337 -0.309217  
 O2 5.488689 0.367424 -0.287298  
 O3 3.943160 1.997715 -0.554090  
 C4 3.174587 -0.234474 -0.049956  
 H5 2.869065 -0.554828 -1.059911  
 N6 3.714215 -1.353028 0.738608  
 H7 4.705454 -1.395746 0.505100  
 C8 1.952782 0.376382 0.625335  
 S9 0.546634 -0.815175 0.899564  
 H10 2.210673 0.696892 1.638982  
 H11 1.581505 1.233616 0.067810  
 S12 -0.546637 -0.815171 -0.899579  
 C13 -1.952785 0.376384 -0.625343  
 C14 -3.174585 -0.234472 0.049959  
 H15 -1.581506 1.233621 -0.067823  
 H16 -2.210684 0.696890 -1.638990  
 H17 -2.869054 -0.554822 1.059913  
 N18 -3.714216 -1.353030 -0.738597  
 H19 -3.263377 -2.226571 -0.488707  
 H20 -4.705454 -1.395749 -0.505081  
 C21 -4.318990 0.831337 0.309224



O22 -5.488686 0.367422 0.287318  
 O23 -3.943159 1.997718 0.554087  
 H24 3.263380 -2.226571 0.488719

Zero-point correction= 0.172637 (Hartree/Particle)  
 Thermal correction to Energy= 0.188846  
 Thermal correction to Enthalpy= 0.189790  
 Thermal correction to Gibbs Free Energy= 0.124083  
 Sum of electronic and zero-point Energies= -1441.611687  
 Sum of electronic and thermal Energies= -1441.595478  
 Sum of electronic and thermal Enthalpies= -1441.594534  
 Sum of electronic and thermal Free Energies= -1441.660242

### [CySSCy - 2H]<sup>2-</sup>\_11

C1 4.531292 0.998777 -0.041962  
 O2 5.696403 0.610277 0.226920  
 O3 4.106901 2.160416 -0.207883  
 C4 3.480802 -0.173432 -0.276388  
 H5 3.465549 -0.276662 -1.376633  
 N6 3.951291 -1.401308 0.379777  
 H7 4.967174 -1.323732 0.407045  
 C8 2.068859 0.198606 0.175946  
 S9 0.864652 -0.998860 -0.597228  
 H10 1.981591 0.100990 1.258171  
 H11 1.826323 1.210084 -0.141566  
 S12 -0.864653 -0.998857 0.597235  
 C13 -2.068858 0.198609 -0.175941  
 C14 -3.480802 -0.173432 0.276386  
 H15 -1.826325 1.210086 0.141573  
 H16 -1.981584 0.100995 -1.258167  
 H17 -3.465553 -0.276665 1.376631  
 N18 -3.951286 -1.401307 -0.379784  
 H19 -3.679007 -2.229024 0.138552  
 H20 -4.967169 -1.323733 -0.407056  
 C21 -4.531293 0.998775 0.041959  
 O22 -5.696403 0.610274 -0.226930  
 O23 -4.106906 2.160414 0.207886  
 H24 3.679011 -2.229024 -0.138560

Zero-point correction= 0.172612 (Hartree/Particle)  
 Thermal correction to Energy= 0.188903  
 Thermal correction to Enthalpy= 0.189847  
 Thermal correction to Gibbs Free Energy= 0.124146  
 Sum of electronic and zero-point Energies= -1441.611705  
 Sum of electronic and thermal Energies= -1441.595414  
 Sum of electronic and thermal Enthalpies= -1441.594470  
 Sum of electronic and thermal Free Energies= -1441.660172

### [CySSCy - 2H]<sup>2-</sup>\_12

C1 -4.619941 -0.208988 0.601800  
 O2 -5.515270 0.626749 0.884311  
 O3 -4.591787 -1.437387 0.823902  
 C4 -3.393793 0.382730 -0.223532  
 H5 -3.632199 0.100593 -1.263888  
 N6 -3.334896 1.841964 -0.054690  
 H7 -4.283443 2.125156 0.190287  
 C8 -2.069213 -0.285917 0.143941  
 S9 -0.835177 0.025459 -1.215618

H10 -1.681315 0.134808 1.072185  
 H11 -2.211893 -1.360310 0.237182  
 S12 0.869953 -1.108189 -0.720241  
 C13 2.036516 0.104995 0.082180  
 C14 3.488330 -0.323726 -0.144941  
 H15 1.858271 1.081264 -0.365592  
 H16 1.811600 0.143019 1.150210  
 H17 3.648305 -0.395027 -1.225368  
 N18 3.748574 -1.639253 0.479266  
 H19 4.400812 -2.152650 -0.105746  
 H20 4.276092 -1.411851 1.326381  
 C21 4.466558 0.804957 0.388384  
 O22 5.136660 0.501043 1.408855  
 O23 4.465473 1.870495 -0.266075  
 H24 -3.049725 2.308185 -0.908881

Zero-point correction= 0.172623 (Hartree/Particle)  
 Thermal correction to Energy= 0.189170  
 Thermal correction to Enthalpy= 0.190114  
 Thermal correction to Gibbs Free Energy= 0.123503  
 Sum of electronic and zero-point Energies= -1441.611903  
 Sum of electronic and thermal Energies= -1441.595356  
 Sum of electronic and thermal Enthalpies= -1441.594412  
 Sum of electronic and thermal Free Energies= -1441.661024

### [CySSCy - 2H]<sup>2-</sup>\_13

C1 4.408095 -0.030785 0.075131  
 O2 4.990008 0.131424 -1.026525  
 O3 4.667995 -0.836207 0.996809  
 C4 3.218796 0.970511 0.379637  
 H5 3.561327 1.510872 1.275201  
 N6 2.995509 1.945811 -0.702023  
 H7 3.732961 1.740422 -1.380008  
 H8 2.116909 1.743916 -1.171237  
 C9 1.938656 0.268184 0.844998  
 S10 1.080130 -0.654217 -0.529442  
 H11 2.200812 -0.452639 1.617223  
 H12 1.215857 0.990212 1.232090  
 S13 -0.720679 -1.265517 0.367929  
 C14 -1.951195 0.095384 0.034785  
 C15 -3.380477 -0.420171 0.267586  
 H16 -1.746048 0.927471 0.707332  
 H17 -1.818574 0.410875 -1.002216  
 H18 -3.454980 -0.766007 1.305007  
 N19 -3.789170 -1.491673 -0.650538  
 H20 -4.343226 -1.028692 -1.372552  
 H21 -2.980595 -1.934097 -1.077102  
 C22 -4.368527 0.818261 0.147866  
 O23 -5.051437 0.864888 -0.904662  
 O24 -4.340581 1.613161 1.111676

Zero-point correction= 0.173172 (Hartree/Particle)  
 Thermal correction to Energy= 0.189409  
 Thermal correction to Enthalpy= 0.190354  
 Thermal correction to Gibbs Free Energy= 0.125294  
 Sum of electronic and zero-point Energies= -1441.611240  
 Sum of electronic and thermal Energies= -1441.595002  
 Sum of electronic and thermal Enthalpies= -1441.594058  
 Sum of electronic and thermal Free Energies= -1441.659117

**[CySSCy - 2H]<sup>2-</sup>\_14**

C1 4.383943 0.373402 0.583967  
 O2 4.821701 -0.433979 1.439671  
 O3 4.735297 1.555301 0.361713  
 C4 3.212322 -0.159162 -0.344257  
 H5 3.493181 0.122663 -1.366142  
 N6 3.086351 -1.618824 -0.245689  
 H7 3.572840 -1.873893 0.614746  
 H8 2.115372 -1.904498 -0.172411  
 C9 1.941816 0.618406 0.011289  
 S10 0.537612 0.515382 -1.208846  
 H11 1.553458 0.333718 0.992064  
 H12 2.178621 1.685344 0.024737  
 S13 -0.594072 -1.190927 -0.705106  
 C14 -1.948589 -0.657977 0.442008  
 C15 -3.016014 0.280735 -0.115811  
 H16 -2.423742 -1.615190 0.679760  
 H17 -1.505961 -0.236307 1.345797  
 H18 -3.127779 0.054891 -1.190042  
 N19 -2.674810 1.687873 0.123566  
 H20 -2.022209 2.037915 -0.569782  
 H21 -3.550988 2.204384 0.081602  
 C22 -4.458782 -0.025280 0.475053  
 O23 -5.235369 0.961098 0.501696  
 O24 -4.690180 -1.215469 0.787453

Zero-point correction= 0.172763 (Hartree/Particle)  
 Thermal correction to Energy= 0.188923  
 Thermal correction to Enthalpy= 0.189867  
 Thermal correction to Gibbs Free Energy= 0.125019  
 Sum of electronic and zero-point Energies= -1441.611085  
 Sum of electronic and thermal Energies= -1441.594924  
 Sum of electronic and thermal Enthalpies= -1441.593980  
 Sum of electronic and thermal Free Energies= -1441.658828

**[CySSCy - 2H]<sup>2-</sup>\_15**

C1 -4.331597 1.025118 -0.178941  
 O2 -5.525443 0.739602 0.099456  
 O3 -3.872644 2.077596 -0.672513  
 C4 -3.272643 -0.087757 0.209251  
 H5 -2.924370 0.202057 1.214600  
 N6 -3.927612 -1.405406 0.218671  
 H7 -4.903055 -1.221260 0.450173  
 C8 -2.060797 -0.084022 -0.715125  
 S9 -0.779390 -1.373364 -0.292390  
 H10 -2.369670 -0.344060 -1.731166  
 H11 -1.579121 0.891178 -0.730182  
 S12 0.646043 -0.420160 0.933580  
 C13 2.027252 0.028519 -0.236842  
 C14 3.381201 -0.037925 0.473116  
 H15 2.000682 -0.681616 -1.061721  
 H16 1.842197 1.037041 -0.613436  
 H17 3.501145 -1.052716 0.865078  
 N18 3.432207 0.930000 1.589938  
 H19 3.982917 0.527931 2.342458

H20 4.002791 1.698378 1.227572  
 C21 4.543293 0.186905 -0.582300  
 O22 5.180048 1.265281 -0.464116  
 O23 4.698466 -0.733411 -1.415170  
 H24 -3.515788 -2.010269 0.921108

Zero-point correction= 0.172498 (Hartree/Particle)  
 Thermal correction to Energy= 0.189093  
 Thermal correction to Enthalpy= 0.190037  
 Thermal correction to Gibbs Free Energy= 0.122016  
 Sum of electronic and zero-point Energies= -1441.611211  
 Sum of electronic and thermal Energies= -1441.594616  
 Sum of electronic and thermal Enthalpies= -1441.593672  
 Sum of electronic and thermal Free Energies= -1441.661692

**CySSCy - 2H]<sup>2-</sup>\_16**

C1 -3.989976 -1.038848 -0.178001  
 O2 -4.920642 -0.883588 0.653072  
 O3 -4.042047 -1.476872 -1.348079  
 C4 -2.562154 -0.547504 0.303476  
 H5 -1.856221 0.130003 2.116815  
 N6 2.946038 -0.984641 -1.636860  
 H7 3.375590 -1.857507 -1.323933  
 H8 1.965659 -1.159992 -1.833645  
 C9 -2.384295 0.851425 -0.306582  
 S10 -0.939403 1.885885 0.244984  
 H11 -2.359997 0.794861 -1.395289  
 H12 -3.228450 1.485804 -0.010648  
 S13 0.718193 1.297887 -0.917903  
 C14 1.794218 0.280522 0.214056  
 C15 3.104666 -0.058713 -0.504458  
 H16 2.011977 0.880427 1.095956  
 H17 1.250024 -0.622933 0.496953  
 H18 3.545249 0.883443 -0.854474  
 N19 -2.481245 -0.589472 1.763980  
 H20 -1.816852 -1.217282 -0.134909  
 H21 -3.428473 -0.429662 2.105740  
 C22 4.141380 -0.628635 0.559972  
 O23 4.496559 -1.819471 0.388189  
 O24 4.491665 0.185155 1.442259

Zero-point correction= 0.173009 (Hartree/Particle)  
 Thermal correction to Energy= 0.189262  
 Thermal correction to Enthalpy= 0.190207  
 Thermal correction to Gibbs Free Energy= 0.125004  
 Sum of electronic and zero-point Energies= -1441.610852  
 Sum of electronic and thermal Energies= -1441.594599  
 Sum of electronic and thermal Enthalpies= -1441.593654  
 Sum of electronic and thermal Free Energies= -1441.658857

**CySSCy - 2H]<sup>2-</sup>\_17**

C1 4.014858 0.900209 -0.396526  
 O2 4.460982 0.686760 -1.547748  
 O3 4.246672 1.862190 0.375540  
 C4 3.013407 -0.205967 0.145027  
 H5 3.510298 -1.165904 -0.040540  
 N6 2.772500 -0.038790 1.583958  
 H7 1.786626 -0.121201 1.809879

H8 3.084050 0.909037 1.800426  
 C9 1.751991 -0.173305 -0.721615  
 S10 0.650357 -1.671707 -0.633439  
 H11 1.141931 0.709871 -0.518473  
 H12 2.054731 -0.159199 -1.772039  
 S13 -0.639106 -1.411960 1.016448  
 C14 -2.289375 -0.959426 0.282763  
 C15 -2.556008 0.522829 0.058980  
 H16 -2.413798 -1.520446 -0.641197  
 H17 -2.990660 -1.346662 1.028479  
 H18 -1.843245 0.885585 -0.698706  
 N19 -2.458235 1.278999 1.314529  
 H20 -3.119972 2.048728 1.220283  
 C21 -3.984909 0.746348 -0.597420  
 O22 -4.341288 -0.110768 -1.436523  
 O23 -4.587042 1.784772 -0.226691  
 H24 -1.524210 1.649638 1.450460

Zero-point correction= 0.172854 (Hartree/Particle)  
 Thermal correction to Energy= 0.189064  
 Thermal correction to Enthalpy= 0.190008  
 Thermal correction to Gibbs Free Energy= 0.124968  
 Sum of electronic and zero-point Energies= -1441.610386  
 Sum of electronic and thermal Energies= -1441.594176  
 Sum of electronic and thermal Enthalpies= -1441.593232  
 Sum of electronic and thermal Free Energies= -1441.658272

### [CySSCy - 2H]<sup>2-</sup>\_18

C1 4.397428 -0.549068 0.322042  
 O2 5.273282 -0.201172 -0.510083  
 O3 4.296185 -1.624160 0.956339  
 C4 3.324815 0.558427 0.684030  
 H5 3.610902 0.862040 1.704044  
 N6 3.388098 1.748180 -0.179793  
 H7 2.697456 1.630125 -0.919202  
 C8 1.902682 0.015501 0.848804  
 S9 1.082123 -0.504551 -0.746850  
 H10 1.942887 -0.865703 1.487096  
 H11 1.237941 0.766434 1.280219  
 S12 -0.677851 0.646290 -0.841481  
 C13 -2.010644 -0.388303 -0.056339  
 C14 -3.328075 0.386010 -0.103938  
 H15 -2.104887 -1.316613 -0.615534  
 H16 -1.731383 -0.586702 0.978936  
 H17 -3.459708 0.761262 -1.133723  
 N18 -3.356272 1.476817 0.881451  
 H19 -3.028330 2.350338 0.484491  
 H20 -4.335090 1.569676 1.152780  
 C21 -4.591121 -0.562598 0.100762  
 O22 -5.544479 -0.038974 0.730338  
 O23 -4.522682 -1.689650 -0.431234  
 H24 4.290135 1.658181 -0.652479

Zero-point correction= 0.172988 (Hartree/Particle)  
 Thermal correction to Energy= 0.189221  
 Thermal correction to Enthalpy= 0.190165  
 Thermal correction to Gibbs Free Energy= 0.124842  
 Sum of electronic and zero-point Energies= -1441.610236

Sum of electronic and thermal Energies= -1441.594003  
 Sum of electronic and thermal Enthalpies= -1441.593059  
 Sum of electronic and thermal Free Energies= -1441.658382

### [CySSCy - 2H]<sup>2-</sup>\_19

C1 4.351032 0.922150 0.371094  
 O2 5.538189 0.592360 0.120004  
 O3 3.927180 1.852100 1.086989  
 C4 3.253117 0.065130 -0.398853  
 H5 3.041151 0.672821 -1.297159  
 N6 3.812616 -1.248769 -0.747442  
 H7 4.815896 -1.099645 -0.846688  
 C8 1.953145 -0.068839 0.392360  
 S9 0.610423 -0.697215 -0.738863  
 H10 2.073072 -0.801114 1.191243  
 H11 1.659163 0.896597 0.797343  
 S12 -0.862787 -1.518635 0.522120  
 C13 -2.165312 -0.236922 0.836016  
 C14 -3.068175 0.141219 -0.336209  
 H15 -2.779956 -0.729226 1.596250  
 H16 -1.698811 0.651873 1.263403  
 H17 -3.164353 -0.750865 -0.978925  
 N18 -2.542737 1.299012 -1.068006  
 H19 -1.804374 1.034023 -1.711464  
 H20 -3.329031 1.701291 -1.573453  
 C21 -4.564080 0.427279 0.113075  
 O22 -5.198153 1.208996 -0.637977  
 O23 -4.973366 -0.200134 1.116890  
 H24 3.426752 -1.600537 -1.616691

Zero-point correction= 0.172686 (Hartree/Particle)  
 Thermal correction to Energy= 0.188847  
 Thermal correction to Enthalpy= 0.189791  
 Thermal correction to Gibbs Free Energy= 0.124762  
 Sum of electronic and zero-point Energies= -1441.610158  
 Sum of electronic and thermal Energies= -1441.593997  
 Sum of electronic and thermal Enthalpies= -1441.593053  
 Sum of electronic and thermal Free Energies= -1441.658082

### [CySSCy - 2H]<sup>2-</sup>\_20

C1 4.443227 -0.180898 -0.385447  
 O2 5.235594 0.746744 -0.684379  
 O3 4.662693 -1.412613 -0.331220  
 C4 2.996993 0.298580 0.062594  
 H5 3.090532 0.397145 1.157691  
 N6 2.678227 1.577253 -0.583670  
 H7 3.558825 2.079611 -0.673843  
 C8 1.921504 -0.750023 -0.212983  
 S9 0.546519 -0.902132 1.021011  
 H10 1.493954 -0.607761 -1.206420  
 H11 2.382953 -1.740640 -0.152197  
 S12 -0.546520 0.902138 1.021008  
 C13 -1.921505 0.750024 -0.212986  
 C14 -2.996992 -0.298580 0.062594  
 H15 -2.382955 1.740640 -0.152202  
 H16 -1.493954 0.607760 -1.206422

H17 -3.090531 -0.397144 1.157691  
 N18 -2.678225 -1.577254 -0.583668  
 H19 -2.014980 -2.115272 -0.035879  
 H20 -3.558822 -2.079613 -0.673840  
 C21 -4.443227 0.180896 -0.385447  
 O22 -5.235594 -0.746748 -0.684377  
 O23 -4.662695 1.412610 -0.331222  
 H24 2.014983 2.115272 -0.035882

Zero-point correction= 0.172842 (Hartree/Particle)  
 Thermal correction to Energy= 0.188814  
 Thermal correction to Enthalpy= 0.189758  
 Thermal correction to Gibbs Free Energy= 0.125821  
 Sum of electronic and zero-point Energies= -1441.609293  
 Sum of electronic and thermal Energies= -1441.593322  
 Sum of electronic and thermal Enthalpies= -1441.592378  
 Sum of electronic and thermal Free Energies= -1441.656315

### [CySSCy - 2H]<sup>2-</sup>\_21

C1 4.427897 -0.059319 0.178260  
 O2 5.067067 -0.012806 -0.902832  
 O3 4.629375 -0.773913 1.185688  
 C4 3.241939 0.980771 0.322881  
 H5 3.546687 1.600105 1.180197  
 N6 3.094709 1.850752 -0.857607  
 H7 3.858332 1.565253 -1.474831  
 H8 2.234122 1.622452 -1.347718  
 C9 1.925637 0.343591 0.782005  
 S10 1.123275 -0.695954 -0.541856  
 H11 2.132153 -0.302288 1.633460  
 H12 1.197390 1.109700 1.058537  
 S13 -0.724021 -1.210424 0.318159  
 C14 -1.934679 0.107391 -0.198297  
 C15 -3.344876 -0.347606 0.178503  
 H16 -1.696015 1.036024 0.315477  
 H17 -1.855996 0.231502 -1.278633  
 H18 -3.324887 -0.665880 1.235759  
 N19 -3.824573 -1.420543 -0.704786  
 H20 -3.592098 -2.337862 -0.340770  
 H21 -4.837571 -1.309101 -0.739554  
 C22 -4.387970 0.855188 0.182682  
 O23 -5.549956 0.542703 -0.180755  
 O24 -3.960089 1.951590 0.597620

Zero-point correction= 0.173024 (Hartree/Particle)  
 Thermal correction to Energy= 0.189272  
 Thermal correction to Enthalpy= 0.190216  
 Thermal correction to Gibbs Free Energy= 0.125273  
 Sum of electronic and zero-point Energies= -1441.609383  
 Sum of electronic and thermal Energies= -1441.593135  
 Sum of electronic and thermal Enthalpies= -1441.592191  
 Sum of electronic and thermal Free Energies= -1441.657135

### CySSCy - 2H]<sup>2-</sup>\_22

C1 -4.222456 0.626380 -0.379522  
 O2 -5.035628 -0.228433 -0.813124  
 O3 -4.098703 1.830535 -0.701919

C4 -3.286887 0.137240 0.800423  
 H5 -3.710486 0.643416 1.683736  
 N6 -3.347500 -1.313294 1.038343  
 H7 -4.174424 -1.611130 0.516041  
 H8 -2.563551 -1.747450 0.555655  
 C9 -1.858312 0.678042 0.717815  
 S10 -0.808450 -0.013549 -0.659376  
 H11 -1.911948 1.750252 0.531536  
 H12 -1.302964 0.488051 1.638669  
 S13 0.556161 -1.306606 0.290745  
 C14 2.035876 -0.267646 0.738240  
 C15 3.059689 -0.079086 -0.373232  
 H16 1.689936 0.691665 1.117601  
 H17 2.485231 -0.830903 1.561864  
 H18 2.572785 0.490399 -1.181775  
 N19 3.575809 -1.372107 -0.847171  
 H20 2.995801 -1.746147 -1.590426  
 H21 4.510345 -1.176516 -1.203763  
 C22 4.269282 0.837768 0.085300  
 O23 5.368283 0.581568 -0.470418  
 O24 3.999121 1.737887 0.910035

Zero-point correction= 0.172883 (Hartree/Particle)  
 Thermal correction to Energy= 0.189110  
 Thermal correction to Enthalpy= 0.190055  
 Thermal correction to Gibbs Free Energy= 0.124626  
 Sum of electronic and zero-point Energies= -1441.608947  
 Sum of electronic and thermal Energies= -1441.592720  
 Sum of electronic and thermal Enthalpies= -1441.591776  
 Sum of electronic and thermal Free Energies= -1441.657204

### [CySSCy - 2H]<sup>2-</sup>\_23

C1 -3.897143 -0.721450 -0.346994  
 O2 -4.373587 -1.689849 0.294633  
 O3 -4.382275 -0.117833 -1.331359  
 C4 -2.534861 -0.140620 0.230111  
 H5 -2.867107 0.683036 0.883930  
 N6 -1.821131 -1.183661 0.977742  
 H7 -2.536821 -1.812187 1.338344  
 C8 -1.657888 0.464205 -0.864196  
 S9 -0.634673 1.945941 -0.416482  
 H10 -1.008823 -0.300368 -1.292246  
 H11 -2.308994 0.873621 -1.642726  
 S12 0.578204 1.430238 1.225652  
 C13 2.222508 0.923761 0.525305  
 C14 2.314558 -0.468735 -0.088578  
 H15 2.542532 1.681294 -0.187211  
 H16 2.865749 0.977306 1.410484  
 H17 1.685632 -0.474703 -0.993663  
 N18 1.911088 -1.505375 0.865610  
 H19 0.920501 -1.715250 0.779905  
 H20 2.457883 -2.330259 0.625455  
 C21 3.783426 -0.739819 -0.625305  
 O22 4.193560 -1.920265 -0.504544  
 O23 4.364685 0.241514 -1.145581  
 H24 -1.279399 -0.790689 1.740297

Zero-point correction=	0.173382 (Hartree/Particle)
Thermal correction to Energy=	0.189217
Thermal correction to Enthalpy=	0.190161
Thermal correction to Gibbs Free Energy=	0.126888
Sum of electronic and zero-point Energies=	-1441.608528
Sum of electronic and thermal Energies=	-1441.592693
Sum of electronic and thermal Enthalpies=	-1441.591749
Sum of electronic and thermal Free Energies=	-1441.655022

**Cartesian coordinates and energies  
for TS(C-S) in Fig. 2d, optimized  
at B3LYP/6-311++G(d,p)**

C1 -4.890929 -1.094044 -0.507967  
O2 -4.863532 -2.040902 0.207470  
O3 -5.276584 -0.461890 -1.432037  
C4 -3.453824 0.379970 0.726918  
H5 -4.259805 1.108760 0.673774  
N6 -3.294023 -0.237418 2.010436  
H7 -3.826151 -1.101369 2.070557  
H8 -2.314962 -0.454563 2.170569  
C9 -2.440894 0.438088 -0.187137  
S10 -0.338743 2.171395 0.409418  
H11 -1.596879 -0.236179 -0.141741  
H12 -2.550850 1.018201 -1.091389  
S13 1.162333 1.420815 -0.876567  
C14 2.328713 0.469709 0.221672  
C15 3.372054 -0.302548 -0.604546  
H16 2.828428 1.182468 0.878451  
H17 1.729554 -0.218047 0.824638  
H18 3.918821 0.420225 -1.220780  
N19 2.792814 -1.349234 -1.464391  
H20 2.889059 -2.214605 -0.931510  
H21 1.806277 -1.163400 -1.624016  
C22 4.434912 -0.934830 0.383312  
O23 4.309883 -2.166477 0.607851  
O24 5.281150 -0.136777 0.847965  
Zero-point correction= 0.168241 (Hartree/Particle)  
Thermal correction to Energy= 0.186066  
Thermal correction to Enthalpy= 0.187010  
Thermal correction to Gibbs Free Energy= 0.116312  
Sum of electronic and zero-point Energies= -1441.570280  
Sum of electronic and thermal Energies= -1441.552455  
Sum of electronic and thermal Enthalpies= -1441.551511  
Sum of electronic and thermal Free Energies= -1441.622210

**Cartesian coordinates and energies  
for the structure in Fig. 3, optimized  
at B3LYP/6-31+G(d,p)**

**protonated precursor**

C1 0.569816 2.303117 -0.553834  
 O2 -0.626701 2.271759 -0.771025  
 O3 1.488299 2.671170 -1.450564  
 H4 1.049576 2.900972 -2.289542  
 C5 1.216061 1.921150 0.777489  
 H6 1.927971 2.721549 1.025365  
 N7 0.162737 1.804760 1.806026  
 H8 -1.257261 1.002791 1.305374  
 H9 0.552469 1.371866 2.642178  
 H10 -0.142921 2.737800 2.083213  
 C11 2.064224 0.640254 0.659421  
 S12 1.353298 -0.860521 -0.139549  
 H13 2.926902 0.844134 0.018008  
 H14 2.457347 0.367425 1.643223  
 S15 0.081758 -1.699894 1.318201  
 C16 -1.536462 -1.767694 0.435320  
 C17 -2.087123 -0.433866 -0.072932  
 H18 -1.458049 -2.451268 -0.411517  
 H19 -2.211333 -2.231521 1.165571  
 H20 -1.397427 -0.006167 -0.807222  
 N21 -2.214557 0.582331 1.018350  
 H22 -2.675331 0.183768 1.840967  
 H23 -2.815922 1.343259 0.683132  
 C24 -3.462225 -0.560102 -0.734524  
 O25 -4.403701 0.134547 -0.419157  
 O26 -3.467668 -1.494193 -1.686682  
 H27 -4.348540 -1.525695 -2.103280  
 O28 4.164848 -1.337794 -1.198532  
 O29 5.121000 -1.697873 -0.535314

Zero-point correction=	0.219800 (Hartree/Particle)
Thermal correction to Energy=	0.239688
Thermal correction to Enthalpy=	0.240632
Thermal correction to Gibbs Free Energy=	0.166146
Sum of electronic and zero-point Energies=	-1593.158566
Sum of electronic and thermal Energies=	-1593.138679
Sum of electronic and thermal Enthalpies=	-1593.137735
Sum of electronic and thermal Free Energies=	-1593.212220

**Cartesian coordinates and energies  
for the structure in Fig. 4, optimized  
at B3LYP/6-31+G(d,p)**

**deprotonated precursor**

C1 -0.415747 -2.166697 -0.097807  
 O2 0.019821 -2.432693 1.043953  
 O3 0.268598 -1.901977 -1.144042  
 H4 1.723109 -1.620620 -1.119531  
 C5 -1.957013 -2.117892 -0.267290  
 H6 -2.196086 -2.131205 -1.334851  
 N7 -2.628959 -3.257916 0.385772  
 H8 -2.133462 -3.422043 1.263802  
 C9 -2.549392 -0.843762 0.366171  
 S10 -2.058736 0.751568 -0.430166  
 H11 -3.639616 -0.878425 0.274748  
 H12 -2.293017 -0.794260 1.428357  
 S13 -0.469629 1.426684 0.724888  
 C14 1.041428 1.065002 -0.277624  
 C15 2.023790 0.198137 0.532398  
 H16 0.704091 0.566992 -1.187160  
 H17 1.492468 2.031367 -0.524472  
 H18 1.477650 -0.655001 0.948086  
 N19 2.585614 0.986445 1.629720  
 H20 2.881092 0.365318 2.377956  
 H21 3.432058 1.443185 1.290206  
 C22 3.104672 -0.364752 -0.426908  
 O23 4.243302 0.089152 -0.426069  
 O24 2.724316 -1.335010 -1.233841  
 H25 -2.479510 -4.093604 -0.176084  
 O26 -0.901938 3.699080 -0.208268  
 O27 -2.066343 3.833492 -0.661571

Zero-point correction= 0.192102 (Hartree/Particle)  
 Thermal correction to Energy= 0.211186  
 Thermal correction to Enthalpy= 0.212130  
 Thermal correction to Gibbs Free Energy= 0.142757  
 Sum of electronic and zero-point Energies= -1592.303809  
 Sum of electronic and thermal Energies= -1592.284725  
 Sum of electronic and thermal Enthalpies= -1592.283781  
 Sum of electronic and thermal Free Energies= -1592.353154

**[TS – H]<sup>-</sup>**

C1 -1.128304 -1.834832 0.113621  
 O2 -0.769124 -1.888464 1.312605  
 O3 -0.410356 -2.072199 -0.915242  
 H4 1.071971 -2.236454 -0.864882  
 C5 -2.587970 -1.386537 -0.153133  
 H6 -2.827471 -1.561002 -1.206132  
 N7 -3.563487 -2.110358 0.682707  
 H8 -3.151714 -2.195228 1.613094  
 C9 -2.759523 0.110791 0.166950  
 S10 -1.798042 1.258529 -0.910704  
 H11 -3.807648 0.394064 0.031579  
 H12 -2.489110 0.303914 1.210475  
 S13 -0.033118 1.595501 0.310876  
 C14 1.289943 0.629160 -0.520087  
 C15 1.943998 -0.345562 0.478602

H16 0.823008 0.113852 -1.359910  
 H17 2.002535 1.382966 -0.872927  
 H18 1.154952 -0.906365 0.992688  
 N19 2.710364 0.403591 1.466080  
 H20 2.830768 -0.156903 2.304858  
 H21 3.644940 0.575901 1.097528  
 C22 2.785364 -1.373042 -0.323908  
 O23 4.007438 -1.307125 -0.339766  
 O24 2.108933 -2.297093 -0.978536  
 H25 -3.660487 -3.060910 0.331870  
 O26 0.559336 3.176345 -0.195153  
 O27 -0.194025 4.242185 0.204243

Zero-point correction= 0.191567 (Hartree/Particle)  
 Thermal correction to Energy= 0.209583  
 Thermal correction to Enthalpy= 0.210528  
 Thermal correction to Gibbs Free Energy= 0.144829  
 Sum of electronic and zero-point Energies= -1592.292843  
 Sum of electronic and thermal Energies= -1592.274826  
 Sum of electronic and thermal Enthalpies= -1592.273882  
 Sum of electronic and thermal Free Energies= -1592.339581

**[CySS(OO)Cy – H]<sup>-</sup>**

C1 -0.970720 -1.852512 0.179973  
 O2 -0.608037 -1.708341 1.371685  
 O3 -0.233634 -2.172129 -0.811932  
 H4 1.260298 -2.190945 -0.762935  
 C5 -2.462493 -1.569923 -0.126171  
 H6 -2.667136 -1.836375 -1.167105  
 N7 -3.373765 -2.335239 0.745260  
 H8 -2.993310 -2.292472 1.691384  
 C9 -2.782707 -0.080553 0.094814  
 S10 -1.891396 1.084926 -1.019370  
 H11 -3.846646 0.096705 -0.088844  
 H12 -2.570872 0.199201 1.132356  
 S13 -0.152935 1.581655 0.252111  
 C14 1.236490 0.689354 -0.573255  
 C15 2.002456 -0.158273 0.459873  
 H16 0.793767 0.082460 -1.363529  
 H17 1.864265 1.481051 -0.994481  
 H18 1.276215 -0.750666 1.029106  
 N19 2.724957 0.714798 1.374979  
 H20 2.914603 0.222857 2.243328  
 H21 3.631312 0.943783 0.968855  
 C22 2.907714 -1.159620 -0.304985  
 O23 4.119811 -0.998062 -0.353725  
 O24 2.296699 -2.172463 -0.889416  
 H25 -3.347480 -3.316243 0.475047  
 O26 0.258573 3.103593 -0.182705  
 O27 -0.664476 4.050852 0.352317

Zero-point correction= 0.192381 (Hartree/Particle)  
 Thermal correction to Energy= 0.210766  
 Thermal correction to Enthalpy= 0.211710  
 Thermal correction to Gibbs Free Energy= 0.145328  
 Sum of electronic and zero-point Energies= -1592.292818  
 Sum of electronic and thermal Energies= -1592.274434  
 Sum of electronic and thermal Enthalpies= -1592.273489  
 Sum of electronic and thermal Free Energies= -1592.339871



**di-deprotonated precursor**

C1 -4.655582 -0.643768 -0.333297  
 O2 -5.130771 -1.670060 0.221330  
 O3 -4.932648 -0.135028 -1.446784  
 C4 -3.534812 0.126765 0.495187  
 H5 -3.839064 1.182874 0.492964  
 N6 -3.464295 -0.375162 1.873436  
 H7 -3.988433 -1.254247 1.862065  
 H8 -2.506915 -0.562659 2.159702  
 C9 -2.220246 0.014875 -0.290024  
 S10 -0.945716 1.146162 0.472045  
 H11 -1.837351 -1.009965 -0.264692  
 H12 -2.390114 0.329738 -1.320771  
 S13 0.727459 0.889877 -0.775075  
 C14 2.019723 0.035426 0.211460  
 C15 2.903177 -0.878155 -0.664035  
 H16 2.630991 0.838816 0.662903  
 H17 1.515804 -0.529904 1.000444  
 H18 3.409942 -0.256282 -1.411257  
 N19 2.190853 -1.980962 -1.313168  
 H20 2.273317 -2.775802 -0.675457  
 H21 1.208216 -1.766875 -1.463768  
 C22 4.036427 -1.466362 0.288951  
 O23 3.808309 -2.625548 0.729576  
 O24 5.005604 -0.703222 0.507373  
 O25 1.669009 3.024161 -0.297333  
 O26 2.660207 2.933182 0.490214

Zero-point correction= 0.177857 (Hartree/Particle)  
 Thermal correction to Energy= 0.197458  
 Thermal correction to Enthalpy= 0.198402  
 Thermal correction to Gibbs Free Energy= 0.124436  
 Sum of electronic and zero-point Energies= -1591.682648  
 Sum of electronic and thermal Energies= -1591.663048  
 Sum of electronic and thermal Enthalpies= -1591.662104  
 Sum of electronic and thermal Free Energies= -1591.736069

**[TS - 2H]<sup>2-</sup>**

C1 4.849554 -0.176767 0.172908  
 O2 5.244827 -1.052838 0.987445  
 O3 5.338441 0.946635 -0.096372  
 C4 3.510524 -0.531874 -0.610259  
 H5 3.657232 -0.191289 -1.643305  
 N6 3.269775 -1.975322 -0.577808  
 H7 3.776904 -2.319211 0.240701  
 H8 2.280811 -2.195742 -0.490029  
 C9 2.396566 0.321648 0.025545  
 S10 0.810126 0.128767 -0.929738  
 H11 2.212265 -0.002941 1.054973  
 H12 2.680713 1.374747 0.008953  
 S13 -0.627926 0.654798 0.563324  
 C14 -2.183212 0.179807 -0.292470  
 C15 -3.201268 -0.465687 0.668005  
 H16 -2.531642 1.145257 -0.699122  
 H17 -1.918592 -0.506333 -1.100780  
 H18 -3.499664 0.275496 1.416050  
 N19 -2.744553 -1.697039 1.319164

H20 -2.972145 -2.454511 0.671649  
 H21 -1.743137 -1.694381 1.498341  
 C22 -4.486089 -0.800810 -0.213873  
 O23 -4.481782 -1.957055 -0.718356  
 O24 -5.326809 0.119369 -0.322081  
 O25 -0.918069 2.476465 0.662859  
 O26 -1.587976 3.039985 -0.361424

Zero-point correction= 0.177432 (Hartree/Particle)  
 Thermal correction to Energy= 0.196122  
 Thermal correction to Enthalpy= 0.197066  
 Thermal correction to Gibbs Free Energy= 0.125089  
 Sum of electronic and zero-point Energies= -1591.680175  
 Sum of electronic and thermal Energies= -1591.661485  
 Sum of electronic and thermal Enthalpies= -1591.660541  
 Sum of electronic and thermal Free Energies= -1591.732518

**[CySS(OO)Cy - 2H]<sup>2-</sup>**

C1 4.814471 -0.250905 0.180517  
 O2 5.144883 -1.129686 1.020717  
 O3 5.370034 0.837882 -0.101632  
 C4 3.471827 -0.547820 -0.619704  
 H5 3.647037 -0.219133 -1.651963  
 N6 3.165358 -1.978171 -0.584698  
 H7 3.628890 -2.338408 0.252224  
 H8 2.164784 -2.152143 -0.529190  
 C9 2.389648 0.358201 -0.000692  
 S10 0.804160 0.238215 -0.970807  
 H11 2.181022 0.047130 1.028462  
 H12 2.720169 1.397657 -0.016781  
 S13 -0.636767 0.686513 0.561512  
 C14 -2.191990 0.198392 -0.309944  
 C15 -3.202893 -0.441491 0.657834  
 H16 -2.533615 1.155779 -0.729140  
 H17 -1.910794 -0.497618 -1.103852  
 H18 -3.512360 0.306989 1.393983  
 N19 -2.737717 -1.659054 1.328601  
 H20 -2.953376 -2.428948 0.691869  
 H21 -1.739671 -1.647097 1.524698  
 C22 -4.481925 -0.801342 -0.225000  
 O23 -4.471362 -1.969240 -0.700267  
 O24 -5.321549 0.115680 -0.361559  
 O25 -0.842432 2.342902 0.760008  
 O26 -1.399408 3.046276 -0.319391

Zero-point correction= 0.178092 (Hartree/Particle)  
 Thermal correction to Energy= 0.197077  
 Thermal correction to Enthalpy= 0.198021  
 Thermal correction to Gibbs Free Energy= 0.125786  
 Sum of electronic and zero-point Energies= -1591.680116  
 Sum of electronic and thermal Energies= -1591.661131  
 Sum of electronic and thermal Enthalpies= -1591.660187  
 Sum of electronic and thermal Free Energies= -1591.732422