

3'_Skew (opt. @S₀)

E(RB3LYP) = -6155.75051019

| | | | |
|----|-----------------|-----------------|-----------------|
| C | -3.938043057553 | -0.325970323411 | -1.325167485448 |
| C | -4.395243704499 | 0.303041658102 | -0.206443626604 |
| C | -2.370401949643 | -0.370149914487 | 0.298308424777 |
| C | -2.624398737670 | -0.761359112088 | -0.997125644542 |
| C | -1.210688851425 | -0.440696699010 | 1.178381171935 |
| O | -1.127903106930 | 0.148125506771 | 2.235081863743 |
| C | -0.087363299209 | -1.433908295936 | 0.820677375854 |
| O | -0.287384143785 | -2.601413126406 | 1.098031511837 |
| C | 1.196199201698 | -0.951464383891 | 0.315295056360 |
| C | 1.591111009211 | 0.249091033489 | -0.240361228066 |
| C | 2.947080039169 | 0.274498812754 | -0.655059420353 |
| C | 3.571254301035 | -0.917563596692 | -0.412251272211 |
| S | 2.530578431390 | -2.085137794368 | 0.307195642593 |
| Br | 0.470719341238 | 1.755811732747 | -0.521237320923 |
| H | -4.453562398557 | -0.467105439882 | -2.261514172286 |
| H | -5.328991149977 | 0.785802148050 | 0.034601051846 |
| H | 3.418618661486 | 1.135770545946 | -1.107772690426 |
| H | 4.601728091277 | -1.169574833620 | -0.619234691418 |
| O | -3.470420248258 | 0.293254941114 | 0.773864644916 |
| Br | -1.462056868997 | -1.649336299182 | -2.182222881585 |

3'_Skew (opt. @T₁)

E(UB3LYP) = -6155.66675402

| | | | |
|---|-----------------|-----------------|-----------------|
| C | -4.509694449685 | -0.656758464500 | -0.885795455940 |
| C | -4.625010603548 | -0.126185038053 | 0.363759819561 |
| C | -2.465497553631 | -0.323274662391 | 0.012287651354 |
| C | -3.114014869955 | -0.764806212511 | -1.130141693889 |
| C | -1.071335715045 | -0.114935610666 | 0.370655599375 |
| O | -0.741596560167 | 0.886478995493 | 1.044029392940 |
| C | -0.095576472161 | -1.127615102592 | -0.041665339178 |
| O | -0.471805758612 | -2.276211764814 | -0.356419070498 |
| C | 1.328190922355 | -0.804106314518 | 0.031359891950 |

| | | | |
|----|-----------------|-----------------|-----------------|
| C | 2.032253275667 | 0.317803731010 | -0.367589004888 |
| C | 3.429189650367 | 0.226089204854 | -0.136609836551 |
| C | 3.785613705731 | -0.978776443937 | 0.401695809443 |
| S | 2.434526953470 | -2.025902344811 | 0.633888278993 |
| Br | 1.296190284182 | 1.808753581241 | -1.278221026478 |
| H | -5.305382531847 | -0.928690003442 | -1.560798528871 |
| H | -5.470788126801 | 0.126976658737 | 0.982530105596 |
| H | 4.124347997033 | 1.019786817325 | -0.373270181625 |
| H | 4.776686202937 | -1.307028751188 | 0.680159297260 |
| O | -3.408214116352 | 0.098531515743 | 0.912877724523 |
| Br | -2.357250673939 | -1.278413230982 | -2.769687123077 |

3'_Int_a (opt. @S₀)

E(RB3LYP) = -6155.75114629

| | | | |
|----|-----------------|-----------------|-----------------|
| C | -0.074094397562 | -4.376637488039 | 0.502126342770 |
| C | -0.788022762953 | -3.547662172330 | -0.318088707331 |
| C | -0.355239649430 | -2.201639960863 | -0.207405144033 |
| C | 0.679941480683 | -2.016152181368 | 0.687884327977 |
| S | 1.117125716291 | -3.544375104093 | 1.424482444552 |
| C | 1.403726702918 | -0.826346545282 | 1.135051636772 |
| C | 1.329194440495 | 0.478919670578 | 0.313722125691 |
| O | 2.162290706045 | -0.838264622886 | 2.085663049502 |
| C | 0.534732721941 | 1.556733900392 | 0.878704294324 |
| O | 1.990851834380 | 0.572904734969 | -0.698138960974 |
| C | 0.283419853033 | 2.854930362711 | 0.503188591803 |
| C | -0.645573921092 | 3.392774175154 | 1.437449601337 |
| C | -0.901297244496 | 2.384398329228 | 2.317897294752 |
| O | -0.204578933305 | 1.273411580227 | 2.001169779684 |
| Br | 1.002323151005 | 3.770568051029 | -0.968529059813 |
| Br | -1.219252086305 | -0.830698135208 | -1.198782245787 |
| H | -0.188598633624 | -5.445980265898 | 0.610057358902 |
| H | -1.586208176540 | -3.867751263264 | -0.973487540704 |
| H | -1.055641113115 | 4.390060161405 | 1.442113493162 |
| H | -1.530708689764 | 2.311240243684 | 3.190312839787 |

3'_Int_a (opt. @T₁)

E(UB3LYP) = -6155.66946694

| | | | |
|----|-----------------|-----------------|-----------------|
| C | 0.677453041507 | -4.536990430427 | 0.104379224668 |
| C | -0.248938232861 | -3.956384666648 | -0.715709471393 |
| C | -0.515004456693 | -2.609836957601 | -0.355818484290 |
| C | 0.243344044567 | -2.160619709725 | 0.709644275126 |
| S | 1.243225442369 | -3.461865797456 | 1.329954783783 |
| C | 0.263799039865 | -0.862022307006 | 1.395637901452 |
| C | 0.418165780665 | 0.338448439673 | 0.537100184588 |
| O | 0.230972235796 | -0.825280179104 | 2.637695568755 |
| C | 0.229507351847 | 1.657771061204 | 1.087999048913 |
| O | 0.711661956843 | 0.169184997824 | -0.668430243002 |
| C | 0.342237329797 | 2.905501720014 | 0.507770354090 |
| C | 0.028428297165 | 3.865040038466 | 1.510261975044 |
| C | -0.260053098028 | 3.142612419119 | 2.627562524978 |
| O | -0.147342808607 | 1.813173498258 | 2.391052066230 |
| Br | 0.827980854168 | 3.290875645394 | -1.265543000172 |
| Br | -1.892469926571 | -1.627064182706 | -1.209017492598 |
| H | 1.065807188848 | -5.543802492257 | 0.049489040704 |
| H | -0.737101119001 | -4.459135924648 | -1.539167686542 |
| H | 0.021439658693 | 4.937686517152 | 1.400402843408 |
| H | -0.548721581761 | 3.413141780617 | 3.630128108629 |

3'_Int_b (opt. @S₀)

E(RB3LYP) = -6155.74807639

| | | | |
|---|-----------------|-----------------|-----------------|
| C | -4.387910493840 | -1.312776127287 | -0.669203357196 |
| C | -4.986054450095 | -0.259957759986 | -0.045345713775 |
| C | -2.838267856516 | -0.006805370284 | 0.324822329136 |
| C | -2.995253915419 | -1.149858357150 | -0.430503704523 |
| C | -1.699181703913 | 0.765992779578 | 0.810877389115 |
| O | -1.790893626279 | 1.926699908432 | 1.164606409600 |
| C | -0.358883498852 | 0.027770130436 | 0.983634999198 |
| O | -0.359168597587 | -0.996933449737 | 1.633901645598 |
| C | 0.839563421943 | 0.641934097341 | 0.405133696457 |

| | | | |
|----|-----------------|-----------------|-----------------|
| C | 2.091443825353 | 0.074830734423 | 0.238310061223 |
| C | 3.016179400130 | 0.905590269964 | -0.441650512654 |
| C | 2.463494908439 | 2.108073820553 | -0.785716576883 |
| S | 0.824250557171 | 2.254929197954 | -0.288545636411 |
| Br | 2.599415919481 | -1.663884631756 | 0.792864322654 |
| H | -4.859841753061 | -2.104668496092 | -1.228333871726 |
| H | -6.016202723299 | 0.039253484233 | 0.065913811147 |
| H | 4.034938151971 | 0.613538680926 | -0.655708872855 |
| H | 2.948095361698 | 2.931929697849 | -1.290480366839 |
| O | -4.076920162708 | 0.539276778358 | 0.545032280241 |
| Br | -1.666243484619 | -2.283346607756 | -1.131331221509 |

3'_Int_b (opt. @T₁)

E(UB3LYP) = -6155.67211059

| | | | |
|----|-----------------|-----------------|-----------------|
| C | -4.611150845285 | -1.473410417267 | -0.218056862517 |
| C | -5.013083388463 | -0.348521036132 | 0.434110446457 |
| C | -2.870246977371 | -0.062504140628 | 0.047333467228 |
| C | -3.227145489978 | -1.285199858526 | -0.490559742425 |
| C | -1.651759270192 | 0.750608187800 | 0.032291178886 |
| O | -1.706512946142 | 1.967422593790 | -0.198672930563 |
| C | -0.384694290463 | 0.054108089156 | 0.330036413990 |
| O | -0.467631651296 | -1.124863589756 | 0.780116089174 |
| C | 0.878977076187 | 0.712351412157 | 0.118914280130 |
| C | 2.141360720587 | 0.166359743353 | 0.306213872233 |
| C | 3.206110782354 | 1.047023139703 | 0.003239900290 |
| C | 2.749871930166 | 2.265318140188 | -0.415535989306 |
| S | 1.024179207219 | 2.371166508685 | -0.449296488501 |
| Br | 2.464872300707 | -1.600874460701 | 0.914416202221 |
| H | -5.210794399645 | -2.327618699748 | -0.489002641825 |
| H | -5.956062271518 | -0.033316425117 | 0.850847749988 |
| H | 4.249650247890 | 0.778904773559 | 0.095723171737 |
| H | 3.338543323642 | 3.124959283990 | -0.702815049568 |
| O | -3.984837121133 | 0.519829498173 | 0.586549497608 |
| Br | -2.187087657266 | -2.450153962678 | -1.537575455238 |

3'_TP (opt. @S₀)

E(RB3LYP) = -6155.74960051

| | | | |
|----|-----------------|-----------------|-----------------|
| C | -4.981138751883 | -0.452081814782 | -0.430982900440 |
| C | -4.072446493264 | -1.403475597151 | -0.789401256930 |
| C | -2.899609625579 | 0.191891446760 | 0.154160202866 |
| C | -4.221642849030 | 0.584895542655 | 0.174743839686 |
| C | -1.676987756349 | 0.851696842409 | 0.589607920899 |
| O | -1.662243503978 | 2.004438185478 | 0.983891321513 |
| C | -0.380039211914 | 0.011910497044 | 0.611664584542 |
| O | -0.431982140711 | -1.128491914793 | 1.022727925502 |
| C | 0.859489824361 | 0.672812761630 | 0.179682749587 |
| C | 2.093577534933 | 0.085573224405 | -0.050331040415 |
| C | 3.081056344581 | 0.979677330285 | -0.531823628120 |
| C | 2.595683468863 | 2.251185158301 | -0.661792842359 |
| S | 0.946582061178 | 2.387670744322 | -0.195822065322 |
| Br | 2.517377158384 | -1.745854800641 | 0.192230573479 |
| H | -6.049632882652 | -0.473775084475 | -0.573495194671 |
| H | -4.164165640635 | -2.360318887885 | -1.278320797324 |
| H | 4.093741767520 | 0.680207677463 | -0.763646405601 |
| H | 3.136271924167 | 3.128228255466 | -0.989261909028 |
| O | -2.822790608471 | -1.039068992981 | -0.448069026210 |
| Br | -4.937907599520 | 2.174636566491 | 0.869203658349 |

3'_TP (opt. @T₁)

E(UB3LYP) = -6155.67648896

| | | | |
|---|-----------------|-----------------|-----------------|
| C | -5.096967450498 | -0.509866314521 | -0.028652259959 |
| C | -4.287513125031 | -1.595453454337 | -0.164640751970 |
| C | -2.932919303591 | 0.128733012578 | -0.046916391618 |
| C | -4.223421637578 | 0.610974218091 | 0.048197405967 |
| C | -1.661490194051 | 0.819990201840 | -0.026408340041 |
| O | -1.598490698523 | 2.051696346717 | 0.091568068793 |
| C | -0.386474440207 | 0.028590622657 | -0.150932965384 |
| O | -0.436911116534 | -1.225066707891 | -0.271475047520 |
| C | 0.873087305571 | 0.727481350411 | -0.129370318227 |

| | | | |
|----|-----------------|-----------------|-----------------|
| C | 2.132441428248 | 0.145774555682 | -0.232825621939 |
| C | 3.204613930181 | 1.065193814839 | -0.183044630905 |
| C | 2.760028559203 | 2.349684495914 | -0.041245330494 |
| S | 1.036055058833 | 2.472753613023 | 0.034875796766 |
| Br | 2.444925008249 | -1.715557918538 | -0.425994212395 |
| H | -6.174331594890 | -0.493388155445 | 0.013073415173 |
| H | -4.474173494375 | -2.652588722432 | -0.260871078430 |
| H | 4.244618129736 | 0.776337092803 | -0.249800252132 |
| H | 3.356521356734 | 3.248679416546 | 0.024247949547 |
| O | -2.983654326008 | -1.228717137675 | -0.177358916427 |
| Br | -4.772750375470 | 2.396506809738 | 0.242539191193 |