# (*S*)-Proline-Catalyzed Nitro-Michael Reactions: Towards a Better Understanding of the Catalytic Mechanism and Enantioselectivity

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## Supporting Information

**Table S1**. Cartesian coordinates, total energies (E, Hartrees) and number of imaginary frequencies (in parenthesis) of the M06-2X/6-31G** optimized geometries of all calculated structures.

| **TS1-α1-*RS*** E = -1031.6034955 (1) | | | | **TS1-α1-*SR*** E = -1031.5956026 (1) | | | |
|---|---|---|---|---|---|---|---|
| C | -3.002192 | 1.138477 | -1.229298 | C | -2.887746 | 0.597634 | 0.698302 |
| H | -2.506700 | 1.154768 | -2.204083 | H | -3.358053 | 0.816372 | 1.666445 |
| H | -3.483840 | 2.105733 | -1.044230 | C | -0.871786 | 1.924334 | 0.838690 |
| C | -3.875727 | -0.366045 | 0.428967 | H | -0.490467 | 2.213393 | 1.825507 |
| C | -2.387016 | -0.155048 | 0.759154 | H | -0.040317 | 1.947574 | 0.132529 |
| H | -2.223580 | 0.199473 | 1.779914 | N | -1.425571 | 0.561395 | 0.901918 |
| N | -1.987572 | 0.899704 | -0.185156 | C | -0.755281 | -0.490176 | 1.365044 |
| C | -0.995327 | 1.763444 | 0.028260 | H | -1.343743 | -1.393897 | 1.501974 |
| C | 0.097424 | 1.533186 | 0.862838 | C | 0.626095 | -0.496706 | 1.546714 |
| H | 0.016952 | 0.698685 | 1.559971 | H | 1.115262 | 0.466979 | 1.667325 |
| C | 0.932174 | 2.708319 | 1.305654 | C | 1.269061 | -1.666939 | 2.242302 |
| H | 0.492496 | 3.202431 | 2.177272 | H | 0.745462 | -2.595844 | 1.996482 |
| H | 1.940376 | 2.390563 | 1.582465 | H | 1.256360 | -1.549663 | 3.330346 |
| C | 1.355332 | 0.516419 | -0.473654 | H | 2.315636 | -1.772068 | 1.940534 |
| H | 1.577838 | 1.430439 | -1.018165 | C | -3.044319 | 1.795899 | -0.230007 |
| C | 0.594592 | -0.434744 | -1.166492 | H | -4.070647 | 2.165201 | -0.252820 |
| H | 0.557684 | -1.486774 | -0.931079 | C | -3.517347 | -0.754478 | 0.293330 |
| N | -0.269514 | -0.007367 | -2.131163 | O | -3.826419 | -1.519620 | 1.174447 |
| O | -1.134767 | -0.820203 | -2.601261 | O | -3.804150 | -0.964889 | -0.978559 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -0.247902 | 1.175045 | -2.511836 | H | -3.099941 | -0.612574 | -1.589148 |
| C | 2.412800 | 0.044891 | 0.450921 | C | 1.300850 | -0.717855 | -0.479030 |
| C | 4.464768 | -0.829893 | 2.138149 | H | 1.187551 | -1.791404 | -0.355683 |
| C | 2.210189 | -1.052446 | 1.298411 | C | 0.406992 | -0.124877 | -1.370316 |
| C | 3.646487 | 0.704374 | 0.470561 | H | 0.544024 | 0.806443 | -1.897720 |
| C | 4.669937 | 0.266137 | 1.305398 | N | -0.806301 | -0.728392 | -1.557074 |
| C | 3.233464 | -1.483966 | 2.133861 | O | -1.657566 | -0.176537 | -2.316845 |
| H | 1.246910 | -1.557272 | 1.319338 | O | -1.065024 | -1.780614 | -0.951416 |
| H | 3.804309 | 1.557711 | -0.183689 | C | 2.680057 | -0.193808 | -0.362549 |
| H | 5.625012 | 0.781077 | 1.304682 | C | 5.315366 | 0.741919 | -0.166061 |
| H | 3.066198 | -2.332842 | 2.788504 | C | 2.954716 | 1.179262 | -0.396869 |
| H | 5.259675 | -1.171513 | 2.793103 | C | 3.746232 | -1.088070 | -0.220054 |
| H | -4.471273 | 0.334631 | 1.021624 | C | 5.055345 | -0.624001 | -0.125584 |
| C | -1.601122 | -1.470646 | 0.649735 | C | 4.260076 | 1.643327 | -0.302335 |
| O | -1.018226 | -1.892010 | 1.622727 | H | 2.137077 | 1.889426 | -0.491413 |
| O | -1.692475 | -2.162174 | -0.477755 | H | 3.544338 | -2.155430 | -0.201462 |
| H | -1.620144 | -1.621493 | -1.335094 | H | 5.871227 | -1.331652 | -0.022174 |
| H | -1.020825 | 2.654495 | -0.594593 | H | 4.456817 | 2.710052 | -0.330371 |
| H | 1.012894 | 3.451000 | 0.505117 | H | 6.334635 | 1.105582 | -0.089599 |
| H | -4.205034 | -1.380373 | 0.661494 | H | -2.736939 | 1.522145 | -1.242538 |
| C | -3.975866 | -0.024779 | -1.061744 | C | -2.054777 | 2.795784 | 0.381473 |
| H | -4.989674 | 0.243745 | -1.362624 | H | -2.507229 | 3.290253 | 1.245690 |
| H | -3.650404 | -0.868748 | -1.673838 | H | -1.741909 | 3.568830 | -0.321703 |

**TS1-β1-*RS*** E = -1031.6033799 (1)

| | | | |
|---|---|---|---|
| C | -1.087960 | 1.967971 | -0.583449 |
| H | -0.994725 | 2.261812 | -1.636103 |
| H | -0.122127 | 2.111303 | -0.094278 |
| C | -3.437565 | 1.781568 | -0.108564 |
| H | -4.259015 | 1.963970 | 0.585343 |
| C | -2.820898 | 0.406528 | 0.094436 |
| H | -2.668760 | 0.217780 | 1.169347 |
| N | -1.491033 | 0.551120 | -0.531760 |
| C | -0.805513 | -0.426372 | -1.108698 |

**TS1-β1-*SR*** E = -1031.5895171 (1)

| | | | |
|---|---|---|---|
| C | -3.278546 | -1.469331 | -1.094999 |
| H | -3.659556 | -1.042756 | -2.023363 |
| H | -4.119644 | -1.679130 | -0.428288 |
| C | -2.448733 | -2.740907 | -1.301575 |
| H | -1.766087 | -2.625518 | -2.149355 |
| H | -3.063757 | -3.626668 | -1.467270 |
| C | -1.655065 | -2.818008 | -0.002172 |
| H | -0.731711 | -3.398238 | -0.068284 |
| H | -2.273830 | -3.210694 | 0.813070 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.298731 | -1.391554 | -1.168085 | C | -2.317071 | -0.503410 | -0.379560 |
| C | 0.540426 | -0.320337 | -1.460305 | H | -1.787153 | 0.151532 | -1.074079 |
| H | 0.947130 | 0.681708 | -1.575952 | N | -1.343975 | -1.407903 | 0.262720 |
| C | 1.155584 | -1.385960 | -2.329671 | C | -0.345996 | -1.003662 | 1.031589 |
| H | 0.723042 | -2.366158 | -2.106170 | H | 0.278813 | -1.803109 | 1.430171 |
| H | 2.235879 | -1.442062 | -2.168951 | C | 0.039673 | 0.328263 | 1.224938 |
| H | 0.992388 | -1.181321 | -3.391952 | H | -0.722064 | 1.072362 | 1.014673 |
| C | -3.622253 | -0.753826 | -0.503508 | C | 0.954671 | 0.655184 | 2.375754 |
| O | -4.454193 | -0.591233 | -1.356853 | H | 1.469610 | 1.601854 | 2.179678 |
| O | -3.324805 | -1.952539 | -0.007463 | H | 1.711396 | -0.121622 | 2.521337 |
| H | -2.600495 | -1.896145 | 0.661860 | H | 0.392649 | 0.772258 | 3.306148 |
| C | 1.363924 | -0.666297 | 0.429424 | C | -3.066892 | 0.323587 | 0.686551 |
| H | 1.224577 | -1.738343 | 0.315943 | O | -3.655582 | -0.236593 | 1.576281 |
| C | 0.606648 | -0.071711 | 1.447898 | O | -3.050347 | 1.638713 | 0.543977 |
| H | 0.851632 | 0.845359 | 1.961898 | H | -2.405792 | 1.947091 | -0.145854 |
| N | -0.572302 | -0.641793 | 1.838981 | C | 1.119667 | 2.115140 | -0.519643 |
| O | -0.946661 | -1.707687 | 1.264431 | H | 1.944213 | 2.742495 | -0.221914 |
| O | -1.274985 | -0.099263 | 2.706914 | C | 1.069042 | 0.710345 | -0.439876 |
| C | 2.746350 | -0.174654 | 0.202647 | H | 0.345692 | 0.249734 | -1.109064 |
| C | 5.377665 | 0.707025 | -0.192967 | N | -0.018845 | 2.807382 | -0.842766 |
| C | 3.050264 | 1.192052 | 0.213229 | O | -1.059459 | 2.141281 | -1.167672 |
| C | 3.778999 | -1.090382 | -0.020586 | O | -0.033281 | 4.034905 | -0.821407 |
| C | 5.086707 | -0.653100 | -0.213958 | C | 2.326684 | -0.070244 | -0.303105 |
| C | 4.354241 | 1.629684 | 0.020843 | C | 4.639099 | -1.638501 | -0.051376 |
| H | 2.254762 | 1.917489 | 0.367438 | C | 2.351405 | -1.391998 | -0.764332 |
| H | 3.553465 | -2.153208 | -0.027709 | C | 3.480634 | 0.453284 | 0.287936 |
| H | 5.877425 | -1.377367 | -0.379662 | C | 4.627145 | -0.326286 | 0.412431 |
| H | 4.574111 | 2.692204 | 0.032739 | C | 3.495501 | -2.171063 | -0.643726 |
| H | 6.395660 | 1.049519 | -0.345737 | H | 1.458090 | -1.802171 | -1.232370 |
| H | -3.819291 | 1.852992 | -1.131217 | H | 3.486603 | 1.473959 | 0.656588 |
| C | -2.233236 | 2.698800 | 0.123922 | H | 5.514925 | 0.095559 | 0.872056 |
| H | -2.372311 | 3.709534 | -0.262092 | H | 3.499112 | -3.190089 | -1.016952 |
| H | -2.019784 | 2.760243 | 1.195346 | H | 5.535372 | -2.242408 | 0.043897 |

**TS1-β2-*RS*** E = -1031.58810471 (1)

| | | | |
|---|---|---|---|
| C | 1.069502 | -1.182932 | -1.313029 |
| H | 0.208520 | -1.672166 | -0.854011 |
| C | 2.926217 | -1.723860 | 0.106305 |
| H | 3.977186 | -1.995059 | 0.206437 |
| C | 2.742688 | -0.203376 | 0.178977 |
| H | 2.652192 | 0.154113 | 1.212177 |
| N | 1.457741 | -0.001283 | -0.509814 |
| C | 0.740769 | 1.110409 | -0.391176 |
| C | -0.624215 | 1.178264 | -0.740533 |
| H | -0.942271 | 0.456941 | -1.492661 |
| C | -1.242783 | 2.551843 | -0.876961 |
| H | -0.898366 | 3.206174 | -0.070046 |
| H | -2.332470 | 2.485408 | -0.820954 |
| C | -1.491541 | 0.386470 | 0.783007 |
| H | -1.495909 | 1.315958 | 1.351504 |
| C | -0.734372 | -0.641114 | 1.399369 |
| H | -0.936594 | -1.699634 | 1.340549 |
| N | 0.379790 | -0.288291 | 2.103687 |
| O | 1.108508 | -1.158083 | 2.620807 |
| O | 0.675057 | 0.936361 | 2.162842 |
| C | -2.828096 | -0.001638 | 0.240699 |
| C | -5.355150 | -0.719495 | -0.738694 |
| C | -2.984897 | -1.130383 | -0.570942 |
| C | -3.954558 | 0.766970 | 0.544999 |
| C | -5.210599 | 0.409364 | 0.061455 |
| C | -4.237095 | -1.489883 | -1.054224 |
| H | -2.114868 | -1.731260 | -0.826783 |
| H | -3.843997 | 1.643295 | 1.177874 |
| H | -6.076074 | 1.013841 | 0.312430 |
| H | -4.342285 | -2.370075 | -1.680186 |
| H | -6.332722 | -0.998300 | -1.117688 |
| H | 1.225688 | 1.935094 | 0.122337 |
| H | -0.987045 | 3.021352 | -1.830609 |

**TS1-β2-*SR*** E = -1031.59139217 (1)

| | | | |
|---|---|---|---|
| C | -0.608949 | -1.926997 | -0.000166 |
| H | -0.911555 | -1.005922 | 0.495768 |
| C | -1.683616 | -2.451395 | -0.959922 |
| H | -2.449345 | -3.010835 | -0.422284 |
| C | 0.390485 | -2.444125 | -2.164124 |
| H | 0.249655 | -1.708108 | -2.964348 |
| N | 0.536322 | -1.697607 | -0.891895 |
| C | 1.529790 | -0.841479 | -0.679069 |
| H | 2.307226 | -0.839360 | -1.436856 |
| C | 1.536190 | 0.115624 | 0.355373 |
| H | 0.948401 | -0.142979 | 1.235231 |
| C | 2.852377 | 0.796429 | 0.658907 |
| H | 2.683475 | 1.717914 | 1.221859 |
| H | 3.372717 | 1.053724 | -0.269083 |
| H | 3.510695 | 0.159702 | 1.256193 |
| C | -0.321202 | -2.957896 | 1.105806 |
| O | -1.178778 | -3.276146 | 1.881275 |
| O | 0.910707 | -3.485553 | 1.156165 |
| H | 1.460741 | -3.097106 | 0.462156 |
| C | 0.389890 | 1.525486 | -0.338238 |
| H | 1.192563 | 1.975819 | -0.920421 |
| C | -0.674876 | 1.035314 | -1.130558 |
| H | -1.711346 | 0.978781 | -0.833557 |
| N | -0.384279 | 0.524722 | -2.362885 |
| O | 0.817194 | 0.532894 | -2.738943 |
| O | -1.281130 | 0.010659 | -3.064775 |
| C | 0.023590 | 2.288072 | 0.891458 |
| C | -0.652102 | 3.761148 | 3.179180 |
| C | -0.948158 | 1.818071 | 1.781812 |
| C | 0.656590 | 3.502470 | 1.169916 |
| C | 0.319315 | 4.236458 | 2.304096 |
| C | -1.285935 | 2.548212 | 2.914775 |
| H | -1.447644 | 0.871422 | 1.587588 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.925244 | 0.513001 | -0.488006 | H | 1.409189 | 3.878401 | 0.482119 |
| O | 5.039285 | 0.384215 | -0.066554 | H | 0.816295 | 5.180581 | 2.501711 |
| O | 3.668671 | 1.271296 | -1.569625 | H | -2.041917 | 2.169143 | 3.594512 |
| H | 2.729543 | 1.228483 | -1.791635 | H | -0.914083 | 4.330119 | 4.064974 |
| H | 2.351028 | -2.169955 | 0.921726 | H | -2.128741 | -1.603275 | -1.487646 |
| H | 0.797938 | -0.866366 | -2.325601 | H | 1.293183 | -3.029066 | -2.360592 |
| C | 2.319537 | -2.065300 | -1.258073 | C | -0.861875 | -3.293321 | -1.942893 |
| H | 3.009681 | -1.789028 | -2.062837 | H | -1.387968 | -3.475207 | -2.880204 |
| H | 2.074143 | -3.122142 | -1.369952 | H | -0.604238 | -4.259788 | -1.495671 |

**TS1-β3-*RS*** E = -1031.59995960 (1)

| | | | |
|---|---|---|---|
| C | -0.753775 | 0.650208 | -1.921338 |
| H | -1.220788 | 1.174580 | -1.083598 |
| C | -2.224846 | -1.171881 | -2.439747 |
| H | -2.711619 | -1.794344 | -3.190782 |
| C | -0.901176 | -1.780545 | -1.956246 |
| H | -1.057865 | -2.496204 | -1.137370 |
| N | -0.169712 | -0.620227 | -1.456195 |
| C | 0.963013 | -0.730470 | -0.780590 |
| C | 1.517926 | 0.331686 | -0.049667 |
| H | 1.247423 | 1.331196 | -0.386233 |
| C | 2.928356 | 0.185112 | 0.467616 |
| H | 3.101627 | -0.835951 | 0.821878 |
| H | 3.104768 | 0.870306 | 1.301570 |
| C | 0.370476 | 0.306173 | 1.577528 |
| H | 0.960085 | -0.481072 | 2.043685 |
| C | -0.964183 | -0.057563 | 1.307917 |
| H | -1.805838 | 0.616151 | 1.259512 |
| N | -1.243637 | -1.365402 | 1.016165 |
| O | -2.402962 | -1.704238 | 0.701195 |
| O | -0.299058 | -2.194006 | 1.023695 |
| C | 0.606323 | 1.669627 | 2.130671 |
| C | 1.045234 | 4.218137 | 3.215900 |
| C | -0.003748 | 2.798655 | 1.572275 |

**TS1-β3-*SR*** E = -1031.60020372 (1)

| | | | |
|---|---|---|---|
| C | -1.866918 | 2.131580 | -1.697422 |
| H | -2.418115 | 2.381735 | -0.783525 |
| C | -2.211642 | -0.204809 | -2.181427 |
| H | -2.382246 | -0.977916 | -2.932644 |
| C | -0.715403 | 0.003948 | -1.894655 |
| H | -0.310735 | -0.749366 | -1.219606 |
| N | -0.689443 | 1.334476 | -1.303780 |
| C | 0.278174 | 1.817278 | -0.544953 |
| C | 1.275582 | 1.033042 | 0.056320 |
| H | 1.535109 | 0.108306 | -0.455977 |
| C | 2.437141 | 1.744594 | 0.707519 |
| H | 3.188448 | 2.051257 | -0.025919 |
| H | 2.930218 | 1.091163 | 1.432493 |
| C | 0.261303 | 0.207428 | 1.572721 |
| H | 0.390592 | 1.088072 | 2.198672 |
| C | -1.078174 | -0.072749 | 1.242522 |
| H | -1.484097 | -1.047612 | 1.017868 |
| N | -1.965167 | 0.968652 | 1.138510 |
| O | -3.139527 | 0.753683 | 0.772779 |
| O | -1.552500 | 2.129853 | 1.368254 |
| C | 1.138741 | -0.942343 | 1.930142 |
| C | 2.791872 | -3.092344 | 2.649749 |
| C | 1.138263 | -2.126248 | 1.183368 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.448573 | 1.839926 | 3.232749 | C | 1.987396 | -0.851669 | 3.037172 |
| C | 1.664639 | 3.104621 | 3.774168 | C | 2.806293 | -1.918931 | 3.396770 |
| C | 0.209426 | 4.061326 | 2.111209 | C | 1.953812 | -3.192925 | 1.540400 |
| H | -0.647123 | 2.682530 | 0.702843 | H | 0.491152 | -2.214027 | 0.313543 |
| H | 1.925408 | 0.969383 | 3.674776 | H | 1.992427 | 0.060925 | 3.626916 |
| H | 2.316991 | 3.217793 | 4.633953 | H | 3.454210 | -1.832020 | 4.262920 |
| H | -0.272837 | 4.926341 | 1.667416 | H | 1.938891 | -4.103909 | 0.950865 |
| H | 1.214052 | 5.204406 | 3.635339 | H | 3.430587 | -3.924344 | 2.927109 |
| H | 1.363157 | -1.733949 | -0.686966 | H | 0.166554 | 2.861488 | -0.268796 |
| H | 3.669250 | 0.405535 | -0.306006 | H | 2.091852 | 2.639312 | 1.235260 |
| C | -0.118350 | -2.462504 | -3.067715 | C | 0.083269 | 0.004011 | -3.191566 |
| O | 0.989684 | -2.164051 | -3.433607 | O | 0.428408 | 0.983734 | -3.798632 |
| O | -0.824615 | -3.472352 | -3.599127 | O | 0.316147 | -1.252461 | -3.607164 |
| H | -0.266230 | -3.882578 | -4.277308 | H | 0.782515 | -1.190008 | -4.455176 |
| H | -2.876292 | -1.078358 | -1.566855 | H | -2.704146 | -0.477448 | -1.243995 |
| H | 0.034903 | 1.281201 | -2.341717 | H | -1.540352 | 3.045084 | -2.199675 |
| C | -1.789398 | 0.202704 | -2.956140 | C | -2.662114 | 1.196309 | -2.613543 |
| H | -1.314315 | 0.109427 | -3.938303 | H | -2.401482 | 1.376136 | -3.660471 |
| H | -2.615177 | 0.910529 | -3.041460 | H | -3.736102 | 1.337256 | -2.489549 |

**TS2-α1-*RS*** E = -1110.19473893 (1)

| | | | |
|---|---|---|---|
| C | -2.048940 | 1.080824 | -1.047833 |
| H | -2.455062 | 1.294836 | -0.056072 |
| C | -2.820799 | 1.787263 | -2.177543 |
| H | -3.643246 | 1.176085 | -2.553683 |
| C | -0.515755 | 2.426391 | -2.404944 |
| N | -0.704719 | 1.668381 | -1.153307 |
| C | 0.145412 | 1.799106 | -0.134993 |
| H | 0.940471 | 2.519517 | -0.301906 |
| C | 0.149106 | 0.994157 | 1.005687 |
| H | -0.746455 | 0.392347 | 1.172692 |
| C | 0.849473 | 1.466723 | 2.267780 |
| H | 1.184473 | 0.572213 | 2.806962 |
| C | 2.072953 | 2.343310 | 1.992678 |

**TS2-α1-*SR*** E = -1110.18782243 (1)

| | | | |
|---|---|---|---|
| C | 2.889577 | 0.594065 | -0.675891 |
| H | 3.373449 | 0.745304 | -1.650227 |
| C | 0.845491 | 1.844222 | -0.981230 |
| H | 0.493335 | 2.032776 | -2.002648 |
| H | -0.011531 | 1.908052 | -0.309719 |
| N | 1.433393 | 0.496981 | -0.902170 |
| C | 0.804084 | -0.614193 | -1.274160 |
| H | 1.426918 | -1.502883 | -1.308205 |
| C | -0.574423 | -0.681713 | -1.474711 |
| H | -1.081123 | 0.253917 | -1.707063 |
| C | -1.199937 | -1.920427 | -2.085126 |
| H | -2.207418 | -2.014294 | -1.656032 |
| C | 2.991438 | 1.870113 | 0.150698 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.634427 | 2.503827 | 2.916389 | H | 4.006369 | 2.270140 | 0.164253 |
| H | 1.776187 | 3.328991 | 1.617823 | C | 3.546258 | -0.701215 | -0.147432 |
| H | 2.750348 | 1.896258 | 1.257467 | O | 3.901308 | -1.523942 | -0.956940 |
| C | -0.143420 | 2.200640 | 3.177507 | O | 3.799277 | -0.804853 | 1.143787 |
| H | 0.335378 | 2.492732 | 4.117092 | H | 3.073472 | -0.418325 | 1.708864 |
| H | -1.003174 | 1.568540 | 3.416189 | C | -1.297058 | -0.690757 | 0.540029 |
| H | -0.513391 | 3.107442 | 2.686894 | H | -1.188354 | -1.771816 | 0.530853 |
| C | 1.286186 | -0.622814 | 0.330758 | C | -0.420812 | -0.011040 | 1.387078 |
| H | 2.210016 | -0.054170 | 0.387373 | H | -0.572127 | 0.965556 | 1.820357 |
| C | 0.857777 | -0.954776 | -0.962306 | N | 0.790210 | -0.585203 | 1.653412 |
| H | 0.195199 | -1.771357 | -1.202507 | O | 1.624065 | 0.042380 | 2.374086 |
| N | 1.188640 | -0.129060 | -1.994764 | O | 1.067905 | -1.688448 | 1.154767 |
| O | 0.619968 | -0.283251 | -3.127966 | C | -2.674706 | -0.181462 | 0.352805 |
| O | 1.997051 | 0.798731 | -1.818629 | C | -5.308500 | 0.725968 | 0.032845 |
| C | 1.072902 | -1.605223 | 1.419782 | C | -2.950893 | 1.187637 | 0.247426 |
| C | 0.755444 | -3.485130 | 3.466198 | C | -3.739323 | -1.086737 | 0.288333 |
| C | -0.119227 | -2.332646 | 1.530902 | C | -5.047351 | -0.636742 | 0.132303 |
| C | 2.093714 | -1.820467 | 2.352132 | C | -4.255310 | 1.637953 | 0.091484 |
| C | 1.939032 | -2.759538 | 3.367100 | H | -2.135899 | 1.905997 | 0.282466 |
| C | -0.271468 | -3.266648 | 2.548952 | H | -3.537099 | -2.150344 | 0.379670 |
| H | -0.934761 | -2.157190 | 0.832886 | H | -5.861514 | -1.352648 | 0.090677 |
| H | 3.017680 | -1.253641 | 2.269511 | H | -4.452672 | 2.701920 | 0.011348 |
| H | 2.741805 | -2.923112 | 4.078537 | H | -6.326948 | 1.078543 | -0.091584 |
| H | -1.199089 | -3.823814 | 2.628003 | H | 2.667362 | 1.673425 | 1.175889 |
| H | 0.630411 | -4.215743 | 4.258749 | C | 1.990068 | 2.785812 | -0.565372 |
| C | -2.120790 | -0.445377 | -1.203538 | H | 2.452009 | 3.223718 | -1.454652 |
| O | -2.626123 | -1.104783 | -0.323894 | H | 1.635502 | 3.602565 | 0.064857 |
| O | -1.738532 | -0.975463 | -2.357194 | C | -0.422936 | -3.200146 | -1.765678 |
| H | -0.879079 | -0.604309 | -2.751364 | H | 0.512090 | -3.242966 | -2.334336 |
| H | 0.424430 | 2.112453 | -2.866971 | H | -0.165989 | -3.274609 | -0.703891 |
| H | -3.235100 | 2.722864 | -1.790342 | H | -1.011565 | -4.077954 | -2.043679 |
| H | -0.471954 | 3.496385 | -2.170443 | C | -1.370015 | -1.751762 | -3.599554 |
| C | -1.747960 | 2.074173 | -3.233682 | H | -1.874221 | -2.621222 | -4.032211 |
| H | -2.031216 | 2.882472 | -3.909590 | H | -1.961741 | -0.862866 | -3.836934 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.548052 | 1.182873 | -3.832559 | H | -0.392876 | -1.649491 | -4.082890 |

**TS2-β1-*RS*** E = -1110.19506826 (1)

| | | | |
|---|---|---|---|
| C | -2.374539 | -1.805514 | -0.300636 |
| H | -2.984548 | -0.894621 | -0.186060 |
| C | -2.731598 | -2.511436 | -1.599073 |
| H | -3.810793 | -2.573265 | -1.744233 |
| C | -0.689340 | -1.296491 | -1.974157 |
| H | 0.087143 | -2.032346 | -2.216418 |
| H | -0.319554 | -0.301952 | -2.232489 |
| N | -0.977243 | -1.385972 | -0.531728 |
| C | -0.055164 | -1.254897 | 0.412449 |
| H | -0.358676 | -1.539047 | 1.412935 |
| C | 1.167640 | -0.611335 | 0.211339 |
| H | 1.520411 | -0.537111 | -0.816477 |
| C | 2.266919 | -0.722741 | 1.251485 |
| H | 2.830752 | 0.219435 | 1.222033 |
| C | 1.731530 | -0.915430 | 2.672572 |
| H | 2.538264 | -0.789194 | 3.398704 |
| H | 1.328125 | -1.924915 | 2.806713 |
| H | 0.934968 | -0.204799 | 2.917961 |
| C | 3.241955 | -1.847642 | 0.884930 |
| H | 4.064882 | -1.896488 | 1.604311 |
| H | 3.669825 | -1.694122 | -0.109951 |
| H | 2.727875 | -2.814423 | 0.889334 |
| C | 0.517821 | 1.366295 | 0.326292 |
| H | 0.560278 | 1.335441 | 1.411670 |
| C | -0.764936 | 1.528769 | -0.215802 |
| H | -0.991227 | 1.963127 | -1.177849 |
| N | -1.855994 | 1.085493 | 0.475751 |
| O | -2.993943 | 1.187080 | -0.011179 |
| O | -1.671650 | 0.527453 | 1.599740 |
| C | 1.648217 | 2.069297 | -0.332328 |
| C | 3.777279 | 3.443490 | -1.531983 |

**TS2-β1-*SR*** E = -1110.18152497 (1)

| | | | |
|---|---|---|---|
| C | 2.621448 | 3.089187 | -1.117778 |
| H | 3.620697 | 3.539730 | -1.101639 |
| C | 3.176013 | 0.951150 | -1.995295 |
| H | 2.886997 | 0.089553 | -2.597867 |
| C | 2.844727 | 0.740231 | -0.507390 |
| H | 1.974544 | 0.097825 | -0.358674 |
| N | 2.521254 | 2.100229 | -0.036165 |
| C | 2.266585 | 2.412211 | 1.223067 |
| C | 2.082054 | 1.487779 | 2.262330 |
| H | 2.495491 | 0.503105 | 2.066094 |
| C | 2.247882 | 1.929125 | 3.707774 |
| H | 1.494482 | 1.384331 | 4.295380 |
| C | 0.220575 | 0.863186 | 2.005722 |
| H | 0.294799 | 0.771348 | 0.923814 |
| C | 0.147004 | -0.369820 | 2.687752 |
| H | -0.243312 | -0.525884 | 3.680223 |
| N | 0.778334 | -1.465798 | 2.166391 |
| O | 0.825389 | -2.522121 | 2.791794 |
| O | 1.318694 | -1.361055 | 1.011098 |
| C | 4.071435 | 0.191142 | 0.253862 |
| O | 5.095151 | 0.827163 | 0.277951 |
| O | 3.938686 | -0.994011 | 0.824242 |
| H | 2.991299 | -1.299820 | 0.861196 |
| C | -0.628287 | 1.999931 | 2.450419 |
| C | -2.112646 | 4.249726 | 3.230251 |
| C | -0.903563 | 3.029112 | 1.541582 |
| C | -1.124616 | 2.108570 | 3.752750 |
| C | -1.858913 | 3.227054 | 4.138860 |
| C | -1.637372 | 4.144774 | 1.923423 |
| H | -0.529648 | 2.944086 | 0.522608 |
| H | -0.934124 | 1.322969 | 4.476280 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.782840 | 2.101260 | -1.725484 | H | -2.233175 | 3.297747 | 5.154849 |
| C | 2.602568 | 2.728105 | 0.448879 | H | -1.843644 | 4.930633 | 1.203973 |
| C | 3.658388 | 3.413200 | -0.146325 | H | -2.683931 | 5.120531 | 3.534156 |
| C | 2.835421 | 2.784389 | -2.320983 | C | 2.043381 | 3.428162 | 3.937664 |
| H | 1.058011 | 1.580737 | -2.346961 | H | 2.864961 | 4.004908 | 3.497007 |
| H | 2.504332 | 2.713053 | 1.530998 | H | 2.038344 | 3.639781 | 5.010048 |
| H | 4.386721 | 3.924109 | 0.474750 | H | 1.869880 | 3.870276 | -0.981647 |
| H | 2.925387 | 2.800182 | -3.402234 | H | 1.097700 | 3.791925 | 3.522828 |
| H | 4.600782 | 3.974691 | -1.997432 | H | 2.079906 | 3.470543 | 1.398696 |
| C | -2.527669 | -2.660231 | 0.961272 | C | 3.629133 | 1.490549 | 4.209848 |
| O | -2.583477 | -3.861258 | 0.923408 | H | 4.419765 | 1.972736 | 3.625176 |
| O | -2.595317 | -1.973549 | 2.099613 | H | 3.757355 | 0.408828 | 4.112443 |
| H | -2.501075 | -1.001801 | 1.946456 | H | 3.764127 | 1.759790 | 5.261801 |
| H | -2.322161 | -3.525568 | -1.576674 | H | 4.253993 | 1.108161 | -2.092813 |
| C | -2.030582 | -1.628425 | -2.635974 | C | 2.427408 | 2.235677 | -2.365908 |
| H | -2.603468 | -0.707708 | -2.782174 | H | 2.823313 | 2.714346 | -3.262801 |
| H | -1.898684 | -2.112878 | -3.604405 | H | 1.362719 | 2.033614 | -2.518500 |

**TS2-β2-*RS*** E = -1110.18026554 (1)

| | | | |
|---|---|---|---|
| C | 1.100303 | -0.454109 | -1.658029 |
| H | 0.227663 | -1.083517 | -1.477139 |
| C | 2.930798 | -1.603615 | -0.617372 |
| H | 3.976912 | -1.908756 | -0.641228 |
| C | 2.763506 | -0.273155 | 0.125359 |
| H | 2.666629 | -0.413590 | 1.209214 |
| N | 1.488332 | 0.233106 | -0.405904 |
| C | 0.790862 | 1.191188 | 0.194196 |
| C | -0.570971 | 1.433219 | -0.088954 |
| H | -0.882156 | 1.141036 | -1.093199 |
| C | -1.189146 | 2.744520 | 0.381252 |
| H | -2.261842 | 2.553011 | 0.515478 |
| C | -1.476749 | 0.043601 | 0.874983 |
| H | -1.520925 | 0.615318 | 1.801199 |
| C | -0.723658 | -1.152360 | 0.991630 |

**TS2-β2-*SR*** E = -1110.18386010 (1)

| | | | |
|---|---|---|---|
| C | -1.696732 | 0.902794 | -0.416392 |
| H | -0.654358 | 1.003608 | -0.724369 |
| C | -2.610284 | 0.468891 | -1.560418 |
| H | -2.902474 | 1.322671 | -2.170650 |
| C | -3.093148 | -0.949931 | 0.319935 |
| H | -2.811249 | -1.965850 | 0.018118 |
| N | -1.839053 | -0.196764 | 0.549302 |
| C | -0.957550 | -0.559991 | 1.468329 |
| H | -1.283191 | -1.365278 | 2.116754 |
| C | 0.371705 | -0.078843 | 1.517666 |
| H | 0.519561 | 0.918098 | 1.098578 |
| C | 1.171552 | -0.308069 | 2.794357 |
| H | 2.229862 | -0.297820 | 2.503706 |
| C | -2.129400 | 2.262315 | 0.171146 |
| O | -2.584896 | 3.130794 | -0.518707 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.914292 | -2.073837 | 0.462927 | O | -1.913738 | 2.456233 | 1.482212 |
| N | 0.371359 | -1.150706 | 1.804420 | H | -1.579735 | 1.652552 | 1.904428 |
| O | 1.098585 | -2.159599 | 1.898102 | C | 1.274283 | -1.072760 | 0.120582 |
| O | 0.654835 | -0.078511 | 2.406560 | H | 1.484141 | -1.922274 | 0.768440 |
| C | -2.792353 | -0.066512 | 0.174893 | C | 0.423570 | -1.387687 | -0.965597 |
| C | -5.284050 | -0.285719 | -1.092882 | H | 0.443671 | -0.922674 | -1.939771 |
| C | -2.908228 | -0.698326 | -1.067800 | N | -0.557602 | -2.318128 | -0.775611 |
| C | -3.942428 | 0.461839 | 0.767084 | O | -0.646026 | -2.862059 | 0.356916 |
| C | -5.180645 | 0.351002 | 0.139713 | O | -1.376507 | -2.570238 | -1.683834 |
| C | -4.142666 | -0.811103 | -1.696092 | C | 2.472294 | -0.234260 | -0.182071 |
| H | -2.020483 | -1.104142 | -1.547757 | C | 4.751869 | 1.301275 | -0.741686 |
| H | -3.864494 | 0.950097 | 1.734796 | C | 2.381237 | 0.920383 | -0.967161 |
| H | -6.064384 | 0.761699 | 0.616936 | C | 3.722622 | -0.602834 | 0.322213 |
| H | -4.215448 | -1.306752 | -2.658718 | C | 4.855478 | 0.157013 | 0.042715 |
| H | -6.247778 | -0.371460 | -1.583713 | C | 3.509877 | 1.681199 | -1.247344 |
| H | 1.291012 | 1.680848 | 1.022530 | H | 1.418184 | 1.226541 | -1.369481 |
| C | 3.960627 | 0.648908 | -0.146627 | H | 3.806317 | -1.501916 | 0.927032 |
| O | 5.070547 | 0.324616 | 0.167094 | H | 5.818996 | -0.147696 | 0.437911 |
| O | 3.721487 | 1.821063 | -0.762668 | H | 3.420618 | 2.572975 | -1.858981 |
| H | 2.783245 | 1.900383 | -0.978815 | H | 5.632825 | 1.896263 | -0.958263 |
| H | 2.338508 | -2.356883 | -0.091393 | H | -2.092666 | -0.281887 | -2.163527 |
| H | 0.847687 | 0.288746 | -2.422021 | H | -3.677453 | -0.987946 | 1.242819 |
| C | 2.339259 | -1.288520 | -1.994813 | C | -3.778990 | -0.185685 | -0.814215 |
| H | 3.044182 | -0.693412 | -2.585725 | H | -4.357325 | -0.856055 | -1.450249 |
| H | 2.083120 | -2.179398 | -2.569636 | H | -4.449102 | 0.584240 | -0.417955 |
| C | -1.046626 | 3.829819 | -0.689534 | C | 0.955378 | 0.841265 | 3.783800 |
| H | -1.530890 | 4.756962 | -0.369357 | H | 1.580729 | 0.714881 | 4.672494 |
| H | 0.010844 | 4.050063 | -0.874512 | H | 1.197347 | 1.808757 | 3.333860 |
| H | -1.500211 | 3.519526 | -1.635396 | H | -0.089744 | 0.870627 | 4.115270 |
| C | -0.615731 | 3.221334 | 1.719021 | C | 0.866954 | -1.657058 | 3.452674 |
| H | -1.243825 | 4.010390 | 2.139317 | H | 0.824532 | -2.474594 | 2.725642 |
| H | -0.538618 | 2.410562 | 2.450912 | H | 1.629402 | -1.894193 | 4.198490 |
| H | 0.386334 | 3.644306 | 1.585543 | H | -0.095684 | -1.628645 | 3.975357 |

**TS2-β3-*RS*** E = -1110.19193505 (1)

| | | | |
|---|---|---|---|
| C | -2.336658 | -1.717113 | 0.069581 |
| H | -2.776680 | -1.007311 | 0.783810 |
| C | -3.025890 | -1.643160 | -1.299509 |
| H | -3.914384 | -2.273099 | -1.345991 |
| C | -0.671838 | -1.378208 | -1.674697 |
| H | 0.254755 | -1.937398 | -1.835016 |
| N | -0.965182 | -1.318208 | -0.232275 |
| C | -0.075992 | -1.075485 | 0.717862 |
| H | -0.412821 | -1.270548 | 1.728208 |
| C | 1.138057 | -0.412720 | 0.470794 |
| H | 1.525936 | -0.511536 | -0.543504 |
| C | 2.212697 | -0.402799 | 1.546370 |
| H | 2.786686 | 0.524024 | 1.410877 |
| C | 1.630856 | -0.401531 | 2.962871 |
| H | 2.409034 | -0.159826 | 3.691146 |
| H | 1.238890 | -1.391131 | 3.222350 |
| H | 0.813787 | 0.319222 | 3.074213 |
| C | 3.181009 | -1.574988 | 1.359228 |
| H | 3.978675 | -1.543336 | 2.107741 |
| H | 3.644580 | -1.552831 | 0.368573 |
| H | 2.650807 | -2.527300 | 1.465674 |
| C | 0.538191 | 1.471761 | 0.295594 |
| H | 0.591605 | 1.641830 | 1.369132 |
| C | -0.759121 | 1.591778 | -0.243497 |
| H | -0.998603 | 1.900948 | -1.249408 |
| N | -1.828651 | 1.229631 | 0.528244 |
| O | -2.983650 | 1.254383 | 0.054490 |
| O | -1.609707 | 0.821475 | 1.697257 |
| C | 1.652288 | 2.088744 | -0.479452 |
| C | 3.740038 | 3.296141 | -1.912134 |
| C | 1.788243 | 1.880366 | -1.856555 |
| C | 2.585579 | 2.902367 | 0.168884 |
| C | 3.620617 | 3.504500 | -0.541883 |

**TS2-β3-*SR*** E = -1110.19204406 (1)

| | | | |
|---|---|---|---|
| C | -1.047979 | -1.318155 | -1.377145 |
| H | -1.442520 | -0.571079 | -0.689529 |
| C | -1.455198 | -1.051034 | -2.835586 |
| H | -2.472402 | -1.385123 | -3.047016 |
| H | -1.366494 | 0.022585 | -3.023515 |
| C | -0.373631 | -1.803257 | -3.621318 |
| H | -0.270362 | -1.427432 | -4.639576 |
| H | -0.604121 | -2.871796 | -3.662001 |
| C | 0.899324 | -1.562627 | -2.804390 |
| H | 1.563498 | -2.429717 | -2.782827 |
| H | 1.447575 | -0.677080 | -3.147043 |
| N | 0.405446 | -1.281785 | -1.443044 |
| C | 1.218206 | -1.076335 | -0.421694 |
| H | 2.271219 | -1.178493 | -0.658661 |
| C | 0.808310 | -0.559573 | 0.819435 |
| H | -0.220601 | -0.777938 | 1.106315 |
| C | 1.783498 | -0.585706 | 1.986336 |
| H | 1.517387 | 0.257190 | 2.638076 |
| C | 1.617318 | -1.868807 | 2.806771 |
| H | 2.291415 | -1.869460 | 3.668868 |
| H | 1.846253 | -2.746590 | 2.193204 |
| H | 0.593227 | -1.973238 | 3.176789 |
| C | 3.239852 | -0.406075 | 1.548097 |
| H | 3.870533 | -0.185301 | 2.412822 |
| H | 3.355931 | 0.401113 | 0.817015 |
| H | 3.626352 | -1.324608 | 1.092720 |
| C | 0.524349 | 1.372840 | 0.397655 |
| H | 1.574627 | 1.607685 | 0.556938 |
| C | 0.080597 | 1.579345 | -0.922642 |
| H | -0.925194 | 1.837983 | -1.217929 |
| N | 0.963041 | 1.389854 | -1.954073 |
| O | 0.573672 | 1.491403 | -3.136367 |
| O | 2.142133 | 1.062211 | -1.677340 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.819470 | 2.480701 | -2.568477 | C | -0.377062 | 1.812752 | 1.500033 |
| H | 1.079661 | 1.235873 | -2.371792 | C | -2.040383 | 2.682998 | 3.586626 |
| H | 2.487234 | 3.073728 | 1.237438 | C | -1.749554 | 1.538442 | 1.483254 |
| H | 4.332657 | 4.137840 | -0.022761 | C | 0.147152 | 2.524301 | 2.583312 |
| H | 2.909164 | 2.309702 | -3.636424 | C | -0.677236 | 2.958672 | 3.617936 |
| H | 4.547073 | 3.762937 | -2.467101 | C | -2.574829 | 1.970995 | 2.514121 |
| C | -2.362926 | -3.111448 | 0.676814 | H | -2.178813 | 0.982512 | 0.652936 |
| O | -1.397761 | -3.769332 | 0.970879 | H | 1.210088 | 2.749415 | 2.603890 |
| O | -3.625022 | -3.527810 | 0.863283 | H | -0.252293 | 3.514508 | 4.447424 |
| H | -3.576541 | -4.403312 | 1.277015 | H | -3.636902 | 1.750354 | 2.482843 |
| H | -3.310515 | -0.600136 | -1.462249 | H | -2.684282 | 3.018746 | 4.392745 |
| H | -0.551647 | -0.367960 | -2.073646 | C | -1.505848 | -2.701893 | -0.934772 |
| C | -1.908164 | -2.069328 | -2.256146 | O | -0.821472 | -3.691157 | -0.915660 |
| H | -2.092810 | -1.775918 | -3.290575 | O | -2.808773 | -2.688902 | -0.605660 |
| H | -1.773577 | -3.155650 | -2.226424 | H | -3.053583 | -3.598900 | -0.376606 |

**TS3-α1-*RS*** E = -1110.19888369 (1)

| | | | |
|---|---|---|---|
| C | 3.169248 | 0.915424 | -0.128773 |
| H | 3.032599 | 1.327661 | 0.875596 |
| H | 3.615773 | 1.676758 | -0.779351 |
| C | 3.400088 | -1.164599 | -1.303089 |
| C | 1.895298 | -0.856271 | -1.229821 |
| H | 1.419495 | -0.848069 | -2.213245 |
| N | 1.857074 | 0.506636 | -0.668135 |
| C | 0.857270 | 1.377673 | -0.916943 |
| C | -0.424326 | 0.915802 | -1.238032 |
| H | -0.519943 | -0.145574 | -1.459889 |
| C | -1.447977 | 1.798022 | -1.908279 |
| H | -1.186764 | 1.996157 | -2.953261 |
| H | -2.422634 | 1.306294 | -1.903139 |
| C | -1.186711 | 0.685105 | 0.750751 |
| H | -1.167907 | 1.757549 | 0.928096 |
| C | -0.269512 | -0.074363 | 1.479670 |
| H | -0.340165 | -1.138235 | 1.642639 |

**TS3-α1-*SR*** E = -1110.18848496 (1)

| | | | |
|---|---|---|---|
| C | 1.009258 | 0.821042 | 0.717529 |
| H | 1.489004 | 0.077967 | 1.366679 |
| H | 0.045528 | 1.077058 | 1.154520 |
| C | 1.388822 | 1.499096 | -1.571426 |
| H | 1.766550 | 1.204810 | -2.551911 |
| C | 2.496220 | 2.072025 | -0.685862 |
| H | 3.354141 | 1.388212 | -0.682799 |
| N | 1.861575 | 2.030349 | 0.650740 |
| C | 2.273497 | 2.655870 | 1.771215 |
| C | 1.633621 | 2.368410 | 2.989922 |
| H | 1.122872 | 1.414083 | 3.054923 |
| C | 3.429443 | 3.623346 | 1.708352 |
| H | 3.338826 | 4.293086 | 0.854423 |
| H | 3.374595 | 4.264546 | 2.588907 |
| C | 4.770253 | 2.877719 | 1.680461 |
| H | 5.591413 | 3.593697 | 1.753539 |
| H | 4.902327 | 2.332705 | 0.743207 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 0.880305 | 0.519847 | 1.924106 | H | 4.850609 | 2.174992 | 2.515417 |
| O | 1.825187 | -0.209414 | 2.366254 | C | 2.179818 | 2.876049 | 4.302413 |
| O | 1.014648 | 1.751197 | 1.863164 | H | 1.563603 | 2.504581 | 5.124221 |
| C | -2.510610 | 0.106095 | 0.432594 | H | 2.177374 | 3.970312 | 4.358048 |
| C | -5.043968 | -0.935910 | -0.130400 | H | 3.207600 | 2.542423 | 4.482980 |
| C | -2.651815 | -1.231266 | 0.039070 | C | -0.254114 | 3.405147 | 2.840085 |
| C | -3.648035 | 0.915295 | 0.524602 | H | 0.264963 | 4.291879 | 3.191421 |
| C | -4.909405 | 0.395916 | 0.251495 | C | -0.676001 | 3.452613 | 1.513033 |
| C | -3.913261 | -1.744385 | -0.238759 | H | -1.447886 | 2.855982 | 1.052740 |
| H | -1.773818 | -1.863401 | -0.073721 | N | 0.047506 | 4.230962 | 0.651137 |
| H | -3.538984 | 1.955182 | 0.820725 | O | -0.209184 | 4.186689 | -0.588109 |
| H | -5.784877 | 1.031571 | 0.334642 | O | 0.975967 | 4.925676 | 1.087997 |
| H | -4.012629 | -2.779880 | -0.547066 | C | 3.073472 | 3.388302 | -1.237067 |
| H | -6.026084 | -1.342298 | -0.349123 | O | 4.248217 | 3.421701 | -1.518458 |
| H | 3.790535 | -0.790927 | -2.254496 | O | 2.265488 | 4.397698 | -1.485735 |
| C | 1.152260 | -1.939019 | -0.430868 | H | 1.323011 | 4.311612 | -1.167470 |
| O | 0.262712 | -2.563096 | -0.963149 | H | 0.604194 | 2.251308 | -1.694922 |
| O | 1.597638 | -2.244830 | 0.781785 | C | 0.884553 | 0.325162 | -0.731752 |
| H | 1.842631 | -1.456715 | 1.364424 | H | 1.523771 | -0.548280 | -0.885409 |
| H | -1.562562 | 2.764237 | -1.406353 | H | -0.139433 | 0.038893 | -0.976436 |
| H | 3.602131 | -2.235708 | -1.244464 | C | -1.048195 | 2.678468 | 3.854670 |
| C | 3.990350 | -0.371069 | -0.135765 | C | -2.547964 | 1.359857 | 5.822944 |
| H | 5.056143 | -0.171439 | -0.258293 | C | -1.748410 | 1.503835 | 3.551472 |
| H | 3.851187 | -0.904881 | 0.806759 | C | -1.106390 | 3.175393 | 5.161413 |
| C | 1.160437 | 2.853348 | -0.831673 | C | -1.852955 | 2.523487 | 6.138125 |
| H | 1.912673 | 3.043311 | -0.067085 | C | -2.493155 | 0.851610 | 4.525903 |
| H | 0.260639 | 3.380157 | -0.505765 | H | -1.709822 | 1.094878 | 2.545262 |
| C | 1.622983 | 3.385100 | -2.194946 | H | -0.568388 | 4.087325 | 5.405097 |
| H | 1.859391 | 4.449549 | -2.130479 | H | -1.892554 | 2.926690 | 7.144636 |
| H | 2.519338 | 2.859119 | -2.537854 | H | -3.031182 | -0.056635 | 4.274954 |
| H | 0.849645 | 3.253644 | -2.955799 | H | -3.129196 | 0.848866 | 6.583267 |

**TS3-β1-*RS*** E = -1110.19118181 (1)

| | | | |
|---|---|---|---|
| C | 2.610368 | -0.703527 | -0.217401 |

**TS3-β1-*SR*** E = -1110.18722312 (1)

| | | | |
|---|---|---|---|
| C | -3.202846 | -1.562799 | -0.903748 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.354540 | -1.480247 | 0.519275 | H | -3.712612 | -1.132622 | -1.766580 |
| C | 3.258021 | -1.373592 | -1.422458 | H | -3.946894 | -1.832721 | -0.148668 |
| H | 4.064447 | -2.046736 | -1.126978 | C | -2.339822 | -2.777027 | -1.241247 |
| C | 0.901368 | -1.111689 | -1.855148 | H | -1.762101 | -2.596886 | -2.153489 |
| H | -0.023724 | -1.623613 | -1.578456 | H | -2.919405 | -3.692068 | -1.373466 |
| N | 1.342554 | -0.194795 | -0.779229 | C | -1.398552 | -2.857778 | -0.044024 |
| C | 0.633620 | 0.905481 | -0.467151 | H | -0.464934 | -3.369326 | -0.282362 |
| C | -0.714308 | 0.979800 | -0.845800 | H | -1.874422 | -3.362964 | 0.805800 |
| H | -1.068994 | 0.250035 | -1.564155 | C | -2.206761 | -0.572594 | -0.278971 |
| C | -1.487711 | 2.276908 | -0.841146 | H | -1.774511 | 0.100496 | -1.022598 |
| H | -1.617631 | 2.683809 | 0.168345 | N | -1.153594 | -1.444007 | 0.281243 |
| H | -1.003058 | 3.050743 | -1.445281 | C | -0.172822 | -0.986876 | 1.072650 |
| H | -2.486596 | 2.110524 | -1.248450 | C | 0.081779 | 0.390810 | 1.180374 |
| C | 3.560294 | 0.285954 | 0.467584 | H | -0.719740 | 1.048330 | 0.868823 |
| O | 4.373483 | 0.927377 | -0.147569 | C | 0.920915 | 0.972782 | 2.285103 |
| O | 3.487671 | 0.312371 | 1.796329 | H | 1.254850 | 1.971658 | 1.982591 |
| H | 2.655293 | -0.117527 | 2.103791 | H | 1.807616 | 0.377792 | 2.517284 |
| C | -0.849234 | -1.291116 | 1.043385 | H | 0.336494 | 1.092471 | 3.202719 |
| H | -1.178873 | -2.260557 | 0.702093 | C | -2.902785 | 0.228510 | 0.838226 |
| C | -1.519518 | -0.086818 | 0.837398 | O | -3.328938 | -0.330703 | 1.815915 |
| H | -1.253456 | 0.723175 | 1.512122 | O | -3.050678 | 1.531361 | 0.631139 |
| N | 0.356341 | -1.308925 | 1.696336 | H | -2.485403 | 1.865418 | -0.105076 |
| O | 0.841461 | -0.224638 | 2.125871 | C | 1.104201 | 2.135346 | -0.690954 |
| O | 0.972183 | -2.377768 | 1.824834 | H | 1.941993 | 2.778263 | -0.472977 |
| C | -2.931952 | -0.117339 | 0.389736 | C | 1.075046 | 0.739586 | -0.562395 |
| C | -5.615202 | -0.146335 | -0.416232 | H | 0.320539 | 0.237130 | -1.163480 |
| C | -3.853848 | 0.770045 | 0.952611 | N | -0.061035 | 2.808220 | -0.980968 |
| C | -3.371538 | -1.014146 | -0.591532 | O | -1.111876 | 2.127943 | -1.211337 |
| C | -4.702046 | -1.030590 | -0.989679 | O | -0.075560 | 4.035143 | -1.017170 |
| C | -5.187752 | 0.753349 | 0.555298 | C | 2.335071 | -0.027991 | -0.421970 |
| H | -3.520922 | 1.470424 | 1.713431 | C | 4.646404 | -1.587998 | -0.119586 |
| H | -2.660244 | -1.694977 | -1.053303 | C | 2.392953 | -1.330442 | -0.933294 |
| H | -5.028449 | -1.730370 | -1.752052 | C | 3.456026 | 0.482770 | 0.241337 |
| H | -5.892373 | 1.444811 | 1.005524 | C | 4.601350 | -0.293528 | 0.392244 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -6.653799 | -0.157943 | -0.729568 | C | 3.538055 | -2.104831 | -0.787269 |
| H | 0.709319 | -0.512943 | -2.752608 | H | 1.524058 | -1.730811 | -1.452448 |
| H | 3.668465 | -0.599504 | -2.077017 | H | 3.428776 | 1.488062 | 0.650513 |
| C | 2.063912 | -2.094784 | -2.045439 | H | 5.462593 | 0.115687 | 0.910239 |
| H | 1.863061 | -3.015931 | -1.491408 | H | 3.568242 | -3.109407 | -1.196957 |
| H | 2.208888 | -2.351744 | -3.095870 | H | 5.541823 | -2.189332 | -0.002534 |
| C | 1.256937 | 2.078922 | 0.243972 | C | 0.680022 | -1.987643 | 1.802123 |
| H | 1.926204 | 1.773525 | 1.042442 | H | 0.789711 | -2.909067 | 1.226732 |
| H | 0.456367 | 2.639224 | 0.731868 | H | 1.686223 | -1.579029 | 1.920642 |
| C | 1.986465 | 2.978456 | -0.765699 | C | 0.053279 | -2.287592 | 3.173157 |
| H | 2.805806 | 2.435349 | -1.240701 | H | -0.976400 | -2.639226 | 3.065256 |
| H | 2.409507 | 3.846024 | -0.254909 | H | 0.631019 | -3.051217 | 3.698101 |
| H | 1.304910 | 3.336047 | -1.542726 | H | 0.028949 | -1.386460 | 3.790090 |

**TS3-β2-*RS*** E = -1110.18466800 (1)

| | | | |
|---|---|---|---|
| C | 1.112157 | -0.347835 | -1.649920 |
| H | 0.249071 | -0.993991 | -1.478762 |
| C | 2.932508 | -1.533061 | -0.659186 |
| H | 3.976750 | -1.846991 | -0.688280 |
| C | 2.760512 | -0.237863 | 0.153099 |
| H | 2.649468 | -0.448865 | 1.221394 |
| N | 1.505962 | 0.322467 | -0.384777 |
| C | 0.768965 | 1.265750 | 0.225921 |
| C | -0.594688 | 1.405313 | -0.139769 |
| H | -0.848388 | 1.015874 | -1.122630 |
| C | -1.364822 | 2.657267 | 0.215600 |
| H | -2.435566 | 2.478393 | 0.094170 |
| C | -1.452475 | -0.026230 | 0.889756 |
| H | -1.428195 | 0.529884 | 1.826808 |
| C | -0.716928 | -1.232158 | 0.920127 |
| H | -0.938051 | -2.116433 | 0.342326 |
| N | 0.385834 | -1.316816 | 1.723998 |
| O | 1.072908 | -2.355596 | 1.740199 |
| O | 0.705319 | -0.308427 | 2.402951 |

**TS3-β2-*SR*** E = -1110.18856632 (1)

| | | | |
|---|---|---|---|
| C | -1.645037 | 0.861819 | -0.305032 |
| H | -0.635922 | 0.934565 | -0.703928 |
| C | -2.655141 | 0.497545 | -1.398631 |
| H | -2.958004 | 1.380127 | -1.962646 |
| C | -3.030066 | -0.999428 | 0.432518 |
| H | -2.764007 | -1.987354 | 0.034939 |
| N | -1.771107 | -0.247616 | 0.654369 |
| C | -0.830873 | -0.610107 | 1.540697 |
| C | 0.467887 | -0.052487 | 1.469481 |
| H | 0.530305 | 0.913630 | 0.975075 |
| C | 1.417426 | -0.178684 | 2.641540 |
| H | 2.358123 | 0.321035 | 2.402654 |
| H | 1.651573 | -1.223613 | 2.869088 |
| H | 1.019066 | 0.281798 | 3.551047 |
| C | -1.979352 | 2.231223 | 0.311456 |
| O | -1.898073 | 3.233161 | -0.343260 |
| O | -2.381346 | 2.252644 | 1.591242 |
| H | -2.362372 | 1.354781 | 1.951935 |
| C | 1.319176 | -1.105770 | 0.020949 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.800147 | -0.100323 | 0.250865 | H | 1.488904 | -1.966580 | 0.665577 |
| C | -5.350449 | -0.270232 | -0.901403 | C | 0.448617 | -1.363042 | -1.058116 |
| C | -2.976381 | -0.679018 | -1.010412 | H | 0.450146 | -0.849924 | -2.008003 |
| C | -3.919108 | 0.401666 | 0.920605 | N | -0.545546 | -2.288627 | -0.892901 |
| C | -5.186404 | 0.314382 | 0.350717 | O | -0.617367 | -2.896582 | 0.204000 |
| C | -4.240288 | -0.766880 | -1.581828 | O | -1.385520 | -2.478434 | -1.795814 |
| H | -2.112459 | -1.062904 | -1.548956 | C | 2.537386 | -0.293622 | -0.260538 |
| H | -3.792161 | 0.854368 | 1.900151 | C | 4.854143 | 1.196545 | -0.779708 |
| H | -6.045638 | 0.703836 | 0.886897 | C | 2.473210 | 0.887234 | -1.008340 |
| H | -4.360295 | -1.220783 | -2.560197 | C | 3.777270 | -0.709771 | 0.232024 |
| H | -6.337159 | -0.336649 | -1.347507 | C | 4.929049 | 0.027378 | -0.028820 |
| C | 3.977162 | 0.667117 | -0.053033 | C | 3.621510 | 1.625587 | -1.268554 |
| O | 5.004757 | 0.491863 | 0.536343 | H | 1.515768 | 1.235094 | -1.390137 |
| O | 3.864791 | 1.628732 | -0.995456 | H | 3.836186 | -1.623861 | 0.816494 |
| H | 2.952424 | 1.657144 | -1.315553 | H | 5.884917 | -0.313021 | 0.355819 |
| H | 2.335948 | -2.309193 | -0.172571 | H | 3.554091 | 2.539183 | -1.849967 |
| H | 0.842410 | 0.406941 | -2.396465 | H | 5.750273 | 1.774012 | -0.981067 |
| C | 2.351994 | -1.160295 | -2.023530 | H | -2.199826 | -0.240842 | -2.064525 |
| H | 3.058576 | -0.541661 | -2.587289 | H | -3.578932 | -1.120202 | 1.369989 |
| H | 2.097687 | -2.026717 | -2.635552 | C | -3.782273 | -0.158125 | -0.597966 |
| H | -1.098844 | 3.495606 | -0.434854 | H | -4.434584 | -0.777134 | -1.214437 |
| H | -1.192181 | 2.965273 | 1.250724 | H | -4.393756 | 0.604606 | -0.102872 |
| C | 1.388617 | 2.121896 | 1.302713 | C | -1.219215 | -1.585178 | 2.620173 |
| H | 0.659138 | 2.208658 | 2.111480 | H | -1.867830 | -2.361476 | 2.215284 |
| H | 2.249660 | 1.618677 | 1.744250 | H | -0.319075 | -2.091284 | 2.971304 |
| C | 1.790419 | 3.513904 | 0.791304 | C | -1.899217 | -0.840535 | 3.778536 |
| H | 2.166083 | 4.110058 | 1.625803 | H | -1.263323 | -0.042177 | 4.171967 |
| H | 2.589069 | 3.454782 | 0.048728 | H | -2.847646 | -0.391239 | 3.460674 |
| H | 0.945262 | 4.047710 | 0.352139 | H | -2.125677 | -1.526395 | 4.597430 |

**TS3-β3-*RS*** E = -1110.19608907 (1)

| | | | |
|---|---|---|---|
| C | 0.988307 | -0.698509 | -1.695938 |
| H | 0.112922 | -1.309131 | -1.459788 |
| C | 2.821676 | -1.709528 | -0.540446 |

**TS3-β3-*SR*** E = -1110.19717316 (1)

| | | | |
|---|---|---|---|
| C | -2.971378 | -0.831053 | 0.218327 |
| H | -2.763011 | -1.828834 | -0.187923 |
| C | -2.525585 | 0.774792 | -1.517010 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.869245 | -2.016664 | -0.532358 | H | -2.814734 | 1.697776 | -2.022770 |
| C | 2.630767 | -0.301557 | 0.052112 | C | -1.538438 | 1.029502 | -0.368620 |
| H | 2.563150 | -0.332515 | 1.144897 | H | -0.521865 | 1.164567 | -0.733811 |
| N | 1.359848 | 0.128527 | -0.529411 | N | -1.677868 | -0.161857 | 0.459621 |
| C | 0.662876 | 1.198540 | -0.128868 | C | -0.798960 | -0.539839 | 1.391014 |
| C | -0.694493 | 1.299753 | -0.506333 | C | 0.505392 | -0.003300 | 1.399366 |
| H | -0.983071 | 0.723883 | -1.381330 | H | 0.623275 | 0.971866 | 0.935339 |
| C | -1.460635 | 2.591562 | -0.357545 | C | 1.428549 | -0.221881 | 2.575355 |
| H | -1.261877 | 3.079643 | 0.601108 | H | 1.037802 | 0.217823 | 3.498651 |
| H | -2.534053 | 2.394747 | -0.415888 | H | 2.396428 | 0.241353 | 2.372042 |
| C | -1.544233 | 0.036102 | 0.829211 | C | 1.357775 | -1.052999 | -0.129933 |
| H | -1.490971 | 0.766097 | 1.635340 | H | 1.469364 | -1.944005 | 0.484354 |
| C | -0.789286 | -1.128858 | 1.046260 | C | 0.493060 | -1.204257 | -1.224086 |
| H | -0.993742 | -2.099339 | 0.620813 | H | 0.517734 | -0.624748 | -2.134660 |
| N | 0.325324 | -1.067824 | 1.844417 | N | -0.528825 | -2.121897 | -1.149207 |
| O | 1.022256 | -2.086101 | 2.015822 | O | -1.353442 | -2.204774 | -2.080796 |
| O | 0.639303 | 0.032955 | 2.354862 | O | -0.629502 | -2.827955 | -0.121562 |
| C | -2.896367 | -0.138696 | 0.229207 | C | 2.606478 | -0.268387 | -0.329537 |
| C | -5.463830 | -0.481682 | -0.846962 | C | 4.985850 | 1.172551 | -0.695506 |
| C | -3.098206 | -0.949806 | -0.893088 | C | 2.607811 | 0.943991 | -1.028947 |
| C | -3.999303 | 0.506857 | 0.795361 | C | 3.814303 | -0.739973 | 0.192726 |
| C | -5.274578 | 0.334583 | 0.263958 | C | 4.996178 | -0.027493 | 0.008802 |
| C | -4.370102 | -1.123577 | -1.425175 | C | 3.786175 | 1.656988 | -1.213829 |
| H | -2.246823 | -1.445224 | -1.354523 | H | 1.675981 | 1.334195 | -1.432180 |
| H | -3.852734 | 1.140881 | 1.665493 | H | 3.823603 | -1.678211 | 0.740600 |
| H | -6.120324 | 0.839222 | 0.719668 | H | 5.925473 | -0.411982 | 0.416524 |
| H | -4.509175 | -1.757356 | -2.295095 | H | 3.768839 | 2.594405 | -1.760331 |
| H | -6.456672 | -0.614920 | -1.263677 | H | 5.905650 | 1.730092 | -0.837988 |
| H | -1.216859 | 3.302395 | -1.153186 | H | 1.609811 | -1.285257 | 2.763525 |
| C | 3.767790 | 0.595854 | -0.398466 | C | -1.950582 | 2.252703 | 0.440970 |
| O | 3.757992 | 1.296752 | -1.380774 | O | -2.566292 | 2.230228 | 1.475478 |
| O | 4.832164 | 0.470714 | 0.407135 | O | -1.573722 | 3.385686 | -0.175276 |
| H | 5.536744 | 1.024790 | 0.037079 | H | -1.899924 | 4.124051 | 0.362192 |
| H | 2.241426 | -2.402037 | 0.074897 | H | -2.051583 | 0.091905 | -2.227563 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.749224 | -0.044315 | -2.539493 | H | -3.534106 | -0.921266 | 1.150190 |
| C | 2.225707 | -1.562578 | -1.940865 | C | -3.677983 | 0.063443 | -0.803176 |
| H | 2.920548 | -1.033284 | -2.598980 | H | -4.317656 | 0.789405 | -0.292567 |
| H | 1.971341 | -2.519168 | -2.399986 | H | -4.291274 | -0.523010 | -1.487981 |
| C | 1.310134 | 2.231780 | 0.758681 | C | -1.240844 | -1.560765 | 2.403618 |
| H | 0.601208 | 2.493995 | 1.548166 | H | -1.912522 | -2.284569 | 1.943061 |
| H | 2.170752 | 1.806462 | 1.277141 | H | -0.371004 | -2.125430 | 2.743704 |
| C | 1.725117 | 3.477279 | -0.037799 | C | -1.916496 | -0.843638 | 3.582392 |
| H | 0.861123 | 3.972379 | -0.486077 | H | -2.296779 | -1.568712 | 4.305454 |
| H | 2.212786 | 4.194168 | 0.627527 | H | -1.213641 | -0.183608 | 4.097286 |
| H | 2.422922 | 3.214040 | -0.835165 | H | -2.748058 | -0.222612 | 3.236781 |

**TS4-α1-*RS*** E = -1148.29990413 (1)

| | | | |
|---|---|---|---|
| C | -2.740863 | 0.482495 | -1.800631 |
| C | -2.483808 | -1.789215 | -2.515139 |
| H | -2.090321 | -2.480382 | -3.262520 |
| C | -1.496984 | -1.574836 | -1.356000 |
| H | -1.645303 | -2.283721 | -0.537966 |
| N | -1.834288 | -0.219012 | -0.871219 |
| C | -1.622717 | 0.173155 | 0.399415 |
| C | -0.587374 | -0.394161 | 1.155180 |
| H | -0.115442 | -1.289538 | 0.754495 |
| C | -2.450476 | 1.304847 | 0.972564 |
| H | -3.434713 | 1.321927 | 0.498361 |
| H | -1.962847 | 2.250526 | 0.714291 |
| C | -2.602596 | 1.188991 | 2.492196 |
| H | -3.104021 | 2.085293 | 2.868517 |
| C | -0.598193 | -0.293894 | 2.665644 |
| H | 0.422635 | -0.391095 | 3.047079 |
| C | -0.045520 | -1.797962 | -1.817783 |
| O | 0.644180 | -2.600667 | -1.229939 |
| O | 0.360568 | -1.199769 | -2.929159 |
| H | 0.117149 | -0.217160 | -3.005486 |
| C | 0.978412 | 0.888276 | 0.491146 |

**TS4-α1-*SR*** E = -1148.29101301 (1)

| | | | |
|---|---|---|---|
| C | 0.907821 | 0.841262 | 0.675732 |
| H | 1.274980 | 0.102931 | 1.397771 |
| H | -0.100045 | 1.133192 | 0.966901 |
| C | 1.451508 | 1.524393 | -1.564759 |
| H | 1.889757 | 1.264994 | -2.529647 |
| C | 2.485300 | 2.134253 | -0.618337 |
| H | 3.385982 | 1.507934 | -0.591424 |
| N | 1.798657 | 2.026090 | 0.690353 |
| C | 2.219619 | 2.586826 | 1.838900 |
| C | 1.530528 | 2.323988 | 3.040374 |
| H | 0.985973 | 1.385918 | 3.087096 |
| C | 3.437287 | 3.487076 | 1.773653 |
| H | 4.188230 | 3.004823 | 1.138802 |
| H | 3.159709 | 4.417153 | 1.270045 |
| C | 4.033326 | 3.793371 | 3.149125 |
| H | 4.718525 | 4.639479 | 3.054123 |
| H | 4.626812 | 2.938446 | 3.495986 |
| C | 2.097579 | 2.814215 | 4.354482 |
| H | 1.277683 | 2.986608 | 5.061359 |
| H | 2.721475 | 2.032060 | 4.807857 |
| C | -0.317142 | 3.376113 | 2.924133 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.537043 | 1.788223 | 0.912415 | H | 0.192468 | 4.259354 | 3.299128 |
| C | 1.025095 | 0.833680 | -0.906061 | C | -0.751043 | 3.448114 | 1.599652 |
| H | 1.665545 | 0.175488 | -1.471694 | H | -1.532457 | 2.859105 | 1.145755 |
| N | 0.146852 | 1.579242 | -1.642818 | N | -0.026678 | 4.221686 | 0.740127 |
| O | -0.547183 | 2.457719 | -1.110186 | O | -0.280789 | 4.172112 | -0.501533 |
| O | 0.031791 | 1.345718 | -2.889747 | O | 0.898856 | 4.920036 | 1.179423 |
| C | 2.094908 | 0.298515 | 1.263618 | C | 3.008025 | 3.498101 | -1.122761 |
| C | 4.218723 | -0.751640 | 2.748901 | O | 4.188459 | 3.593894 | -1.363361 |
| C | 2.590260 | 0.984768 | 2.377216 | O | 2.157857 | 4.463560 | -1.390784 |
| C | 2.665007 | -0.930716 | 0.906867 | H | 1.214130 | 4.340449 | -1.077648 |
| C | 3.721023 | -1.447583 | 1.647764 | H | 0.639928 | 2.243042 | -1.716495 |
| C | 3.651179 | 0.465816 | 3.113242 | C | 0.959571 | 0.319607 | -0.765960 |
| H | 2.144625 | 1.935366 | 2.658884 | H | 1.679166 | -0.500211 | -0.844586 |
| H | 2.266674 | -1.492836 | 0.064735 | H | -0.011618 | -0.049277 | -1.099106 |
| H | 4.154292 | -2.401834 | 1.366862 | C | -1.138730 | 2.639076 | 3.911662 |
| H | 4.031765 | 1.011379 | 3.970538 | C | -2.722764 | 1.306563 | 5.801934 |
| H | 5.042838 | -1.161204 | 3.323879 | C | -1.736565 | 1.410610 | 3.603611 |
| H | -2.373935 | 1.501379 | -1.958959 | C | -1.340398 | 3.182939 | 5.184430 |
| H | -1.153683 | -1.152937 | 3.066617 | C | -2.130182 | 2.523760 | 6.122206 |
| H | -3.247670 | 0.335017 | 2.733805 | C | -2.523020 | 0.750676 | 4.538926 |
| C | -1.246091 | 0.995608 | 3.163655 | H | -1.576393 | 0.964743 | 2.625105 |
| H | -1.354450 | 0.963353 | 4.251709 | H | -0.886866 | 4.139205 | 5.430329 |
| H | -0.600748 | 1.854104 | 2.935004 | H | -2.282124 | 2.963191 | 7.102472 |
| H | -3.414838 | -2.203109 | -2.116323 | H | -2.978795 | -0.200900 | 4.285692 |
| H | -3.750794 | 0.520412 | -1.376058 | H | -3.336009 | 0.789765 | 6.532607 |
| C | -2.718441 | -0.378613 | -3.060099 | C | 2.935756 | 4.076315 | 4.168532 |
| H | -1.898186 | -0.067242 | -3.709354 | H | 3.363048 | 4.388635 | 5.125708 |
| H | -3.649349 | -0.295230 | -3.623414 | H | 2.307006 | 4.899175 | 3.803271 |

**TS4-β1-*RS*** E = -1148.29349361 (1)

| | | | |
|---|---|---|---|
| C | 2.743369 | -0.770489 | -0.194774 |
| C | 1.029544 | -1.475336 | -1.724307 |
| N | 1.441575 | -0.398815 | -0.790658 |
| C | 0.709085 | 0.719012 | -0.650336 |

**TS4-β1-*SR*** E = -1148.28954041 (1)

| | | | |
|---|---|---|---|
| C | 1.380011 | 2.996655 | -0.600349 |
| H | 0.342271 | 3.176080 | -0.315091 |
| H | 1.922948 | 3.950517 | -0.588720 |
| C | 2.915016 | 1.668674 | -1.839940 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.653311 | 0.687076 | -0.996771 | H | 3.075109 | 0.840969 | -2.531597 |
| H | -0.993664 | -0.152079 | -1.594060 | C | 3.010865 | 1.208237 | -0.373563 |
| C | -1.437406 | 1.961426 | -1.218662 | H | 2.748177 | 0.156452 | -0.251261 |
| H | -1.350754 | 2.248737 | -2.275911 | N | 2.021669 | 2.055646 | 0.326875 |
| C | -1.389539 | -0.165719 | 0.817646 | C | 1.860613 | 2.064612 | 1.652121 |
| H | -1.129839 | 0.703957 | 1.415176 | C | 2.444587 | 1.066276 | 2.463422 |
| C | -0.687758 | -1.333855 | 1.126898 | H | 3.280765 | 0.548053 | 2.011542 |
| H | -1.003237 | -2.336297 | 0.880432 | C | 0.963496 | 3.127526 | 2.232883 |
| N | 0.514820 | -1.273069 | 1.775550 | H | 1.401125 | 4.096241 | 1.952946 |
| O | 0.969073 | -0.144327 | 2.124685 | H | -0.021703 | 3.081331 | 1.753917 |
| O | 1.158002 | -2.311680 | 1.987723 | C | 0.809252 | 3.036655 | 3.752179 |
| C | -2.817848 | -0.282266 | 0.438812 | H | 0.066857 | 2.270725 | 4.003754 |
| C | -5.533957 | -0.480079 | -0.220772 | H | 0.424748 | 3.990808 | 4.123134 |
| C | -3.745030 | 0.625356 | 0.959756 | C | 2.592980 | 1.294835 | 3.958308 |
| C | -3.269341 | -1.284429 | -0.428217 | H | 2.014267 | 0.540095 | 4.507336 |
| C | -4.616045 | -1.384368 | -0.753482 | H | 3.638864 | 1.132510 | 4.232687 |
| C | -5.095179 | 0.525006 | 0.635715 | C | 1.272181 | -0.522699 | 2.174530 |
| H | -3.401729 | 1.409692 | 1.629091 | H | 1.282651 | -0.435592 | 1.090239 |
| H | -2.556344 | -1.984335 | -0.857772 | C | 2.004166 | -1.613954 | 2.684020 |
| H | -4.951626 | -2.165977 | -1.427218 | H | 1.871314 | -2.075430 | 3.648924 |
| H | -5.803154 | 1.233751 | 1.052533 | N | 3.109629 | -2.053745 | 2.006134 |
| H | -6.585285 | -0.557488 | -0.477125 | O | 3.828881 | -2.930689 | 2.478581 |
| H | 0.805590 | -1.013224 | -2.692126 | O | 3.369312 | -1.530230 | 0.869493 |
| C | 1.306384 | 1.983522 | -0.067404 | C | 4.429031 | 1.486183 | 0.167825 |
| H | 2.351699 | 2.060351 | -0.368690 | O | 4.840740 | 2.617708 | 0.222485 |
| H | 1.282472 | 1.916475 | 1.024329 | O | 5.157973 | 0.434554 | 0.507557 |
| H | 2.528705 | -1.451954 | 0.643671 | H | 4.622955 | -0.397663 | 0.579580 |
| H | -2.500905 | 1.770033 | -1.045521 | H | 3.676695 | 2.432646 | -2.018330 |
| C | -0.935650 | 3.110717 | -0.351019 | C | 1.523552 | 2.294061 | -1.945066 |
| H | -1.445833 | 4.038819 | -0.624920 | H | 0.755882 | 1.519586 | -2.040448 |
| H | -1.167222 | 2.918611 | 0.705160 | H | 1.427978 | 2.983008 | -2.785787 |
| C | 0.571498 | 3.246595 | -0.527217 | C | -0.038150 | -0.170354 | 2.774656 |
| H | 0.791100 | 3.434770 | -1.585476 | C | -2.504153 | 0.635793 | 3.847515 |
| H | 0.962937 | 4.098668 | 0.035134 | C | -0.972550 | 0.518896 | 1.990753 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.402427 | -1.570285 | -1.308766 | C | -0.372883 | -0.473000 | 4.099410 |
| H | 4.243906 | -2.158791 | -0.940004 | C | -1.595024 | -0.069883 | 4.630806 |
| H | 0.130309 | -1.981471 | -1.366458 | C | -2.192526 | 0.923278 | 2.519456 |
| C | 3.648473 | 0.343249 | 0.349055 | H | -0.726692 | 0.737664 | 0.952958 |
| O | 4.498718 | 0.861884 | -0.330449 | H | 0.321523 | -1.026624 | 4.722766 |
| O | 3.476876 | 0.635004 | 1.630414 | H | -1.837366 | -0.310551 | 5.660728 |
| H | 2.669779 | 0.187812 | 1.987100 | H | -2.904004 | 1.455107 | 1.895746 |
| H | 3.767536 | -0.879142 | -2.073421 | H | -3.455471 | 0.949224 | 4.264433 |
| C | 2.232909 | -2.424385 | -1.796023 | C | 2.146048 | 2.689431 | 4.399423 |
| H | 2.081528 | -3.261942 | -1.109449 | H | 2.897759 | 3.431211 | 4.101548 |
| H | 2.371918 | -2.824778 | -2.801401 | H | 2.068596 | 2.728615 | 5.489523 |

**TS4-β2-*RS*** E = -1148.28534195 (1)

| | | | |
|---|---|---|---|
| C | 0.964353 | -1.447414 | -1.392983 |
| C | 2.816411 | -2.166102 | -0.068221 |
| H | 3.856003 | -2.488656 | 0.000164 |
| C | 2.685640 | -0.649971 | 0.151975 |
| H | 2.602197 | -0.408069 | 1.217171 |
| N | 1.417526 | -0.328499 | -0.528513 |
| C | 0.743954 | 0.813584 | -0.338457 |
| C | -0.636586 | 0.871673 | -0.684658 |
| H | -0.929306 | 0.147871 | -1.440945 |
| C | 1.481069 | 2.003175 | 0.226060 |
| H | 2.148297 | 2.375995 | -0.566356 |
| H | 2.107322 | 1.698818 | 1.065426 |
| C | 0.517887 | 3.112081 | 0.633142 |
| H | 1.090737 | 3.994685 | 0.928823 |
| C | -1.316519 | 2.231588 | -0.847981 |
| H | -1.715350 | 2.314745 | -1.863281 |
| C | 3.903140 | 0.073121 | -0.431109 |
| O | 4.956850 | 0.090756 | 0.137588 |
| O | 3.756269 | 0.631644 | -1.651575 |
| H | 2.835936 | 0.545960 | -1.935459 |
| C | -1.525642 | 0.000268 | 0.771853 |

**TS4-β2-*SR*** E = -1148.28787139 (1)

| | | | |
|---|---|---|---|
| C | -3.046222 | 0.313222 | 0.655139 |
| H | -3.704401 | 0.989354 | 0.104000 |
| C | -2.425322 | -1.991398 | 0.894303 |
| H | -2.643062 | -3.040797 | 0.692832 |
| C | -1.527726 | -1.392436 | -0.195578 |
| H | -0.480187 | -1.618500 | -0.019275 |
| N | -1.797013 | 0.052585 | -0.100904 |
| C | -0.978184 | 1.020104 | -0.538814 |
| C | 0.367083 | 0.712394 | -0.881009 |
| H | 0.525876 | -0.297537 | -1.253639 |
| C | -1.548131 | 2.421972 | -0.621709 |
| H | -1.648980 | 2.811388 | 0.394323 |
| H | -2.561097 | 2.352020 | -1.035933 |
| C | -0.709759 | 3.368383 | -1.484604 |
| H | -0.902573 | 3.172896 | -2.546659 |
| H | -1.024485 | 4.396552 | -1.287595 |
| C | 0.778039 | 3.180065 | -1.212844 |
| H | 1.368826 | 3.910823 | -1.772315 |
| H | 0.976245 | 3.347894 | -0.146323 |
| C | 1.183533 | 1.763853 | -1.613263 |
| H | 1.052249 | 1.644687 | -2.696348 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.502097 | 0.869975 | 1.427472 | H | 2.245820 | 1.588817 | -1.415217 |
| C | -0.827543 | -1.118328 | 1.294878 | C | -1.881046 | -1.976352 | -1.572593 |
| H | -1.073673 | -2.154213 | 1.118781 | O | -1.604109 | -3.110806 | -1.846347 |
| N | 0.287011 | -0.893614 | 2.045642 | O | -2.539202 | -1.180864 | -2.430801 |
| O | 0.630630 | 0.302122 | 2.248371 | H | -2.637107 | -0.300897 | -2.041244 |
| O | 0.970154 | -1.845601 | 2.472559 | H | -2.765241 | 0.782461 | 1.607350 |
| C | -2.878456 | -0.287579 | 0.202378 | H | -1.921625 | -1.888549 | 1.859256 |
| C | -5.432146 | -0.837268 | -0.818090 | C | -3.651245 | -1.075905 | 0.856360 |
| C | -3.989411 | 0.442404 | 0.631258 | H | -4.300713 | -1.339714 | 0.014239 |
| C | -3.065535 | -1.294019 | -0.751269 | H | -4.238785 | -1.121677 | 1.773603 |
| C | -4.330374 | -1.570140 | -1.256071 | C | 1.287813 | 0.450964 | 0.816648 |
| C | -5.258349 | 0.168712 | 0.126798 | H | 1.423793 | 1.515844 | 0.997407 |
| H | -3.858010 | 1.219881 | 1.378881 | C | 0.501225 | -0.194398 | 1.799355 |
| H | -2.208878 | -1.866085 | -1.101941 | H | 0.590830 | -1.229063 | 2.094796 |
| H | -4.458035 | -2.355811 | -1.993707 | N | -0.506597 | 0.503935 | 2.400404 |
| H | -6.110999 | 0.742462 | 0.475032 | O | -0.672089 | 1.705788 | 2.074826 |
| H | -6.419809 | -1.050066 | -1.213475 | O | -1.272806 | -0.060600 | 3.208604 |
| H | 0.665577 | -1.056644 | -2.371471 | C | 2.537705 | -0.259050 | 0.407745 |
| H | 2.229451 | -2.662627 | 0.709109 | C | 4.915431 | -1.563082 | -0.308053 |
| H | 0.109917 | -1.951045 | -0.938477 | C | 3.755956 | 0.425965 | 0.410031 |
| C | 2.187174 | -2.363806 | -1.447763 | C | 2.528132 | -1.606998 | 0.033208 |
| H | 2.874558 | -2.035517 | -2.235147 | C | 3.705937 | -2.254990 | -0.320213 |
| H | 1.907887 | -3.398448 | -1.651214 | C | 4.937530 | -0.221044 | 0.058291 |
| H | -0.053156 | 2.782543 | 1.508609 | H | 3.774926 | 1.472564 | 0.702348 |
| H | -2.189966 | 2.269741 | -0.185728 | H | 1.591703 | -2.160519 | 0.014174 |
| C | -0.409310 | 3.427186 | -0.537801 | H | 3.678884 | -3.300474 | -0.609110 |
| H | -1.023764 | 4.307329 | -0.329339 | H | 5.874904 | 0.325435 | 0.071189 |
| H | 0.204525 | 3.670790 | -1.414423 | H | 5.834419 | -2.068316 | -0.586037 |

**TS4-β3-*RS*** E = -1148.29670675 (1)

| | | | |
|---|---|---|---|
| C | -0.231371 | 0.567868 | -2.173273 |
| C | 0.241668 | -1.540103 | -3.199611 |
| H | 0.668199 | -2.104216 | -4.030769 |
| C | 1.249836 | -1.357678 | -2.051397 |

**TS4-β3-*SR*** E = -1148.29742699 (1)

| | | | |
|---|---|---|---|
| C | -0.698669 | 1.769316 | -2.548733 |
| C | -0.529911 | -0.528849 | -3.236570 |
| H | -0.146362 | -1.256880 | -3.953581 |
| C | 0.433573 | -0.315792 | -2.059530 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.259193 | -2.228734 | -1.385431 | H | 0.344167 | -1.106305 | -1.317654 |
| N | 0.731030 | -0.187959 | -1.344428 | N | 0.031115 | 0.984874 | -1.534071 |
| C | 1.164981 | 0.211497 | -0.148305 | C | 0.347061 | 1.450693 | -0.328389 |
| C | 0.372066 | 1.116856 | 0.602866 | C | 0.816055 | 0.570305 | 0.679452 |
| H | -0.296292 | 1.733920 | 0.009387 | H | 1.312995 | -0.323537 | 0.313992 |
| C | 2.463310 | -0.338754 | 0.384989 | C | 0.127019 | 2.920022 | -0.070166 |
| H | 3.262633 | 0.168697 | -0.174156 | H | -0.844417 | 3.222931 | -0.461264 |
| H | 2.537714 | -1.407870 | 0.180760 | H | 0.902869 | 3.453628 | -0.640873 |
| C | 2.622303 | -0.057875 | 1.874799 | C | 0.248154 | 3.266457 | 1.409388 |
| H | 3.620355 | -0.368238 | 2.196134 | H | 0.240404 | 4.353506 | 1.527194 |
| C | 0.960080 | 1.830283 | 1.815516 | C | 1.433708 | 1.130362 | 1.956121 |
| H | 0.893660 | 2.912212 | 1.666010 | H | 2.423665 | 0.688070 | 2.101675 |
| C | 2.632718 | -1.084712 | -2.613948 | C | 1.874968 | -0.238328 | -2.544840 |
| O | 3.134757 | 0.004629 | -2.740261 | O | 2.489087 | 0.775745 | -2.752407 |
| O | 3.223906 | -2.221252 | -3.010589 | O | 2.373266 | -1.468154 | -2.758107 |
| H | 4.079677 | -1.977548 | -3.395932 | H | 3.271645 | -1.355076 | -3.105410 |
| C | -1.060653 | -0.050644 | 1.297538 | C | -0.854502 | -0.364719 | 1.236441 |
| H | -0.451345 | -0.437603 | 2.112237 | H | -1.189452 | 0.463726 | 1.857485 |
| C | -1.485934 | -1.035687 | 0.380600 | C | -1.711671 | -0.662086 | 0.158267 |
| H | -2.386460 | -0.998699 | -0.212927 | H | -1.816242 | -1.626160 | -0.316434 |
| N | -0.685661 | -2.123191 | 0.164042 | N | -2.442935 | 0.349889 | -0.408057 |
| O | 0.392429 | -2.208920 | 0.803819 | O | -2.362806 | 1.498131 | 0.088259 |
| O | -1.006270 | -2.980752 | -0.683145 | O | -3.134887 | 0.127304 | -1.422589 |
| C | -2.084282 | 0.949225 | 1.721891 | C | -0.301835 | -1.520310 | 2.000806 |
| C | -4.031002 | 2.791557 | 2.551183 | C | 0.702015 | -3.689970 | 3.471477 |
| C | -2.291205 | 1.206262 | 3.079590 | C | -0.364485 | -1.527672 | 3.396875 |
| C | -2.864289 | 1.636221 | 0.784836 | C | 0.278096 | -2.617424 | 1.353187 |
| C | -3.831208 | 2.546368 | 1.193537 | C | 0.772848 | -3.693652 | 2.079382 |
| C | -3.258599 | 2.119088 | 3.492434 | C | 0.131387 | -2.604372 | 4.127636 |
| H | -1.698266 | 0.672256 | 3.817072 | H | -0.821856 | -0.687091 | 3.911411 |
| H | -2.707159 | 1.456208 | -0.276494 | H | 0.344037 | -2.630416 | 0.267308 |
| H | -4.428112 | 3.068941 | 0.452975 | H | 1.217845 | -4.535824 | 1.559341 |
| H | -3.408321 | 2.302196 | 4.551538 | H | 0.069246 | -2.593486 | 5.210986 |
| H | -4.783611 | 3.504599 | 2.871136 | H | 1.091074 | -4.528755 | 4.039166 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.054946 | 1.623530 | -2.183978 | H | -0.209558 | 2.733108 | -2.706129 |
| H | -0.614484 | -2.086243 | -2.794954 | H | 0.836347 | 0.805987 | 2.818684 |
| H | -1.238427 | 0.474065 | -1.760878 | H | -0.629010 | 2.876070 | 1.939704 |
| C | -0.124643 | -0.096541 | -3.546642 | C | 1.526995 | 2.657536 | 1.976259 |
| H | 0.677020 | 0.374235 | -4.123338 | H | 1.709614 | 3.001892 | 2.998311 |
| H | -1.053776 | -0.014344 | -4.112684 | H | 2.378206 | 2.989779 | 1.368452 |
| H | 1.896752 | -0.661628 | 2.432247 | H | -1.488162 | -0.868720 | -2.833927 |
| H | 0.333397 | 1.616740 | 2.691050 | H | -1.720002 | 1.924704 | -2.176200 |
| C | 2.405284 | 1.431191 | 2.132092 | C | -0.676155 | 0.887594 | -3.799189 |
| H | 2.639166 | 1.691400 | 3.168414 | H | 0.183895 | 1.141705 | -4.425748 |
| H | 3.096963 | 1.999345 | 1.497465 | H | -1.586325 | 1.008266 | -4.387378 |

**β3-*RS*-H** E = -843.089866905 (1)

| | | | |
|---|---|---|---|
| C | 1.079386 | -0.646801 | -1.665707 |
| H | 0.227934 | -1.281395 | -1.408079 |
| C | 2.970266 | -1.603456 | -0.541458 |
| H | 4.024479 | -1.883160 | -0.571186 |
| C | 2.753328 | -0.218865 | 0.064211 |
| H | 2.667371 | -0.233359 | 1.155067 |
| N | 1.456191 | 0.183093 | -0.507779 |
| C | 0.758018 | 1.212260 | -0.064475 |
| C | -0.596092 | 1.415172 | -0.379964 |
| H | -0.939379 | 0.963946 | -1.309521 |
| C | -1.220148 | 2.746929 | -0.040238 |
| H | -0.848615 | 3.108087 | 0.924101 |
| H | -2.307979 | 2.654719 | 0.027621 |
| C | -1.466320 | 0.119316 | 0.864050 |
| H | -1.447623 | 0.828989 | 1.689170 |
| C | -0.698432 | -1.039893 | 1.087612 |
| H | -0.882329 | -2.013623 | 0.660181 |
| N | 0.417838 | -0.948993 | 1.877922 |
| O | 1.143586 | -1.947576 | 2.051730 |
| O | 0.706672 | 0.167137 | 2.375991 |
| C | -2.801533 | -0.055806 | 0.226352 |

**β3-*SR*-H** E = -843.091397276 (1)

| | | | |
|---|---|---|---|
| C | -3.030450 | -0.947347 | 0.408238 |
| H | -2.755754 | -1.968906 | 0.119587 |
| C | -2.633241 | 0.446340 | -1.509044 |
| H | -2.970462 | 1.269111 | -2.141783 |
| C | -1.684049 | 0.911121 | -0.407413 |
| H | -0.654272 | 1.030927 | -0.740686 |
| N | -1.786671 | -0.172378 | 0.579901 |
| C | -0.896548 | -0.456716 | 1.512144 |
| C | 0.408145 | 0.059518 | 1.546180 |
| H | 0.558028 | 1.023787 | 1.065261 |
| C | 1.230907 | -0.171099 | 2.790406 |
| H | 0.993707 | 0.551119 | 3.577471 |
| H | 2.297881 | -0.076746 | 2.569591 |
| C | 1.302228 | -1.072092 | 0.129019 |
| H | 1.468024 | -1.885966 | 0.831703 |
| C | 0.439985 | -1.392478 | -0.933449 |
| H | 0.441697 | -0.933898 | -1.910714 |
| N | -0.544465 | -2.326322 | -0.729978 |
| O | -1.364188 | -2.573745 | -1.638468 |
| O | -0.625517 | -2.877650 | 0.392742 |
| C | 2.509911 | -0.257026 | -0.177167 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -5.335412 | -0.387272 | -0.931638 | C | 4.814840 | 1.240119 | -0.745525 |
| C | -2.970697 | -0.861672 | -0.905431 | C | 2.447163 | 0.863876 | -1.013491 |
| C | -3.920393 | 0.589577 | 0.760389 | C | 3.745262 | -0.609124 | 0.374521 |
| C | -5.179019 | 0.423475 | 0.187904 | C | 4.890002 | 0.131563 | 0.091392 |
| C | -4.225489 | -1.030300 | -1.477583 | C | 3.587900 | 1.604030 | -1.298337 |
| H | -2.106372 | -1.356547 | -1.342477 | H | 1.493786 | 1.157951 | -1.446150 |
| H | -3.801061 | 1.214715 | 1.641085 | H | 3.807334 | -1.480992 | 1.020021 |
| H | -6.037519 | 0.927575 | 0.619810 | H | 5.841046 | -0.160922 | 0.524523 |
| H | -4.339003 | -1.660831 | -2.353605 | H | 3.520700 | 2.468807 | -1.950620 |
| H | -6.315020 | -0.516458 | -1.379829 | H | 5.705178 | 1.819696 | -0.965897 |
| H | 1.237543 | 1.809859 | 0.704386 | H | -1.178242 | -1.259820 | 2.187449 |
| H | -1.000033 | 3.507465 | -0.795162 | H | 1.053845 | -1.175817 | 3.187518 |
| H | 2.424599 | -2.330553 | 0.066792 | H | -2.132207 | -0.309759 | -2.120912 |
| H | 0.795206 | -0.000988 | -2.502929 | H | -3.587574 | -0.972995 | 1.348582 |
| C | 2.340698 | -1.473083 | -1.932135 | C | -3.767003 | -0.215563 | -0.716352 |
| H | 3.009219 | -0.923370 | -2.602718 | H | -4.437524 | 0.546467 | -0.305568 |
| H | 2.108673 | -2.433620 | -2.394991 | H | -4.355626 | -0.905387 | -1.322013 |
| H | 3.529049 | 0.492414 | -0.244247 | H | -2.021453 | 1.850427 | 0.053146 |

**β3-*RS*-Nitro** E = -1047.51726865 (1)

| | | | |
|---|---|---|---|
| C | 1.102192 | -0.637326 | -1.667837 |
| H | 0.240258 | -1.271121 | -1.447363 |
| C | 2.981496 | -1.588560 | -0.508804 |
| H | 4.044788 | -1.827068 | -0.493354 |
| C | 2.707525 | -0.214061 | 0.088490 |
| H | 2.689820 | -0.177084 | 1.182219 |
| N | 1.443548 | 0.167231 | -0.476624 |
| C | 0.748905 | 1.205598 | -0.026447 |
| C | -0.612678 | 1.384070 | -0.339060 |
| H | -0.929427 | 0.940213 | -1.282249 |
| C | -1.232341 | 2.728236 | -0.030730 |
| H | -0.893302 | 3.089546 | 0.945118 |
| H | -2.322321 | 2.649317 | -0.006795 |
| C | -1.473954 | 0.137584 | 0.846686 |

**β3-*SR*-Nitro** E = -1047.51907024 (1)

| | | | |
|---|---|---|---|
| C | -3.062887 | -0.939960 | 0.438699 |
| H | -2.801199 | -1.978646 | 0.208254 |
| C | -2.626188 | 0.415294 | -1.509111 |
| H | -2.925541 | 1.260630 | -2.130143 |
| C | -1.671470 | 0.840505 | -0.398221 |
| H | -0.651852 | 1.046011 | -0.708922 |
| N | -1.795545 | -0.191887 | 0.585475 |
| C | -0.898007 | -0.479512 | 1.519704 |
| C | 0.417795 | 0.018623 | 1.525784 |
| H | 0.555743 | 0.996249 | 1.065860 |
| C | 1.234606 | -0.199739 | 2.779354 |
| H | 0.966535 | 0.513058 | 3.563655 |
| H | 2.299636 | -0.076241 | 2.567145 |
| C | 1.295979 | -1.045042 | 0.148143 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.469516 | 0.824416 | 1.692362 | H | 1.475495 | -1.883018 | 0.819787 |
| C | -0.719366 | -1.040969 | 1.078790 | C | 0.438175 | -1.358631 | -0.931465 |
| H | -0.924968 | -2.016175 | 0.664796 | H | 0.469864 | -0.915717 | -1.915674 |
| N | 0.402629 | -0.947806 | 1.847294 | N | -0.554279 | -2.278450 | -0.727086 |
| O | 1.142166 | -1.939473 | 2.022222 | O | -1.382739 | -2.525288 | -1.629058 |
| O | 0.701503 | 0.182928 | 2.319671 | O | -0.639181 | -2.812697 | 0.406841 |
| C | -2.816420 | -0.044206 | 0.217319 | C | 2.511780 | -0.238056 | -0.164367 |
| C | -5.353686 | -0.389053 | -0.923658 | C | 4.822935 | 1.239643 | -0.744572 |
| C | -2.984267 | -0.837108 | -0.923006 | C | 2.445212 | 0.905574 | -0.967821 |
| C | -3.936623 | 0.581539 | 0.770105 | C | 3.752424 | -0.623819 | 0.350324 |
| C | -5.197878 | 0.408147 | 0.205775 | C | 4.901216 | 0.107431 | 0.060031 |
| C | -4.241658 | -1.012136 | -1.487851 | C | 3.589942 | 1.637623 | -1.258486 |
| H | -2.118466 | -1.318859 | -1.372293 | H | 1.488304 | 1.228057 | -1.372779 |
| H | -3.816842 | 1.197512 | 1.657169 | H | 3.815398 | -1.512495 | 0.972411 |
| H | -6.058523 | 0.896437 | 0.651091 | H | 5.857363 | -0.209913 | 0.463118 |
| H | -4.355551 | -1.632173 | -2.371137 | H | 3.520148 | 2.521801 | -1.883486 |
| H | -6.335324 | -0.523275 | -1.365692 | H | 5.716482 | 1.812368 | -0.969328 |
| H | 1.243436 | 1.834510 | 0.704808 | H | -1.200710 | -1.248103 | 2.223271 |
| H | -0.966983 | 3.475796 | -0.782646 | H | 1.078115 | -1.211354 | 3.166652 |
| H | 2.435258 | -2.306823 | 0.109025 | H | -2.108118 | -0.334359 | -2.114301 |
| H | 0.857605 | 0.032090 | -2.497231 | H | -3.625961 | -0.887371 | 1.372695 |
| C | 2.372128 | -1.460888 | -1.909625 | C | -3.771312 | -0.245439 | -0.729127 |
| H | 3.048803 | -0.912642 | -2.571786 | H | -4.469460 | 0.509725 | -0.359763 |
| H | 2.151660 | -2.425781 | -2.367158 | H | -4.317333 | -0.961723 | -1.342922 |
| N | 3.805831 | 0.755777 | -0.357249 | N | -2.168285 | 2.171836 | 0.187145 |
| O | 3.517729 | 1.647856 | -1.129666 | O | -2.888266 | 2.137827 | 1.162838 |
| O | 4.905918 | 0.532153 | 0.100116 | O | -1.822979 | 3.163758 | -0.421538 |

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**_E_-enamine (E2)** E = -517.6603555 (0)

| | | | |
|---|---|---|---|
| C | -0.054455 | 0.991307 | -1.972836 |
| C | -0.150832 | -0.078330 | -0.865308 |
| H | -1.071865 | -0.666108 | -0.961465 |
| C | -0.130817 | 2.118836 | 0.116255 |
| N | -0.124326 | 0.677016 | 0.387478 |

**iminium-1** E = -518.051614 (0)

| | | | |
|---|---|---|---|
| C | 0.637368 | 0.129653 | 0.696369 |
| H | 0.144592 | 0.428719 | 1.625420 |
| C | 1.964038 | -0.608530 | 0.928833 |
| H | 2.791135 | 0.093292 | 1.031934 |
| C | 0.639022 | -2.025314 | -0.463221 |

| | | | |
|---|---|---|---|
| C | -0.840467 | 0.194373 | 1.490762 |
| C | -1.239503 | -1.066103 | 1.685795 |
| H | -1.029669 | -1.825791 | 0.935720 |
| C | -1.956981 | -1.512138 | 2.924961 |
| H | -2.111598 | -0.676606 | 3.612997 |
| H | -2.937398 | -1.937757 | 2.687648 |
| H | -1.020649 | 0.949661 | 2.254242 |
| H | -1.392592 | -2.285780 | 3.455847 |
| H | -1.059789 | 1.235649 | -2.327226 |
| H | 0.403141 | 2.656387 | 0.905065 |
| H | -1.157565 | 2.511555 | 0.062505 |
| C | 0.548326 | 2.198694 | -1.246845 |
| H | 1.629815 | 2.072901 | -1.129859 |
| H | 0.362758 | 3.144986 | -1.757394 |
| H | 0.529674 | 0.636544 | -2.823047 |
| C | 1.015873 | -1.072956 | -0.955977 |
| O | 1.123362 | -1.843005 | -1.873060 |
| O | 1.905926 | -0.993426 | 0.036313 |
| H | 1.585774 | -0.292052 | 0.635289 |
| H | 0.362312 | -2.305803 | -1.479635 |
| N | -0.190438 | -0.858734 | -0.032993 |
| C | -1.421396 | -0.700556 | -0.356426 |
| H | -1.855740 | -1.503036 | -0.955603 |
| C | -2.300760 | 0.434334 | 0.013604 |
| H | -2.413477 | 1.027749 | -0.904226 |
| H | -1.827021 | 1.085197 | 0.751313 |
| C | -3.671346 | -0.065347 | 0.493005 |
| H | -4.157797 | -0.678735 | -0.269090 |
| H | -4.316015 | 0.790065 | 0.695645 |
| H | -3.585533 | -0.651081 | 1.410158 |
| H | 1.896460 | -1.200621 | 1.845069 |
| H | 0.423227 | -2.850413 | 0.221312 |
| C | 2.067752 | -1.517407 | -0.300030 |
| H | 2.772955 | -2.337152 | -0.163987 |
| H | 2.369451 | -0.946097 | -1.182833 |
| C | 0.790894 | 1.367034 | -0.198225 |
| O | 0.206119 | 1.522869 | -1.236596 |
| O | 1.641313 | 2.223140 | 0.353773 |
| H | 1.715636 | 3.007777 | -0.215394 |

**Z-enamine (Z1)** E = -517.637769662 (0)

| | | | |
|---|---|---|---|
| C | -0.723095 | 1.192459 | -1.705129 |
| H | -0.674585 | 1.708797 | -2.666043 |
| H | -1.756339 | 0.863857 | -1.544622 |
| C | 0.225374 | -0.003544 | -1.642194 |
| H | 1.190343 | 0.228338 | -2.114389 |
| H | -0.181903 | -0.894653 | -2.125889 |
| C | 0.030771 | 0.986733 | 0.543780 |
| H | 0.819311 | 1.302287 | 1.236310 |
| N | 0.422614 | -0.225231 | -0.191175 |
| C | 1.616500 | -0.866755 | 0.210123 |
| H | 2.242599 | -0.295867 | 0.895502 |
| C | 2.000142 | -2.077538 | -0.200010 |

**Z-enamine (Z2)** E = -517.639437993 (0)

| | | | |
|---|---|---|---|
| C | -0.776163 | 0.815142 | -2.187539 |
| H | -0.762059 | 1.190509 | -3.212669 |
| H | -1.821543 | 0.690366 | -1.882991 |
| C | -0.016789 | -0.502489 | -2.042916 |
| H | 0.898368 | -0.482537 | -2.653171 |
| H | -0.602298 | -1.376821 | -2.341370 |
| C | 0.166857 | 0.765836 | -0.005998 |
| H | 1.039243 | 1.029501 | 0.598302 |
| N | 0.333989 | -0.571868 | -0.609669 |
| C | 1.501698 | -1.308693 | -0.306450 |
| H | 2.022298 | -1.687895 | -1.185131 |
| C | 1.991849 | -1.566269 | 0.908899 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.970140 | -2.429173 | 0.138518 | H | 2.931207 | -2.111072 | 0.939149 |
| C | -0.253259 | 2.048272 | -0.526803 | C | -0.041191 | 1.716831 | -1.193049 |
| H | 0.674182 | 2.569017 | -0.785983 | H | 0.930620 | 2.015562 | -1.599507 |
| H | -0.983120 | 2.780981 | -0.179209 | H | -0.592890 | 2.611286 | -0.899343 |
| C | 1.184995 | -2.995162 | -1.064537 | C | 1.373386 | -1.198967 | 2.227458 |
| H | 1.409047 | -2.872599 | -2.131470 | H | 1.517233 | -2.007572 | 2.950149 |
| H | 0.114128 | -2.809941 | -0.927906 | H | 0.297895 | -1.025239 | 2.141019 |
| H | 1.382053 | -4.040168 | -0.811201 | H | 1.825214 | -0.299675 | 2.663401 |
| C | -1.227188 | 0.741134 | 1.396838 | C | -1.069786 | 0.823725 | 0.906301 |
| O | -1.750234 | 1.621787 | 2.027195 | O | -1.396107 | 1.829333 | 1.478579 |
| O | -1.688314 | -0.510226 | 1.364643 | O | -1.766789 | -0.316107 | 0.979156 |
| H | -1.084021 | -0.998377 | 0.762938 | H | -1.268958 | -0.962460 | 0.429820 |

**TS1-Z1-*RS*** E = -1031.58834894 (1)

| | | | |
|---|---|---|---|
| C | -3.693296 | -0.628257 | -0.131116 |
| H | -4.657794 | -1.113312 | -0.289055 |
| H | -3.431296 | -0.703188 | 0.926123 |
| C | -2.592668 | -1.282399 | -0.958044 |
| H | -2.941170 | -1.581186 | -1.954314 |
| H | -2.145678 | -2.129828 | -0.445510 |
| C | -2.260662 | 1.131461 | -1.065091 |
| H | -2.240896 | 1.574773 | -2.064901 |
| N | -1.603440 | -0.202715 | -1.123459 |
| C | -0.331817 | -0.326730 | -1.456493 |
| H | 0.146689 | 0.627859 | -1.679451 |
| C | 0.526183 | -1.423163 | -1.321492 |
| H | 1.477645 | -1.233277 | -1.809817 |
| C | -3.694939 | 0.836790 | -0.598427 |
| H | -4.379191 | 0.973487 | -1.439258 |
| H | -3.993079 | 1.524431 | 0.194608 |
| C | 0.161388 | -2.889852 | -1.225293 |
| H | 1.081822 | -3.479234 | -1.234530 |
| H | -0.439750 | -3.215530 | -2.080237 |
| H | -0.371023 | -3.124773 | -0.303433 |

**TS1-Z2-*RS*** E = -1031.57832398 (1)

| | | | |
|---|---|---|---|
| C | -2.989418 | -1.611152 | 1.541735 |
| H | -3.187879 | -2.368812 | 2.301387 |
| H | -3.031031 | -0.622613 | 2.010546 |
| C | -1.626740 | -1.796839 | 0.876752 |
| H | -1.410192 | -2.855514 | 0.692901 |
| H | -0.812107 | -1.342619 | 1.440841 |
| C | -3.210781 | -0.862730 | -0.729111 |
| H | -3.412500 | -1.252750 | -1.729243 |
| N | -1.794100 | -1.064134 | -0.388353 |
| C | -0.809906 | -0.429275 | -1.019179 |
| H | -1.154174 | 0.361622 | -1.687282 |
| C | 0.567308 | -0.701973 | -0.960201 |
| H | 1.096597 | -0.227702 | -1.780772 |
| C | -3.947086 | -1.678465 | 0.350903 |
| H | -4.061620 | -2.713655 | 0.015398 |
| H | -4.938753 | -1.269283 | 0.545989 |
| C | 1.048998 | -2.098924 | -0.616801 |
| H | 2.062130 | -2.242526 | -0.995527 |
| H | 0.405771 | -2.863266 | -1.065577 |
| H | 1.082562 | -2.287679 | 0.462688 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.416433 | 2.083801 | -0.192027 | C | -3.746983 | 0.585690 | -0.755974 |
| O | -0.526514 | 2.709579 | -0.730386 | O | -4.774135 | 0.767108 | -1.363016 |
| O | -1.701952 | 2.200447 | 1.086221 | O | -3.127557 | 1.544014 | -0.102707 |
| H | -1.895880 | 1.314445 | 1.586396 | H | -2.295259 | 1.324128 | 0.417813 |
| C | 0.204917 | -0.137533 | 1.336259 | C | 1.130364 | 1.805284 | 0.436474 |
| H | 0.299357 | 0.915890 | 1.550566 | H | 1.714094 | 2.621792 | 0.041789 |
| C | 1.148399 | -0.881556 | 0.594493 | C | 1.518574 | 0.459772 | 0.472018 |
| H | 1.177427 | -1.945639 | 0.823820 | H | 1.067913 | -0.141428 | 1.256407 |
| N | -0.952363 | -0.711372 | 1.743133 | N | -0.150180 | 2.125387 | 0.781875 |
| O | -1.184365 | -1.918850 | 1.558363 | O | -0.910064 | 1.158640 | 1.138797 |
| O | -1.834331 | 0.020434 | 2.323104 | O | -0.575130 | 3.273945 | 0.704055 |
| C | 2.454280 | -0.239802 | 0.309519 | C | 2.935952 | 0.143789 | 0.168737 |
| C | 4.938584 | 0.920131 | -0.246288 | C | 5.615095 | -0.459506 | -0.375000 |
| C | 3.618990 | -1.013914 | 0.324813 | C | 3.637559 | -0.760389 | 0.971317 |
| C | 2.543387 | 1.122886 | -0.004783 | C | 3.591585 | 0.735724 | -0.917244 |
| C | 3.780927 | 1.695128 | -0.278239 | C | 4.921409 | 0.436980 | -1.186632 |
| C | 4.855139 | -0.436816 | 0.055192 | C | 4.970948 | -1.056592 | 0.704724 |
| H | 3.551467 | -2.072649 | 0.561462 | H | 3.135157 | -1.223837 | 1.815918 |
| H | 1.646473 | 1.738402 | -0.047780 | H | 3.048664 | 1.426281 | -1.557516 |
| H | 3.839166 | 2.751236 | -0.519944 | H | 5.417980 | 0.901211 | -2.032324 |
| H | 5.752582 | -1.046232 | 0.081115 | H | 5.505874 | -1.754406 | 1.340465 |
| H | 5.901854 | 1.371841 | -0.459394 | H | 6.653363 | -0.692850 | -0.586453 |

**Table S2**. NBO atomic charge of pyrrolidine nitrogen, q(N), of selected transition states, enamine and iminium, calculated at M06-2X/6-31G** level.

| structure | q(N) | structure | q(N) |
|---|---|---|---|
| **TS1-α1-*RS*** | –0.412 | **TS1-β2-*SR*** | –0.424 |
| **TS1-α1-*SR*** | –0.407 | **TS1-β3-*RS*** | –0.393 |
| **TS1-β1-*RS*** | –0.393 | **TS1-β3-*SR*** | –0.385 |
| **TS1-β1-*SR*** | –0.391 | enamine-**1** (**E2**) | –0.548 |
| **TS1-β2-*RS*** | –0.420 | iminium-**1** | –0.314 |

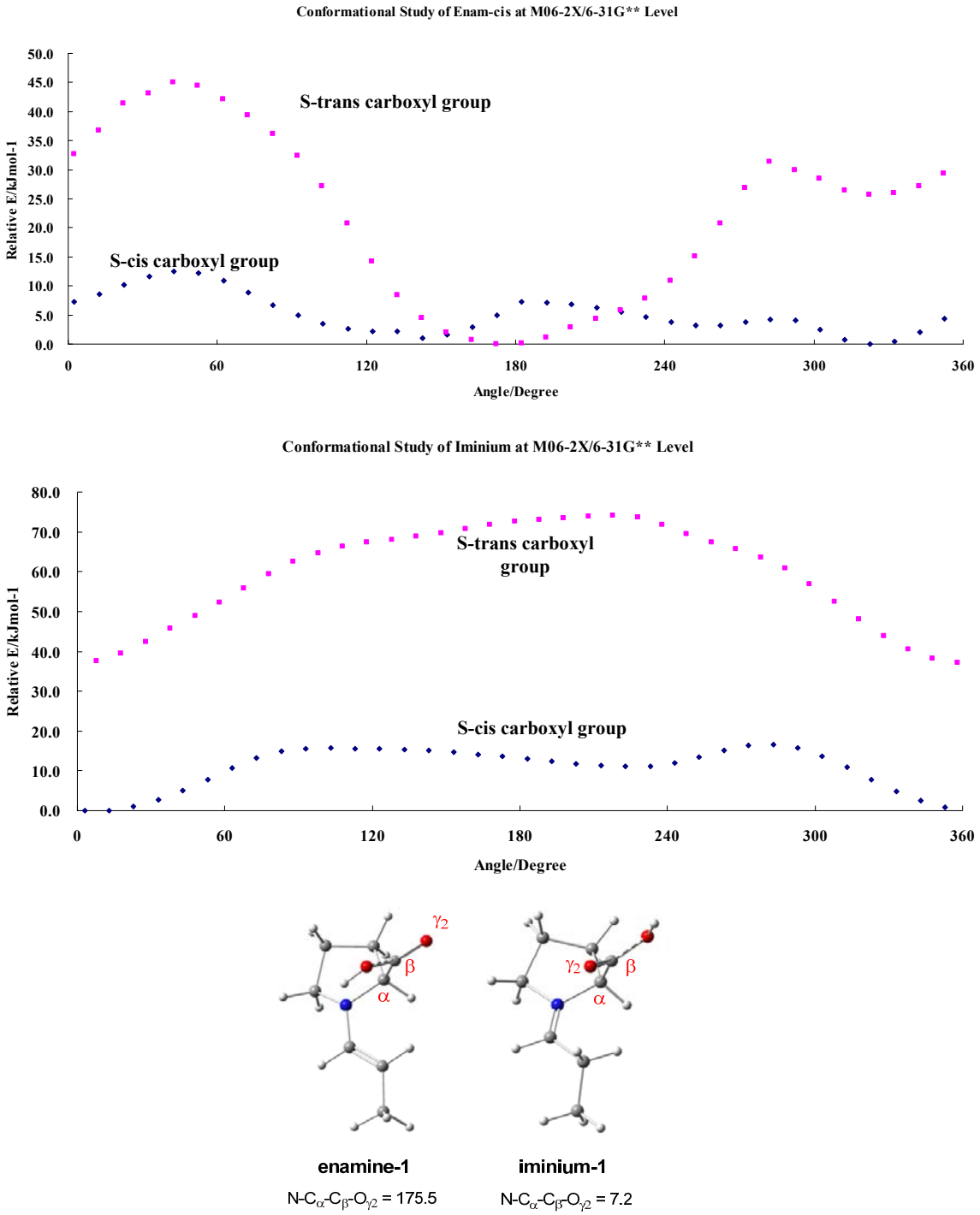
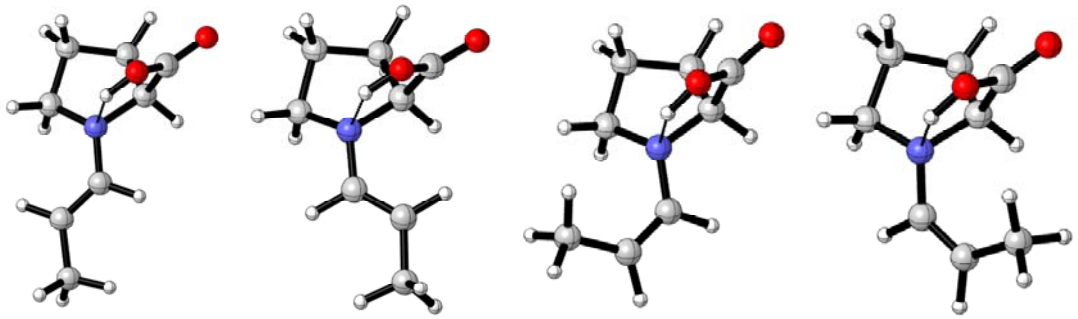


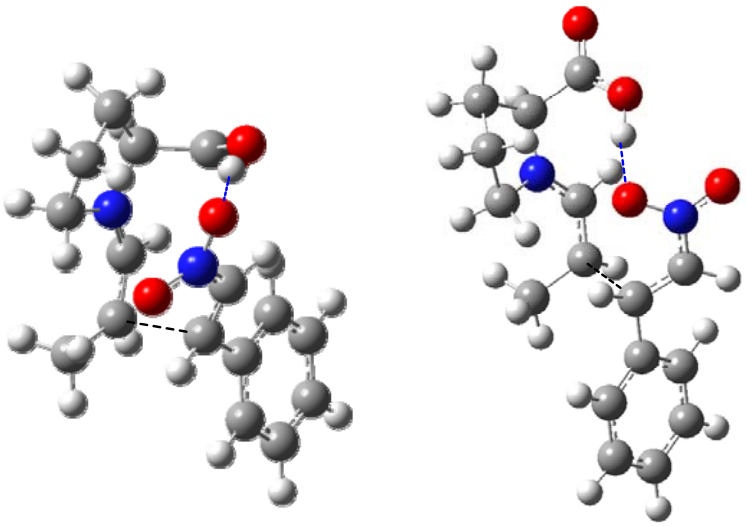

**Figure S1**. Conformational studies of *cis*-enamine and an iminium ion, with respect to the torsional angle of N-$C_\alpha$-$C_\beta$-$O_{\gamma 2}$, at M06-2X/6-31G** level of theory. The optimized geometries of the most favorable enamine and iminium conformations are given at the bottom.



**E1** (0.2) **E2** (0.0) **Z1** (11.1) **Z2** (10.5)

*anti* enamine *syn* enamine

**Figure S2**. M06-2X/6-31G** optimized geometries of the *anti* and *syn* conformations of enamine. Calculated relative enthalpies (MP2/6-311+G**/M06-2X/6-31G*, $\Delta H_{298}$, kJ mol$^{-1}$) are given parenthesis.



**TS1-Z1-*RS*** (58.5) **TS1-Z2-*RS*** (72.8)

**Figure S3**. M06-2X/6-31G** optimized geometries of transition states derived from Z-enamine leading to (*R*,*S*) product of reaction (1). Calculated relative enthalpies (MP2/6-311+G**/M06-2X/6-31G*, $\Delta H_{298}$, kJ mol$^{-1}$), in parenthesis, with respect to **TS1-β1-*RS***.