

Supporting Information: Excited-state Photochemistry Dynamics of 2-(1-naphthyl) phenol: Electronic Structure Calculations and Non-adiabatic Dynamics Simulations

Jiahui Wu,^a Xiaohang Chen,^a Shu-Hua Xia,^{*a} Ganglong Cui^b and Yan Zhang^{*a}

^a College of Life and Environmental Science, Minzu University of China, Beijing 100081, China.

^b Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, China.

Table of Contents

1. CASSCF active space
2. Key dihedral angles and energies of optimized structures
3. The structure of transition state connecting S₀-ENOL-1 and S₀-ENOL-2
4. Schematic plots of S₀-KETO-1 (S₁-KETO-1) and S₀-KETO-2 (S₁-KETO-2) optimized structures in S₀ (S₁) state
5. Structures of the ground state and S₁ excited-state obtained at OM2/MRCI level
6. Structures of four minimum-energy conical intersections obtained at OM2/MRCI level
7. Product distribution
8. Cartesian coordinates of all optimized CASSCF structures
9. Cartesian coordinates of all optimized OM2/MRCI structures

1. CASSCF active space

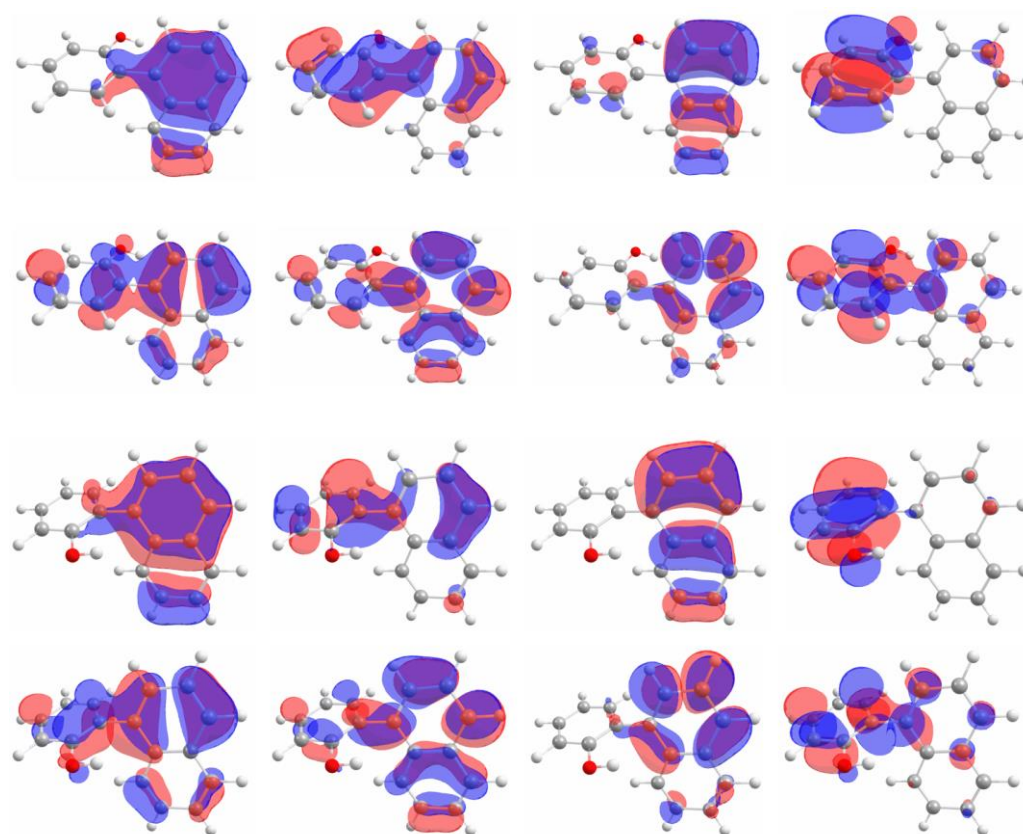


Fig. S1 The active space (10e,8o) of S0-ENOL-1 (top) and S0-ENOL-2 (bottom) used in the CAS(10,8)/6-31G* calculations. See text for simulation details.

2. Table S1 Key dihedral angles (degree) of 2-(1-naphthyl) phenol in different structures from OM2/MRCI and CASSCF optimizations and relative energies ΔE (kcal/mol) from OM2/MRCI and single-point MS-CASPT2 calculations

| structure | C3C4C9C8 | C4C9C8C14 | C9C14C8H7 | ΔE |
|-----------------|----------|-----------|-----------|------------|
| OM2/MRCI | | | | |
| S0-ENOL-1 | 41.2 | 163.6 | -168.2 | 0 |
| S0-ENOL-2 | 108.5 | -179.2 | -179.8 | 0.2 |
| S0-KETO-1 | -13.5 | -134.0 | -124.3 | 33.1 |
| S0-KETO-2 | 121.6 | 178.9 | -178.3 | 59.3 |
| S1-ENOL-1 | 39.7 | 165.4 | -169.1 | 100.1 |

| | | | | |
|---------------|-------|--------|--------|-------|
| S1-ENOL-2 | 143.1 | -163.6 | -173.9 | 98.5 |
| S1S0-ENOL-1 | -9.8 | -105.9 | -130.3 | 80.0 |
| S1S0-ENOL-2 | 172.7 | -107.9 | -113.7 | 102.0 |
| S1S0-KETO-1 | 64.6 | -179.6 | 130.6 | 70.6 |
| S1S0-KETO-2 | 131.6 | -177.9 | -178.1 | 68.8 |
| CASSCF | | | | |
| S0-ENOL-1 | 57.3 | 178.1 | -178.3 | 0.1 |
| S0-ENOL-2 | 120.3 | -179.8 | -178.6 | 0 |
| S0-KETO-1 | -17.3 | -139.6 | 122.9 | 37.2 |
| S0-KETO-2 | 107.5 | 179.3 | -179.3 | 51.2 |
| S1-ENOL-1 | 67.5 | 176.8 | 177.0 | 98.0 |
| S1-ENOL-2 | 127.2 | -176.4 | -173.9 | 97.2 |
| S1-KETO-1 | 85.9 | 179.2 | 122.5 | 82.7 |
| S1-KETO-2 | 95.9 | 179.4 | -179.9 | 96.9 |
| S1S0-ENOL-1 | 7.8 | -109.1 | -132.5 | 84.1 |
| S1S0-ENOL-2 | 148.2 | -135.7 | -96.9 | 101.3 |
| S1S0-KETO-1 | 91.1 | -175.8 | 126.0 | 72.2 |
| S1S0-KETO-2 | 145.0 | 179.3 | 177.3 | 67.8 |

3. The structure of transition state connecting S0-ENOL-1 and S0-ENOL-2

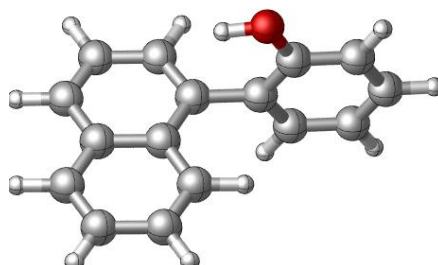


Fig. S2 Structure of the transition state connecting S0-ENOL-1 and S0-ENOL-2 optimized at ω B97X-D/cc-pVTZ level.

4. Schematic plots of S0-KETO-1 (S1-KETO-1) and S0-KETO-2 (S1-KETO-2) optimized structures in S₀ (S₁) state

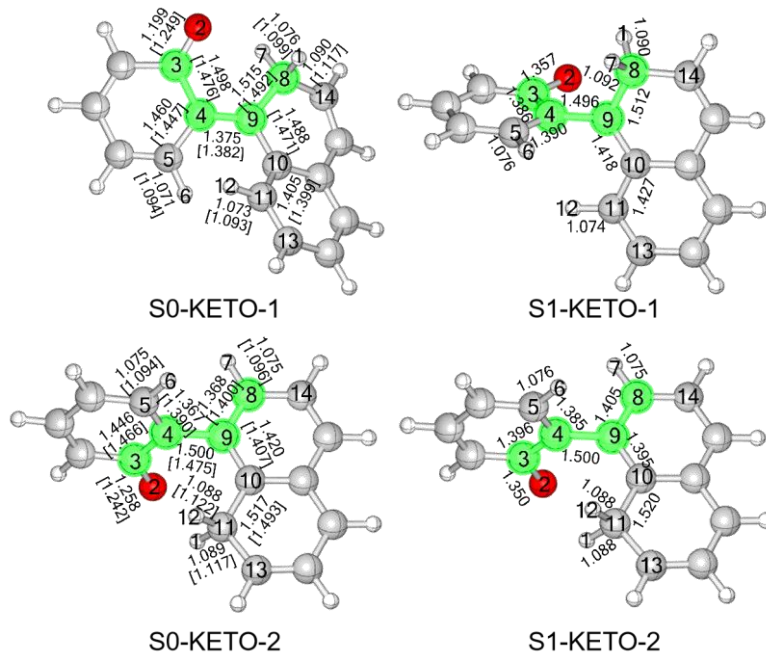


Fig. S3 Optimized keto-type structures in S₀ and S₁ states at CAS(10,8)/6-31G* and OM2/MRCI (in brackets) levels with selected bond distances.

5. Structures of the ground state and S₁ excited-state obtained at OM2/MRCI level

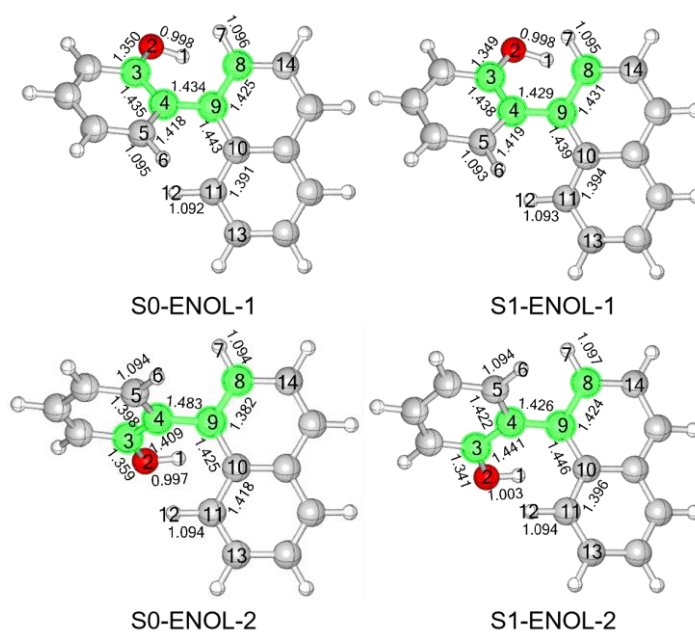


Fig. S4 Structures of the ground state and S₁ excited-state in the enol region,

with selected bond lengths (\AA) obtained at OM2/MRCI level.

6. Structures of four minimum-energy conical intersections obtained at OM2/MRCI level

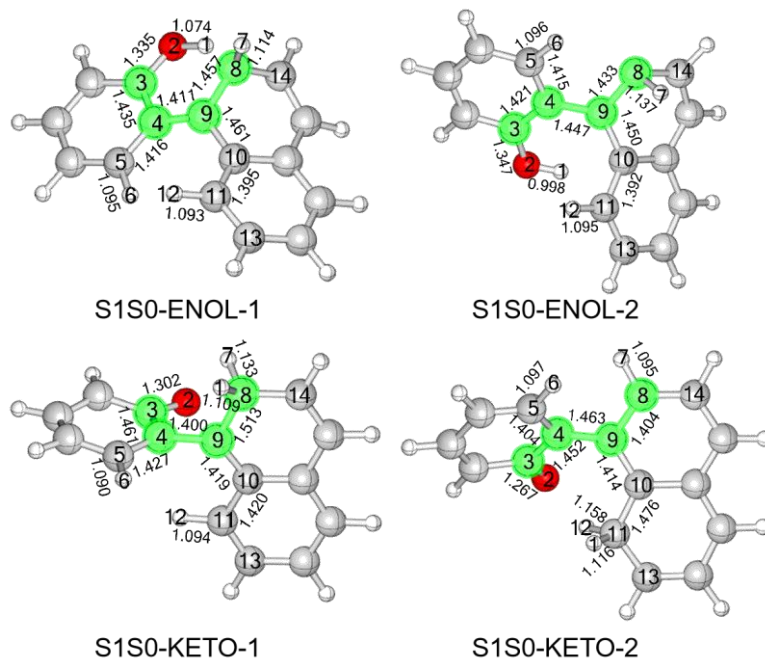


Fig. S5 Structures of four minimum-energy conical intersections, with selected bond lengths (\AA) obtained from OM2/MRCI method.

7. Product distribution

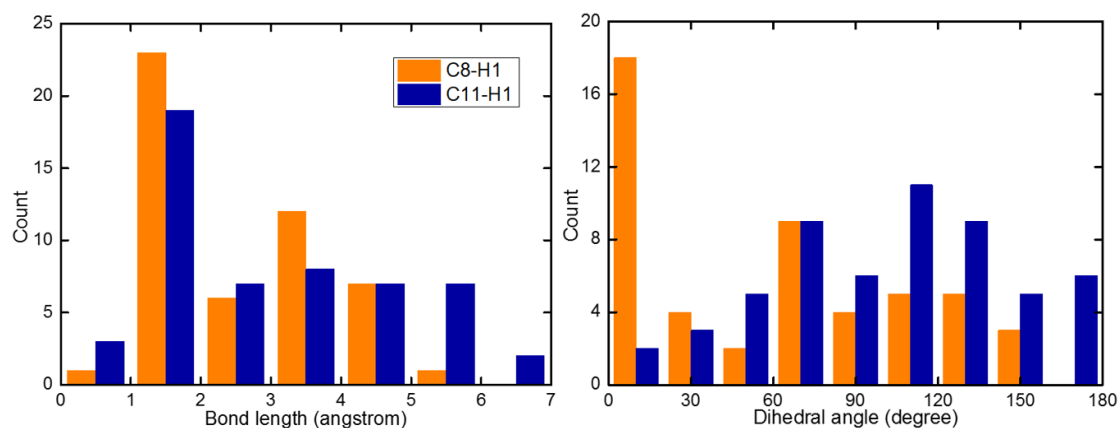


Fig. S6 Distribution of the bond parameters including C8-H1 and C11-H1 (left) and C3C4C9C8 dihedral angle (right) at the end of the 1 ps simulation (orange means starting from S0-ENOL-1 and blue means starting from S0-ENOL-2)

Fig. S6 represents the distributions of two bond distances (C8-H1 and C11-H1) and C3C4C9C8 dihedral angle at the end of the simulation. As shown in Fig. S6, four types of production were observed i.e. S0-ENOL-1, S0-KETO-1, S0-ENOL-2 and S0-KETO-2. We find that more than half trajectories end with enol products in either S0-ENOL-1 or S0-ENOL-2 form while the remaining ones result in keto products (i. e. either C8-H1 or C11-H1 distance closing to 1.0 Å). In addition, the trajectory numbers ended up with S0-ENOL-1, S0-KETO-1, S0-ENOL-2 and S0-KETO-2 products are calculated to be 37, 23, 32 and 15, respectively.

8. Cartesian coordinates of all optimized CASSCF structures

S0-ENOL-1

| | | | |
|---|--------------|--------------|--------------|
| C | 2.411533630 | -0.979888780 | -0.935889250 |
| C | 1.080986350 | -1.316527290 | -1.040091740 |
| C | 0.072928330 | -0.575303100 | -0.393676430 |
| C | 0.482659810 | 0.536201310 | 0.368926610 |
| C | 1.817665710 | 0.868592910 | 0.472962950 |
| C | 2.788688140 | 0.119500080 | -0.177892440 |
| H | 3.152029100 | -1.563866800 | -1.452651570 |
| H | 0.793535670 | -2.156764750 | -1.646869950 |
| H | 2.081918870 | 1.717588880 | 1.076360800 |
| H | 3.823989670 | 0.394234790 | -0.089043990 |
| C | -2.229811600 | 0.012207870 | -1.104949100 |
| C | -1.366905220 | -0.918371170 | -0.566786100 |
| C | -3.603979410 | -0.273984700 | -1.329328410 |
| C | -1.900130360 | -2.218583690 | -0.200990010 |
| C | -4.102530460 | -1.509206530 | -1.016661750 |
| H | -4.236852390 | 0.479043710 | -1.762271480 |
| H | -1.258134650 | 0.933476880 | 1.048088290 |
| C | -3.250960270 | -2.502424470 | -0.436541430 |
| H | -5.136118250 | -1.747525990 | -1.192266970 |
| O | -0.395328420 | 1.322106610 | 1.043650810 |
| C | -3.777196370 | -3.771969010 | -0.075611280 |
| C | -1.103321900 | -3.215091530 | 0.432990080 |
| C | -2.992308220 | -4.705222750 | 0.510654780 |
| C | -1.631373710 | -4.413570770 | 0.776335870 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.815021090 | -3.975702760 | -0.272810400 |
| H | -3.395402500 | -5.663686490 | 0.784569170 |
| H | -1.016874750 | -5.152024040 | 1.259467500 |
| H | -0.074264520 | -3.004691120 | 0.646042180 |
| H | -1.846927350 | 0.975763700 | -1.388962750 |

S0-ENOL-2

| | | | |
|---|-------------|-------------|-------------|
| C | 1.38276675 | 0.76592834 | 1.74045718 |
| C | 0.16315206 | 0.42962226 | 1.20062992 |
| C | 0.02569156 | -0.59770428 | 0.24297463 |
| C | 1.19404906 | -1.29927582 | -0.11133506 |
| C | 2.41664317 | -0.95671771 | 0.43057143 |
| C | 2.52306933 | 0.07649281 | 1.35171299 |
| H | 1.44856672 | 1.56766063 | 2.45402577 |
| H | -0.71544570 | 0.97827197 | 1.48955514 |
| H | 3.27832855 | -1.52499134 | 0.13147797 |
| H | 3.48352368 | 0.32948469 | 1.76223278 |
| C | -2.31637936 | -1.30448545 | 0.61589619 |
| C | -1.32171818 | -0.95727142 | -0.27465804 |
| C | -3.62238303 | -1.66173278 | 0.18552455 |
| C | -1.64887308 | -0.93058483 | -1.69111305 |
| C | -3.92436871 | -1.67373746 | -1.14944503 |
| H | -4.36181281 | -1.93740443 | 0.91540072 |
| H | 0.30422674 | -2.61282554 | -1.18650049 |
| C | -2.93141584 | -1.29581433 | -2.11270600 |
| H | -4.90380583 | -1.95396299 | -1.49291076 |
| O | 1.18719718 | -2.34312525 | -0.97945331 |
| C | -3.25357546 | -1.26456797 | -3.49596275 |
| C | -0.71327958 | -0.49833598 | -2.67653339 |
| C | -2.33993113 | -0.86811225 | -4.41114389 |
| C | -1.04736525 | -0.47011042 | -3.98734077 |
| H | -4.24252314 | -1.55765608 | -3.80207026 |
| H | -2.58907987 | -0.84372209 | -5.45685358 |
| H | -0.33025797 | -0.13782283 | -4.71642429 |
| H | 0.26444385 | -0.18369534 | -2.36932877 |
| H | -2.09034135 | -1.32610374 | 1.66632721 |

S0-KETO-1

| | | | |
|---|-------------|--------------|-------------|
| C | 2.614660480 | -1.910002130 | 0.795575690 |
|---|-------------|--------------|-------------|

| | | | |
|---|--------------|--------------|--------------|
| C | 1.428014340 | -1.361461750 | 0.532616160 |
| C | 1.290979630 | -0.019702900 | -0.027492310 |
| C | 2.559088350 | 0.706812880 | -0.357711740 |
| C | 3.829794280 | 0.023062820 | -0.015950160 |
| C | 3.851424740 | -1.196987450 | 0.499295460 |
| H | 2.673379540 | -2.875816820 | 1.263245440 |
| H | 0.538636070 | -1.884969460 | 0.817160190 |
| H | 4.721306350 | 0.579337220 | -0.238040310 |
| H | 4.787593560 | -1.678937190 | 0.721310680 |
| C | 0.061975280 | 0.573747900 | -0.195579230 |
| C | -1.209395150 | -0.199074250 | -0.200855320 |
| C | -0.115308950 | 2.070950950 | -0.347032200 |
| C | -2.373285740 | 0.397221940 | 0.327160390 |
| C | -1.318972750 | 2.579963850 | 0.407766800 |
| H | -0.207960810 | 2.321098530 | -1.404172620 |
| H | 0.765981150 | 2.588046050 | -0.009740940 |
| C | -2.327806490 | 1.806429090 | 0.756895290 |
| H | -1.322607050 | 3.628190710 | 0.650950920 |
| H | -3.172571850 | 2.198706740 | 1.295629550 |
| O | 2.579569670 | 1.762843570 | -0.924873900 |
| C | -1.314768840 | -1.473918840 | -0.782898590 |
| C | -3.560958980 | -0.321206040 | 0.357680660 |
| H | -0.462509400 | -1.910283520 | -1.267756980 |
| C | -2.524889910 | -2.172348840 | -0.767375900 |
| C | -3.644550110 | -1.595169120 | -0.170354290 |
| H | -4.437010100 | 0.136781330 | 0.783192300 |
| H | -4.577362570 | -2.129126370 | -0.142091060 |
| H | -2.587668710 | -3.144890910 | -1.220262990 |

S0-KETO-2

| | | | |
|---|-------------|-------------|------------|
| C | -3.30322244 | -1.25641545 | 0.25292767 |
| C | -2.00991934 | -0.71542409 | 0.33129597 |
| C | -1.80125668 | 0.62756465 | 0.47719432 |
| C | -2.94972582 | 1.50186384 | 0.55679205 |
| C | -4.26413622 | 0.91717445 | 0.47507243 |
| C | -4.42685094 | -0.42450496 | 0.32599819 |
| H | -3.42646994 | -2.31744082 | 0.13747607 |
| H | -1.16362739 | -1.37565118 | 0.27319098 |
| H | -5.10151371 | 1.58699163 | 0.54016796 |

| | | | |
|---|-------------|-------------|-------------|
| H | -5.41210801 | -0.85067725 | 0.26590513 |
| C | -0.41304340 | 1.17720804 | 0.60090121 |
| C | 0.19460258 | 1.91587399 | -0.44855115 |
| C | 0.28250265 | 0.92504254 | 1.75159244 |
| C | 1.50915358 | 2.37311003 | -0.28523662 |
| C | 1.59841908 | 1.40051454 | 1.92397907 |
| H | -0.96989964 | 1.27504140 | -2.13192204 |
| H | -0.18390788 | 0.36477672 | 2.54182200 |
| C | 2.19551434 | 2.10519871 | 0.93045279 |
| H | 2.12040601 | 1.19734746 | 2.84189971 |
| H | 3.20185431 | 2.46773517 | 1.04802428 |
| O | -2.81850795 | 2.74536751 | 0.69699228 |
| C | -0.56349814 | 2.20265763 | -1.73040802 |
| C | 2.17111524 | 3.08381212 | -1.34465386 |
| H | -1.43035177 | 2.82037585 | -1.50569048 |
| C | 0.25042639 | 2.88846773 | -2.79055246 |
| C | 1.50129093 | 3.29942771 | -2.59805902 |
| H | 3.17993722 | 3.42208757 | -1.20372273 |
| H | 2.03393266 | 3.80196513 | -3.38661729 |
| H | -0.23631510 | 3.05970293 | -3.73520206 |

S1-ENOL-1

| | | | |
|---|--------------|--------------|--------------|
| C | 3.094019000 | -1.323709000 | -1.213998000 |
| C | 1.798750000 | -0.844427000 | -1.199501000 |
| C | 1.364905000 | 0.064549000 | -0.234931000 |
| C | 2.279818000 | 0.482977000 | 0.730460000 |
| C | 3.584789000 | 0.007384000 | 0.724014000 |
| C | 3.987422000 | -0.889493000 | -0.244228000 |
| H | 3.404782000 | -2.020709000 | -1.970734000 |
| H | 1.099969000 | -1.168615000 | -1.950196000 |
| H | 4.259336000 | 0.350311000 | 1.486398000 |
| H | 4.999801000 | -1.252410000 | -0.241571000 |
| C | -0.211749000 | 2.002603000 | -0.594550000 |
| C | -0.025818000 | 0.605693000 | -0.260103000 |
| C | -1.516162000 | 2.564242000 | -0.703160000 |
| C | -1.171897000 | -0.215742000 | -0.007792000 |
| C | -2.665939000 | 1.740728000 | -0.473452000 |
| H | -1.636598000 | 3.596798000 | -0.968777000 |
| H | 1.033423000 | 1.571608000 | 1.676437000 |
| C | -2.522305000 | 0.372694000 | -0.129050000 |
| H | -3.650296000 | 2.162363000 | -0.558665000 |
| O | 1.955280000 | 1.354453000 | 1.710782000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.649271000 | -0.460706000 | 0.116247000 |
| C | -1.083551000 | -1.581000000 | 0.385920000 |
| C | -3.505173000 | -1.757603000 | 0.470480000 |
| C | -2.191845000 | -2.325554000 | 0.614586000 |
| H | -4.631737000 | -0.032551000 | 0.016551000 |
| H | -4.367764000 | -2.372088000 | 0.653397000 |
| H | -2.095927000 | -3.353891000 | 0.912320000 |
| H | -0.112957000 | -2.023198000 | 0.506540000 |
| H | 0.651894000 | 2.602882000 | -0.808718000 |

S1-ENOL-2

| | | | |
|---|-------------|-------------|-------------|
| C | 2.06853740 | -1.30506917 | 1.39684559 |
| C | 0.82001637 | -1.61129877 | 0.92271088 |
| C | -0.00594127 | -0.64267170 | 0.31052169 |
| C | 0.52950368 | 0.65588262 | 0.16032243 |
| C | 1.78484026 | 0.95982878 | 0.63743720 |
| C | 2.55681072 | -0.00831372 | 1.26060174 |
| H | 2.66326218 | -2.06100673 | 1.87771318 |
| H | 0.43612882 | -2.60891345 | 1.04194328 |
| H | 2.15345531 | 1.95943408 | 0.49725276 |
| H | 3.53528055 | 0.24532410 | 1.62688501 |
| C | -1.40703849 | -2.22556239 | -1.06256626 |
| C | -1.33095627 | -1.03505625 | -0.20790510 |
| C | -2.66382219 | -2.62257346 | -1.67015637 |
| C | -2.56090547 | -0.37372201 | 0.13669589 |
| C | -3.85789215 | -1.85314171 | -1.38224887 |
| H | -2.70099896 | -3.46308107 | -2.33377952 |
| H | -0.93280559 | 1.32799058 | -0.86996060 |
| C | -3.80421657 | -0.77318558 | -0.47464700 |
| H | -4.79359517 | -2.12563617 | -1.83082999 |
| O | -0.13842702 | 1.65279219 | -0.47097324 |
| C | -4.98710091 | -0.07776912 | -0.13164656 |
| C | -2.60871359 | 0.65388695 | 1.10555408 |
| C | -4.98115607 | 0.93210797 | 0.78488833 |
| C | -3.77665318 | 1.29219593 | 1.41891897 |
| H | -5.90677921 | -0.37211126 | -0.60539167 |
| H | -5.89273066 | 1.44410808 | 1.03438607 |
| H | -3.77553954 | 2.07082170 | 2.15985563 |
| H | -1.70612099 | 0.93366995 | 1.61193158 |
| H | -0.50482471 | -2.74491448 | -1.31465451 |

S1-KETO-1

| | | | |
|---|-------------|-------------|-------------|
| C | 2.73471628 | -2.00712760 | -0.19993041 |
| C | 1.48962184 | -1.40248765 | -0.14194518 |
| C | 1.34467958 | -0.08300465 | 0.26983958 |
| C | 2.49432063 | 0.60897685 | 0.61689836 |
| C | 3.75192818 | 0.03443956 | 0.56456694 |
| C | 3.86160961 | -1.28329898 | 0.15394611 |
| H | 2.82393068 | -3.02959136 | -0.51832285 |
| H | 0.60958934 | -1.95807999 | -0.41504818 |
| H | 4.61714504 | 0.60763009 | 0.84257630 |
| H | 4.83326217 | -1.74179201 | 0.11176491 |
| C | 0.02171209 | 0.61505903 | 0.30305140 |
| C | -0.87330023 | 0.48793578 | 1.39613818 |
| C | -0.35350085 | 1.38051321 | -0.94586416 |
| C | -2.14067235 | 1.14020444 | 1.35609045 |
| C | -1.69653411 | 2.04875037 | -0.87277400 |
| H | -0.33258884 | 0.70225141 | -1.80083243 |
| H | 0.41324236 | 2.12381084 | -1.16182554 |
| C | -2.49915174 | 1.93312077 | 0.16922289 |
| H | -1.99400254 | 2.63717178 | -1.72400631 |
| H | -3.45556409 | 2.42753629 | 0.17588142 |
| O | 2.36498866 | 1.89748046 | 1.02315077 |
| C | -0.55223092 | -0.26423962 | 2.56496963 |
| C | -3.01750458 | 1.02293196 | 2.43394085 |
| H | 0.39931352 | -0.75821948 | 2.62008901 |
| C | -1.42354405 | -0.36568729 | 3.60516794 |
| C | -2.67556593 | 0.27512173 | 3.56072636 |
| H | -3.97150445 | 1.51919999 | 2.39155573 |
| H | -3.35835384 | 0.19093188 | 4.38608342 |
| H | -1.15204159 | -0.94085899 | 4.47281595 |

S1-KETO-2

| | | | |
|---|-------------|-------------|-------------|
| C | -3.35451786 | -1.24522614 | 0.29386044 |
| C | -2.05722765 | -0.75695794 | 0.35827534 |
| C | -1.78778316 | 0.59707588 | 0.47093906 |
| C | -2.88129058 | 1.46445693 | 0.52483786 |
| C | -4.19841908 | 0.99559851 | 0.45926568 |
| C | -4.42116364 | -0.35579840 | 0.34486727 |
| H | -3.52964768 | -2.30166178 | 0.20689570 |
| H | -1.22727854 | -1.44044786 | 0.32057848 |
| H | -5.01281581 | 1.69518838 | 0.50331863 |
| H | -5.43161997 | -0.72035540 | 0.29627242 |
| C | -0.38237967 | 1.11384183 | 0.56307506 |
| C | 0.30127724 | 1.58389815 | -0.55878880 |

| | | | |
|---|-------------|------------|-------------|
| C | 0.25129058 | 1.10319766 | 1.81770213 |
| C | 1.63479686 | 2.04404094 | -0.41101472 |
| C | 1.54105365 | 1.55283644 | 1.95294102 |
| H | -0.72340304 | 0.60371711 | -2.16842217 |
| H | -0.28914750 | 0.73950587 | 2.67285861 |
| C | 2.23114628 | 2.02203836 | 0.84123802 |
| H | 2.01868444 | 1.54319967 | 2.91646984 |
| H | 3.24262700 | 2.37310616 | 0.94753315 |
| O | -2.67433556 | 2.79368260 | 0.64118826 |
| C | -0.36922291 | 1.60285823 | -1.92312349 |
| C | 2.36074961 | 2.52260405 | -1.56160809 |
| H | -1.26647525 | 2.21710179 | -1.87971932 |
| C | 0.50317218 | 2.10356757 | -3.03865698 |
| C | 1.75466995 | 2.52657846 | -2.85561207 |
| H | 3.36859151 | 2.86898426 | -1.43405861 |
| H | 2.33214613 | 2.88076974 | -3.69177156 |
| H | 0.06646259 | 2.11541016 | -4.02223149 |

S1S0-ENOL-1

| | | | |
|---|-------------|-------------|-------------|
| C | 2.35044333 | -1.26079455 | 0.36902079 |
| C | 1.06752852 | -1.66488638 | 0.05695370 |
| C | 0.05823764 | -0.70715213 | -0.21731188 |
| C | 0.40482700 | 0.67832610 | -0.09388318 |
| C | 1.72669515 | 1.07591135 | 0.18855621 |
| C | 2.68033897 | 0.10741371 | 0.42498142 |
| H | 3.12214482 | -2.00400362 | 0.57621288 |
| H | 0.81731056 | -2.72584126 | 0.03374702 |
| H | 1.95258322 | 2.13650359 | 0.25698917 |
| H | 3.70184497 | 0.40169281 | 0.68032379 |
| C | -2.12710096 | 0.01931285 | -1.19117703 |
| C | -1.23801429 | -1.02419207 | -0.68621273 |
| C | -3.24675391 | 0.27858670 | -0.27849864 |
| C | -1.93204002 | -2.29386249 | -0.46406646 |
| C | -3.78080705 | -0.79712121 | 0.32521923 |
| H | -3.64558631 | 1.28465726 | -0.17088216 |
| H | -1.39126352 | 1.21287032 | -0.66758409 |
| C | -3.23510922 | -2.14266016 | 0.09110221 |
| H | -4.64948816 | -0.71128022 | 0.98055476 |
| O | -0.50631603 | 1.63631503 | -0.23027269 |
| C | -3.96689302 | -3.27799977 | 0.41838885 |
| C | -1.40646470 | -3.56363791 | -0.70318002 |
| C | -3.43152975 | -4.55141442 | 0.17801493 |
| C | -2.16621141 | -4.69280955 | -0.38327559 |
| H | -4.95524548 | -3.17513083 | 0.87306485 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.01475468 | -5.43977316 | 0.43256657 |
| H | -1.76622106 | -5.68911123 | -0.57927196 |
| H | -0.42992243 | -3.67528461 | -1.17314820 |
| H | -2.44060287 | -0.09732477 | -2.24706735 |

S1S0-ENOL-2

| | | | |
|---|--------------|--------------|--------------|
| C | 2.165759630 | 0.563397020 | -1.295268820 |
| C | 0.950982690 | -0.011722610 | -1.597889000 |
| C | 0.127574980 | -0.582449710 | -0.614187860 |
| C | 0.572610750 | -0.526882110 | 0.721235280 |
| C | 1.794939070 | 0.061207660 | 1.024678030 |
| C | 2.584435090 | 0.590837240 | 0.027227180 |
| H | 2.775761420 | 0.981788760 | -2.074156730 |
| H | 0.602564710 | -0.050755730 | -2.609212540 |
| H | 2.094184830 | 0.097159790 | 2.055303200 |
| H | 3.530645860 | 1.033340430 | 0.284789040 |
| C | -1.824412360 | -0.598293610 | -2.197178620 |
| C | -1.158551120 | -1.140601930 | -1.054419710 |
| C | -3.262257570 | -0.386619200 | -2.043004040 |
| C | -1.876799750 | -2.184896740 | -0.354983890 |
| C | -3.922623480 | -0.910762020 | -0.953818490 |
| H | -3.818061060 | -0.007350860 | -2.882017920 |
| H | -0.974125230 | -1.304817200 | 1.532108100 |
| C | -3.258852260 | -1.917692380 | -0.193390290 |
| H | -4.953113050 | -0.688454720 | -0.751163630 |
| O | -0.129036780 | -0.961956390 | 1.781533320 |
| C | -3.997931780 | -2.763051490 | 0.694656330 |
| C | -1.293663760 | -3.333800020 | 0.261287700 |
| C | -3.406036910 | -3.845311220 | 1.286440240 |
| C | -2.033078430 | -4.150327400 | 1.049963210 |
| H | -5.036718710 | -2.551187810 | 0.872509700 |
| H | -3.983471550 | -4.479066410 | 1.936119800 |
| H | -1.591647750 | -5.012381110 | 1.513481250 |
| H | -0.248996710 | -3.526518160 | 0.102377340 |
| H | -2.112909470 | -1.575880670 | -2.694978690 |

S1S0-KETO-1

| | | | |
|---|----------|----------|----------|
| C | -3.24991 | -1.03415 | -1.19913 |
| C | -2.05710 | -0.45540 | -1.52204 |
| C | -1.32388 | 0.18224 | -0.52822 |
| C | -1.95406 | 0.58166 | 0.68427 |
| C | -3.20252 | -0.07050 | 0.97222 |
| C | -3.92428 | -0.63718 | -0.03087 |
| H | -3.76226 | -1.60786 | -1.91701 |

| | | | |
|---|----------|----------|----------|
| H | -1.65889 | -0.66514 | -2.48267 |
| H | -3.62277 | 0.14591 | 1.92170 |
| H | -4.91740 | -0.98263 | 0.13495 |
| C | 1.07133 | -0.30218 | 0.04725 |
| C | 0.05761 | 0.66882 | -0.52903 |
| C | 2.46721 | 0.20805 | 0.14637 |
| C | 0.42180 | 1.98249 | -0.84607 |
| C | 2.78759 | 1.46955 | -0.22905 |
| H | 3.22781 | -0.45865 | 0.54092 |
| H | 0.99275 | -1.25496 | -0.50287 |
| C | 1.76377 | 2.42149 | -0.75418 |
| H | 3.80787 | 1.81734 | -0.13801 |
| O | -1.38117 | 1.31223 | 1.48931 |
| C | 2.06948 | 3.71622 | -1.20651 |
| C | -0.61258 | 2.88705 | -1.33965 |
| C | 1.06825 | 4.53941 | -1.72329 |
| C | -0.28972 | 4.13317 | -1.77638 |
| H | 3.09233 | 4.07568 | -1.16492 |
| H | 1.33834 | 5.53228 | -2.08647 |
| H | -1.05701 | 4.80137 | -2.15010 |
| H | -1.64075 | 2.51805 | -1.34318 |
| H | 0.65478 | -0.53095 | 1.05247 |

S1S0-KETO-2

| | | | |
|---|-------------|-------------|-------------|
| C | -3.94470256 | 0.72217665 | -0.64195983 |
| C | -2.61648239 | 0.85665448 | -0.67007482 |
| C | -1.77277174 | 0.28974662 | 0.36388815 |
| C | -2.39142141 | -0.48120528 | 1.41788475 |
| C | -3.85989481 | -0.51600831 | 1.45338348 |
| C | -4.58597191 | 0.02917019 | 0.46670216 |
| H | -4.58604132 | 1.13187133 | -1.43365442 |
| H | -2.15562830 | 1.39233972 | -1.51333972 |
| H | -4.30082988 | -1.05443917 | 2.29226730 |
| H | -5.68047286 | -0.04114333 | 0.47356587 |
| C | -0.43405831 | 0.77666462 | 0.46488470 |
| C | 0.19678317 | 1.28137826 | 1.62615430 |
| C | 0.37425835 | 0.82943111 | -0.73771893 |
| C | 1.61719288 | 1.73517338 | 1.56884085 |
| C | 1.69034130 | 1.29266132 | -0.79688928 |
| H | -1.26549269 | 2.18430945 | 2.74633013 |
| H | -0.09913657 | 0.52252429 | -1.66939147 |
| C | 2.35515771 | 1.72842165 | 0.33881723 |
| H | 2.21072816 | 1.28070476 | -1.75597343 |
| H | 3.39038406 | 2.06839420 | 0.31685548 |

| | | | |
|---|-------------|-------------|------------|
| O | -1.75539650 | -1.15575563 | 2.26799327 |
| C | -0.50428640 | 1.41709676 | 2.91177218 |
| C | 2.22351803 | 2.15611881 | 2.73730738 |
| H | -1.01848782 | 0.43645248 | 3.10790990 |
| C | 0.28086298 | 1.82551950 | 4.08521363 |
| C | 1.57167169 | 2.21974132 | 4.00469492 |
| H | 3.26713571 | 2.47659667 | 2.67404309 |
| H | 2.12556058 | 2.57542672 | 4.87843959 |
| H | -0.26362190 | 1.84483740 | 5.03812844 |

9 Cartesian coordinates of all optimized OM2/MRCI structures

S0-ENOL-1

| | | | |
|---|--------------|--------------|--------------|
| C | 2.322852041 | -1.118710119 | -0.787355640 |
| C | 0.979963110 | -1.452431513 | -0.804739754 |
| C | 0.002288576 | -0.561328216 | -0.294716721 |
| C | 0.481755955 | 0.669076786 | 0.266131913 |
| C | 1.845519881 | 0.995280905 | 0.306828368 |
| C | 2.759525310 | 0.098682909 | -0.238481657 |
| H | 3.061686409 | -1.795313442 | -1.230840821 |
| H | 0.646766111 | -2.388399881 | -1.266009742 |
| H | 2.161104467 | 1.927521725 | 0.771771463 |
| H | 3.828399115 | 0.336119731 | -0.224966783 |
| C | -2.315017617 | 0.196583144 | -0.697484531 |
| C | -1.403415292 | -0.839943589 | -0.343148896 |
| C | -3.605742933 | -0.121505579 | -1.076032751 |
| C | -1.886379275 | -2.191561608 | -0.189815883 |
| C | -4.090189164 | -1.439861768 | -0.988894231 |
| H | -4.263786858 | 0.656797469 | -1.479988420 |
| H | -1.238957432 | 1.154767710 | 1.002111972 |
| C | -3.242809471 | -2.476770809 | -0.569914215 |
| H | -5.143290074 | -1.646485680 | -1.208698799 |
| O | -0.329909395 | 1.550305117 | 0.888862442 |
| C | -3.720691909 | -3.805559436 | -0.434246543 |
| C | -1.109430633 | -3.174540573 | 0.414366848 |
| C | -2.890082042 | -4.788880182 | 0.080861582 |
| C | -1.608751092 | -4.485327424 | 0.532840714 |
| H | -4.734617466 | -4.042896042 | -0.774217527 |
| H | -3.262153737 | -5.816986883 | 0.169030157 |
| H | -0.993713436 | -5.247794149 | 1.022298262 |
| H | -0.121568001 | -2.951305823 | 0.823610142 |
| H | -1.950932781 | 1.217163433 | -0.860699844 |

S0-ENOL-2

| | | | |
|---|---------------|---------------|---------------|
| C | 1.3947565088 | 0.5607034506 | 1.8425679079 |
| C | 0.1245945985 | 0.2935084351 | 1.3335640933 |
| C | -0.0241857759 | -0.6014209649 | 0.2699497603 |
| C | 1.1257276554 | -1.2148421800 | -0.2667507760 |
| C | 2.4078097395 | -0.9552437817 | 0.2425491465 |
| C | 2.5250303537 | -0.0596137542 | 1.3046399307 |
| H | 1.5090452768 | 1.2636655768 | 2.6742370953 |
| H | -0.7596450140 | 0.7795046261 | 1.7576020166 |
| H | 3.2735458506 | -1.4533794344 | -0.1894923284 |
| H | 3.5163289978 | 0.1560839400 | 1.7191026759 |
| C | -2.2345407321 | -1.6858955368 | 0.4813653146 |
| C | -1.3634120419 | -0.9270918130 | -0.2767034352 |
| C | -3.5051369846 | -2.0199743395 | -0.0273243915 |
| C | -1.7340381064 | -0.4548427368 | -1.5688237026 |
| C | -3.8907929705 | -1.5945509433 | -1.2789311303 |
| H | -4.1798032151 | -2.6289108802 | 0.5838433273 |
| H | 0.1246611704 | -2.1843463766 | -1.6027736959 |
| C | -3.0196521373 | -0.8038458384 | -2.0724925383 |
| H | -4.8773545686 | -1.8600699802 | -1.6784672133 |
| O | 1.0706089309 | -2.0950349599 | -1.3010705978 |
| C | -3.4035230967 | -0.3495497932 | -3.3609505862 |
| C | -0.8741213743 | 0.3490369452 | -2.3597812080 |
| C | -2.5434552812 | 0.4166273860 | -4.1118242917 |
| C | -1.2752519845 | 0.7735943150 | -3.6053328863 |
| H | -4.3944842228 | -0.6198148272 | -3.7466341063 |
| H | -2.8349217933 | 0.7661134494 | -5.1086461872 |
| H | -0.6167094368 | 1.4000556446 | -4.2163435725 |
| H | 0.1082330061 | 0.6272176949 | -1.9657651472 |
| H | -1.9438728013 | -2.0340161683 | 1.4764122883 |

S0-KETO-1

| | | | |
|---|--------------|--------------|--------------|
| C | 2.609224569 | -1.872156954 | 0.887291259 |
| C | 1.387487205 | -1.307343778 | 0.636899978 |
| C | 1.262140508 | 0.017669200 | 0.069684671 |
| C | 2.516466854 | 0.755412305 | -0.179387280 |
| C | 3.780731974 | 0.091286368 | 0.084581139 |
| C | 3.832378999 | -1.157002320 | 0.608744891 |
| H | 2.688631807 | -2.868205795 | 1.332361108 |
| H | 0.475718033 | -1.863632188 | 0.875401501 |
| H | 4.684700344 | 0.667164536 | -0.124052382 |
| H | 4.781774344 | -1.623150562 | 0.894374732 |
| C | 0.033611205 | 0.573879234 | -0.232981706 |
| C | -1.200100728 | -0.226901953 | -0.204249873 |
| C | -0.159862958 | 2.019944013 | -0.543808887 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.376426896 | 0.386074276 | 0.283208821 |
| C | -1.332325319 | 2.558735078 | 0.201389987 |
| H | -0.363380453 | 2.119614343 | -1.637637628 |
| H | 0.741830919 | 2.609040587 | -0.323997623 |
| C | -2.351027159 | 1.792908514 | 0.644648582 |
| H | -1.338149484 | 3.643944926 | 0.366021445 |
| H | -3.179485276 | 2.200194004 | 1.228196815 |
| O | 2.518763751 | 1.911543847 | -0.653113556 |
| C | -1.256015690 | -1.527021209 | -0.718282772 |
| C | -3.576008312 | -0.341958857 | 0.327699042 |
| H | -0.374028647 | -1.984026549 | -1.174620296 |
| C | -2.464452257 | -2.224051071 | -0.698770243 |
| C | -3.611314520 | -1.649715620 | -0.145878451 |
| H | -4.485524022 | 0.134488595 | 0.707442318 |
| H | -4.542791755 | -2.223699960 | -0.102781296 |
| H | -2.508267643 | -3.239230935 | -1.108347729 |

S0-KETO-2

| | | | |
|---|--------------|--------------|--------------|
| C | -3.866194813 | 0.470649092 | -0.683869219 |
| C | -2.534022102 | 0.878151463 | -0.620764225 |
| C | -1.753182666 | 0.576418270 | 0.488650720 |
| C | -2.331019246 | -0.199553550 | 1.589865436 |
| C | -3.731114318 | -0.589731016 | 1.480994188 |
| C | -4.462099264 | -0.253234743 | 0.366313610 |
| H | -4.467105160 | 0.720226174 | -1.566721107 |
| H | -2.100848978 | 1.441248742 | -1.452526074 |
| H | -4.165925835 | -1.144206802 | 2.314097557 |
| H | -5.513498392 | -0.546871338 | 0.280590285 |
| C | -0.361408956 | 1.058941755 | 0.565102630 |
| C | 0.721397699 | 0.166228922 | 0.671005570 |
| C | -0.155860466 | 2.440625595 | 0.477783531 |
| C | 2.030129834 | 0.700069508 | 0.666780538 |
| C | 1.141378684 | 2.955926591 | 0.510972305 |
| H | -0.003643977 | -1.473833179 | 1.813494979 |
| H | -1.012575576 | 3.120495980 | 0.413531472 |
| C | 2.228159348 | 2.096286267 | 0.600874611 |
| H | 1.296626378 | 4.038869216 | 0.466368649 |
| H | 3.248127717 | 2.498789196 | 0.629974579 |
| O | -1.663269715 | -0.520337507 | 2.586522825 |
| C | 0.483401933 | -1.299270297 | 0.823581860 |
| C | 3.160650530 | -0.181655000 | 0.706017641 |
| H | -0.217607244 | -1.649079144 | 0.020400449 |
| C | 1.721262785 | -2.109078128 | 0.769270324 |
| C | 2.980118640 | -1.555722635 | 0.737486533 |

| | | | |
|---|-------------|--------------|-------------|
| H | 4.167151672 | 0.252117563 | 0.680259677 |
| H | 3.859768553 | -2.212906974 | 0.730928625 |
| H | 1.594585552 | -3.198686009 | 0.795294127 |

S1-ENOL-1

| | | | |
|---|--------------|--------------|--------------|
| C | 2.341459318 | -1.193919388 | -0.820142037 |
| C | 1.007183858 | -1.557937232 | -0.770183372 |
| C | 0.023013170 | -0.636267060 | -0.326638290 |
| C | 0.498690219 | 0.644675789 | 0.120296600 |
| C | 1.855732604 | 1.003264623 | 0.083680331 |
| C | 2.769955906 | 0.076788637 | -0.401171341 |
| H | 3.081135067 | -1.897746037 | -1.219002819 |
| H | 0.684672006 | -2.536572389 | -1.134577718 |
| H | 2.163104352 | 1.980764829 | 0.449244128 |
| H | 3.834119653 | 0.331591380 | -0.438052498 |
| C | -2.269654122 | 0.112661866 | -0.801416725 |
| C | -1.377712578 | -0.917251325 | -0.364251106 |
| C | -3.572115704 | -0.202027492 | -1.138493902 |
| C | -1.892694510 | -2.240785392 | -0.131612981 |
| C | -4.083837699 | -1.495263495 | -0.968837166 |
| H | -4.225059598 | 0.571967558 | -1.562538376 |
| H | -1.214483916 | 1.164998272 | 0.851401895 |
| C | -3.259191540 | -2.525127255 | -0.489066249 |
| H | -5.138131966 | -1.699632132 | -1.183925194 |
| O | -0.310807420 | 1.558455139 | 0.694525101 |
| C | -3.768658354 | -3.828658229 | -0.296021942 |
| C | -1.142688391 | -3.220363093 | 0.517061038 |
| C | -2.971191827 | -4.805320528 | 0.287213613 |
| C | -1.684899792 | -4.497529166 | 0.720500621 |
| H | -4.785564437 | -4.065230966 | -0.627332475 |
| H | -3.370521893 | -5.816355743 | 0.430299817 |
| H | -1.089320046 | -5.250832552 | 1.251131765 |
| H | -0.141545883 | -2.999993975 | 0.895605759 |
| H | -1.880586199 | 1.108006424 | -1.041373636 |

S1-ENOL-2

| | | | |
|---|---------------|---------------|--------------|
| C | 2.1822881981 | -1.1519776806 | 1.0714821295 |
| C | 0.8803291697 | -1.5553141208 | 0.8366614124 |
| C | -0.1004142920 | -0.6309083724 | 0.3840590781 |
| C | 0.3687347483 | 0.6955112853 | 0.0726818878 |
| C | 1.6980027962 | 1.0969393911 | 0.3108550766 |
| C | 2.5954193852 | 0.1673565127 | 0.8128709752 |
| H | 2.9058246200 | -1.8637774126 | 1.4851488817 |
| H | 0.5772145604 | -2.5824618416 | 1.0616821725 |

| | | | |
|---|---------------|---------------|---------------|
| H | 2.0032071680 | 2.1063756577 | 0.0428485214 |
| H | 3.6367311250 | 0.4541377395 | 0.9918674804 |
| C | -1.7476388162 | -2.3385679415 | -0.2480290050 |
| C | -1.4608704056 | -1.0183776809 | 0.2033829699 |
| C | -2.9952077713 | -2.6477878579 | -0.7525885900 |
| C | -2.5484995597 | -0.0797980332 | 0.3633971445 |
| C | -4.0231687829 | -1.6878487768 | -0.7681527028 |
| H | -3.1902216760 | -3.6430181193 | -1.1663747185 |
| H | -1.3394134731 | 1.3504442700 | -0.5962051964 |
| C | -3.8319743102 | -0.4259502253 | -0.1938796463 |
| H | -5.0031455362 | -1.9550607372 | -1.1799490197 |
| O | -0.3748452228 | 1.6204086111 | -0.5522280613 |
| C | -4.8910513082 | 0.5125392034 | -0.0928411303 |
| C | -2.4326012512 | 1.0628547564 | 1.1564827609 |
| C | -4.7090716261 | 1.6939059738 | 0.6076479828 |
| C | -3.5044028918 | 1.9595922283 | 1.2607821700 |
| H | -5.8406144890 | 0.2970634060 | -0.5935519611 |
| H | -5.5229364106 | 2.4279969295 | 0.6573250927 |
| H | -3.3908320680 | 2.8661264098 | 1.8634966600 |
| H | -1.5225712103 | 1.2513212656 | 1.7336938157 |
| H | -0.9423700067 | -3.0819223714 | -0.2847551847 |

S1S0-ENOL-1

| | | | |
|---|--------------|--------------|--------------|
| C | 2.302499954 | -1.294756296 | 0.505522347 |
| C | 1.003821276 | -1.681733936 | 0.217465140 |
| C | 0.050974752 | -0.719048182 | -0.196882191 |
| C | 0.457159095 | 0.656746338 | -0.236505036 |
| C | 1.792456449 | 1.029463157 | 0.007892723 |
| C | 2.695838727 | 0.051326111 | 0.389347987 |
| H | 3.036020898 | -2.039209194 | 0.829315709 |
| H | 0.696400017 | -2.726998168 | 0.324963207 |
| H | 2.072224030 | 2.080082558 | -0.055600142 |
| H | 3.730101997 | 0.328866325 | 0.626992454 |
| C | -2.182408661 | 0.008996982 | -1.046236737 |
| C | -1.227575650 | -1.035878553 | -0.701887791 |
| C | -3.257949731 | 0.095350883 | -0.045625836 |
| C | -1.846097219 | -2.358586738 | -0.656093847 |
| C | -3.724245295 | -1.089512645 | 0.405048048 |
| H | -3.679305074 | 1.059381392 | 0.240745417 |
| H | -1.305606935 | 1.198216827 | -0.925847648 |
| C | -3.129729163 | -2.352108652 | -0.047477157 |
| H | -4.560480918 | -1.147657786 | 1.108763765 |
| O | -0.416714486 | 1.629958460 | -0.504124159 |
| C | -3.793143509 | -3.569316833 | 0.143819983 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.258202752 | -3.550778828 | -1.079710409 |
| C | -3.200895256 | -4.756329273 | -0.287091490 |
| C | -1.947908237 | -4.750952629 | -0.896830481 |
| H | -4.767176428 | -3.589198680 | 0.644439690 |
| H | -3.726692693 | -5.707440734 | -0.141885321 |
| H | -1.505077396 | -5.690358072 | -1.242908761 |
| H | -0.290072608 | -3.539168309 | -1.587790566 |
| H | -2.574660385 | -0.040244104 | -2.087575376 |

S1S0-ENOL-2

| | | | |
|---|--------------|--------------|--------------|
| C | 1.725880611 | 1.031034473 | -1.089279205 |
| C | 0.666992499 | 0.236564553 | -1.510869684 |
| C | 0.117076046 | -0.741461992 | -0.648724989 |
| C | 0.701703036 | -0.910821058 | 0.635072221 |
| C | 1.771218572 | -0.101897447 | 1.059455719 |
| C | 2.266806360 | 0.870015069 | 0.195877979 |
| H | 2.138419162 | 1.793868031 | -1.751292824 |
| H | 0.164276740 | 0.304682969 | -2.482170506 |
| H | 2.197365174 | -0.234698179 | 2.055789247 |
| H | 3.080834209 | 1.524915033 | 0.531831106 |
| C | -1.486447099 | -1.009758727 | -2.442804391 |
| C | -0.991724712 | -1.496617466 | -1.189696064 |
| C | -2.783602340 | -0.396051392 | -2.118609035 |
| C | -1.731857746 | -2.433066250 | -0.365745712 |
| C | -3.451807295 | -0.701607533 | -0.961337519 |
| H | -3.230186685 | 0.226891804 | -2.909627218 |
| H | 0.565774368 | -1.827558799 | 2.333476615 |
| C | -3.019972503 | -1.833629931 | -0.178395772 |
| H | -4.364584891 | -0.190750967 | -0.668849521 |
| O | 0.202640093 | -1.895427694 | 1.406496202 |
| C | -3.873457187 | -2.452865820 | 0.760051749 |
| C | -1.371354108 | -3.627818437 | 0.251931220 |
| C | -3.493932370 | -3.619054440 | 1.393125453 |
| C | -2.266503005 | -4.237629857 | 1.117777310 |
| H | -4.849411772 | -1.999213333 | 0.957378101 |
| H | -4.169749039 | -4.089846517 | 2.120833908 |
| H | -2.015732522 | -5.191163855 | 1.588912937 |
| H | -0.389980954 | -4.071260622 | 0.053880866 |
| H | -1.814331580 | -1.888000111 | -3.086027181 |

S1S0-KETO-1

| | | | |
|---|--------------|---------------|--------------|
| C | 2.6003271562 | -1.3158023416 | 0.6734994403 |
| C | 1.3202199880 | -1.8591650020 | 0.7936799002 |
| C | 0.1746551434 | -1.0646213281 | 0.4898591654 |

| | | | |
|---|---------------|---------------|---------------|
| C | 0.4131776158 | 0.2490015789 | -0.1046556670 |
| C | 1.7221961421 | 0.7650579406 | -0.2306273418 |
| C | 2.8047676898 | -0.0149596589 | 0.1756835276 |
| H | 3.4658004751 | -1.9100846629 | 0.9745994135 |
| H | 1.1674222155 | -2.8632611082 | 1.1882337896 |
| H | 1.8740609647 | 1.7838347661 | -0.5990051242 |
| H | 3.8240692052 | 0.3693733830 | 0.0807837623 |
| C | -1.7840594415 | -1.7546891347 | -0.8184495486 |
| C | -1.1575955587 | -1.4935712693 | 0.5340189750 |
| C | -3.1787477547 | -2.2160686539 | -0.7457061350 |
| C | -1.9936390710 | -1.3168114819 | 1.6668485738 |
| C | -3.9240475104 | -2.1477329730 | 0.3552719328 |
| H | -3.6000783001 | -2.6084523076 | -1.6935173124 |
| H | -1.1487403520 | -2.4168013636 | -1.4412711707 |
| C | -3.3512285641 | -1.6531969499 | 1.6176106978 |
| H | -4.9675661862 | -2.4777021632 | 0.3822271042 |
| O | -0.6224396523 | 0.8312744452 | -0.6377712532 |
| C | -4.1528949548 | -1.5203558575 | 2.7676977800 |
| C | -1.4210593947 | -0.8956638476 | 2.8965411839 |
| C | -3.5889879127 | -1.0992406236 | 3.9407334880 |
| C | -2.2292514108 | -0.7652954796 | 4.0172575464 |
| H | -5.2186780195 | -1.7731891216 | 2.7102440218 |
| H | -4.1964699215 | -1.0306607037 | 4.8603759605 |
| H | -1.8025896208 | -0.4146824305 | 4.9633635113 |
| H | -0.3603133859 | -0.6318673448 | 2.9374752780 |
| H | -1.7650664817 | -0.7173577838 | -1.2736715022 |

S1S0-KETO-2

| | | | |
|---|---------------|---------------|---------------|
| C | 2.2266047735 | 0.1702815389 | -1.4758196642 |
| C | 0.9728085792 | -0.3746620449 | -1.6888442863 |
| C | 0.1387309332 | -0.7312609980 | -0.6176663578 |
| C | 0.6438500863 | -0.5733385305 | 0.7341329156 |
| C | 1.9090020284 | 0.1037890684 | 0.9143794857 |
| C | 2.6799278572 | 0.4392755293 | -0.1655763674 |
| H | 2.8731055716 | 0.4135966096 | -2.3260237844 |
| H | 0.6285599914 | -0.5461030658 | -2.7159121086 |
| H | 2.2350232325 | 0.2824083943 | 1.9396361427 |
| H | 3.6618761126 | 0.9071474370 | -0.0278409681 |
| C | -1.9113236465 | -0.2550720200 | -1.8775330128 |
| C | -1.2636321571 | -1.0328942997 | -0.9048503592 |
| C | -3.2586362715 | -0.4544000978 | -2.1729152062 |
| C | -1.9877804072 | -2.0455883182 | -0.2341882844 |
| C | -3.9925120334 | -1.4168237916 | -1.4968664803 |
| H | -3.7434944595 | 0.1696448314 | -2.9323758055 |

| | | | |
|---|---------------|---------------|---------------|
| H | -0.9320701383 | -2.1105650150 | 1.5593089612 |
| C | -3.3682891899 | -2.2119989359 | -0.5146566602 |
| H | -5.0567248982 | -1.5597693446 | -1.7124728723 |
| O | 0.0657416669 | -1.0246859720 | 1.7671714443 |
| C | -4.1239806411 | -3.1768584727 | 0.2145121757 |
| C | -1.3242153747 | -2.8791535002 | 0.7866389012 |
| C | -3.5220145499 | -3.9770908442 | 1.1840801976 |
| C | -2.1703580599 | -3.8777030872 | 1.4286400512 |
| H | -5.1973212122 | -3.2738613862 | 0.0084708499 |
| H | -4.1283046511 | -4.7086350760 | 1.7292711018 |
| H | -1.6903567837 | -4.5462087066 | 2.1555650934 |
| H | -0.4059899133 | -3.3624098264 | 0.3748302501 |
| H | -1.3618493230 | 0.5408546649 | -2.3912565689 |