

Type-I dyotropic rearrangement for 1,2-disubstituted cyclohexanes: substitution effect on activation energy

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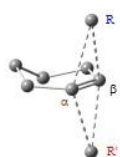
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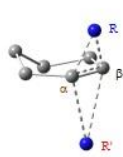
Complete citation for reference 52:

GAUSSIAN09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

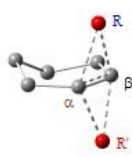
Optimized transition state structures



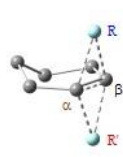
TS1
R/R' = CH₃



TS2
R/R' = NH₂



TS3
R/R' = OH



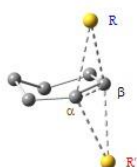
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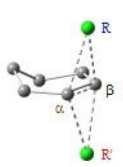
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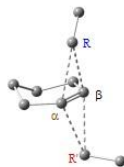
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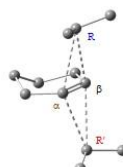
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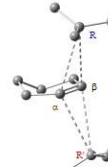
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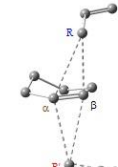
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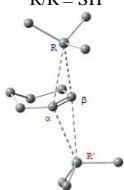
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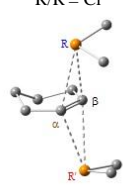
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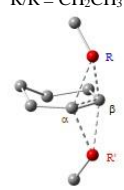
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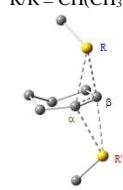
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R/R' = Si(CH₃)₃



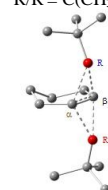
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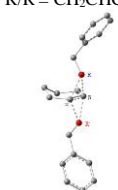
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R/R' = OCH₃



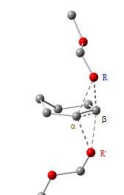
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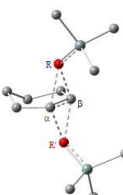
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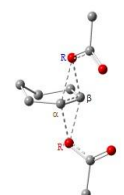
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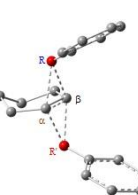
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R/R' = OCH₂OCH₃



TS20
R/R' = OSi(CH₃)₃



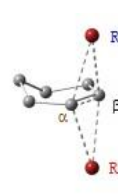
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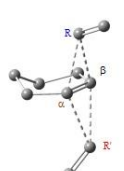
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R/R' = OPh



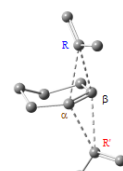
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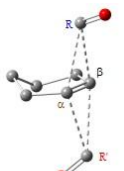
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R/R' = Br



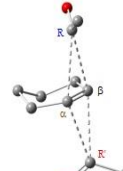
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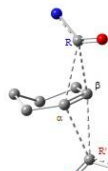
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R/R' = C(CH₃)C(CH₃)₂



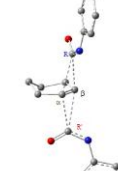
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R/R' = C(O)H



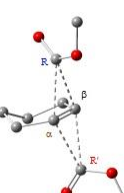
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R/R' = C(O)CH₃



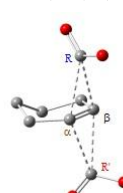
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R/R' = C(O)NH₂



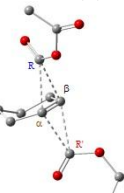
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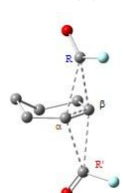
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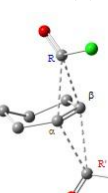
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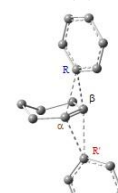
TS33
R/R' = C(O)OC(O)CH₃



TS34
R/R' = C(O)F



TS35
R/R' = C(O)Cl



TS36
R/R' = Ph

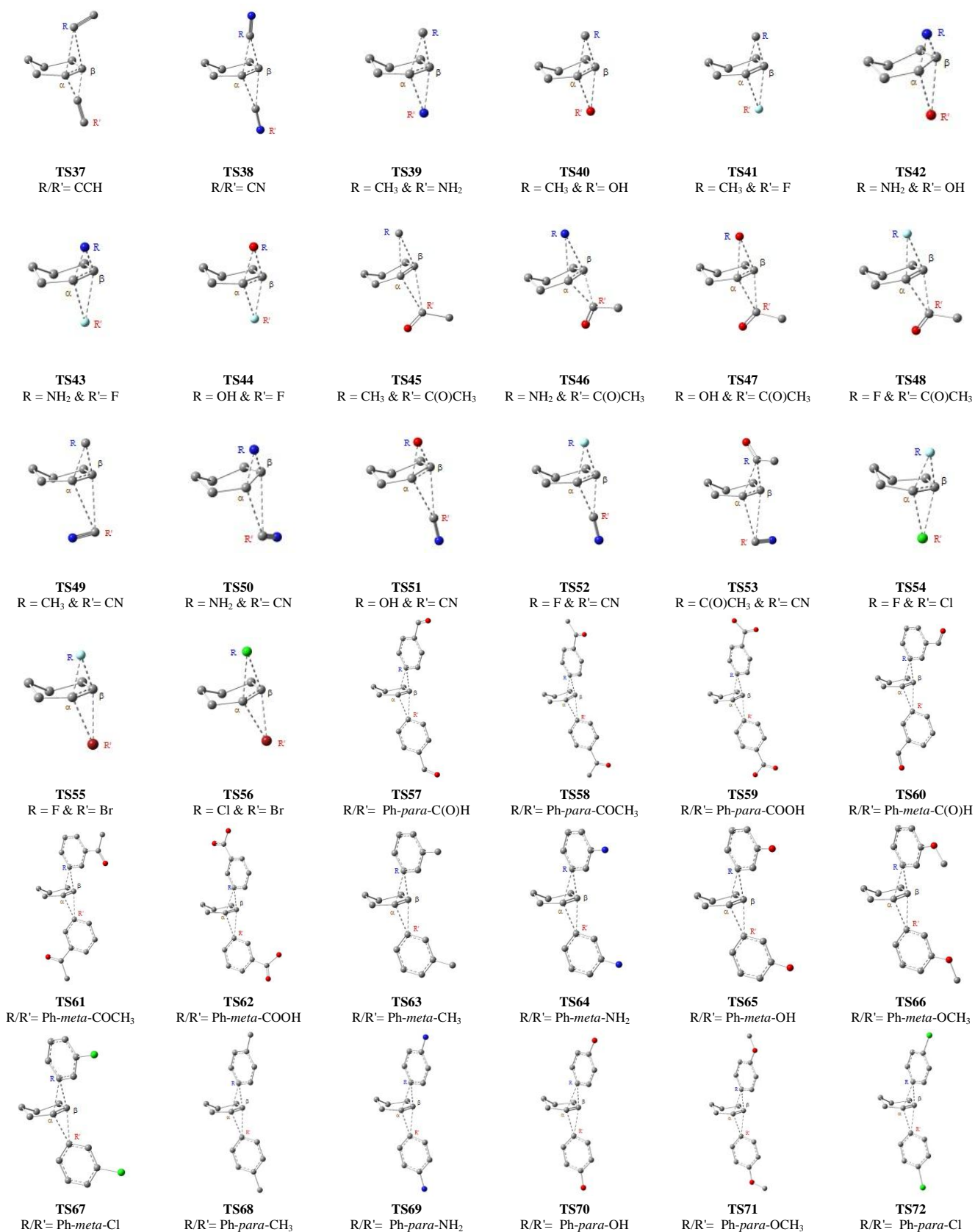
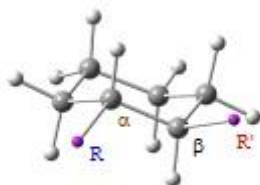


Fig. 1 Optimized transition state structures for type-I dyotropic rearrangement of 1,2-disubstituted cyclohexane motifs; for lucidity, hydrogen atoms are not shown.

Energies for 1,2-disubstituted cyclohexanes



1,2-disubstituted cyclohexane

Fig. 2 Generic representation of 1,2-disubstituted cyclohexanes.

| Entry | Substituents (R and R') | 1,2-Disubstituted cyclohexanes, (Hartree) | | |
|-------|------------------------------------|---|--|-------------------|
| | | Total Electronic Energy | Sum of Electronic and Zero-Point Energies | Gibbs Free Energy |
| S1 | CH ₃ | -314.5326924 | -314.3065740 | -314.3387410 |
| S2 | NH ₂ | -346.6075796 | -346.4030200 | -346.4348830 |
| S3 | OH | -386.3427509 | -386.1640390 | -386.1959290 |
| S4 | F | -434.3884663 | -434.233814 | -434.265325 |
| S5 | SiH ₃ | -817.2798810 | -817.0804440 | -817.1160220 |
| S6 | PH ₂ | -919.7815483 | -919.5959200 | -919.6307440 |
| S7 | SH | -1032.2722078 | -1032.1036000 | -1032.1379060 |
| S8 | Cl | -1155.096159 | -1154.944001 | -1154.977028 |
| S9 | CH ₂ CH ₃ | -393.1637502 | -392.8808020 | -392.9174720 |
| S10 | CH(CH ₃) ₂ | -471.7872252 | -471.4476460 | -471.4868440 |
| S11 | C(CH ₃) ₃ | -550.4098595 | -550.0141710 | -550.0549940 |
| S12 | CH ₂ CHCH ₂ | -469.3276294 | -469.0351620 | -469.0750010 |
| S13 | Si(CH ₃) ₃ | -1053.2645960 | -1052.8924090 | -1052.9415990 |
| S14 | P(CH ₃) ₂ | -1077.0708378 | -1076.7686440 | -1076.8110840 |
| S15 | OCH ₃ | -464.9492652 | -464.7145310 | -464.7514170 |
| S16 | SCH ₃ | -1110.9049075 | -1110.6772110 | -1110.7163390 |
| S17 | OC(CH ₃) ₃ | -700.8681409 | -700.4660900 | -700.5123740 |
| S18 | OCH ₂ Ph | -927.0835523 | -926.6862740 | -926.7407120 |
| S19 | OCH ₂ OCH ₃ | -694.0122519 | -693.7109960 | -693.7559960 |
| S20 | OSi(CH ₃) ₃ | -1203.8016494 | -1203.4202190 | -1203.4741130 |
| S21 | OC(O)CH ₃ | -691.6867218 | -691.4325350 | -691.4774040 |
| S22 | OPh | -848.4604703 | -848.1200190 | -848.1664300 |
| S23 | OC(O)Ph | -1075.1507395 | -1074.7902590 | -1074.8436250 |
| S24 | Br | -5378.160663 | -5378.009397 | -5378.044431 |
| S25 | CHCH ₂ | -390.6944437 | -390.458464 | -390.494087 |
| S26 | C(CH ₃)CH ₂ | -469.3261414 | -469.033544 | -469.072344 |
| S27 | C(O)H | 462.5430736 | -462.355221 | -462.390441 |
| S28 | C(O)CH ₃ | -541.194769 | -540.950479 | -540.989534 |
| S29 | C(O)NH ₂ | -573.3262967 | -573.102645 | -573.142095 |
| S30 | C(O)NHPh | -1035.443042 | -1035.056449 | -1035.109664 |
| S31 | C(O)OCH ₃ | -691.6687055 | -691.412888 | -691.455602 |
| S32 | C(O)OH | -613.0607921 | -612.860646 | -612.898766 |
| S33 | C(O)OC(O)CH ₃ | -918.3540306 | -918.081441 | -918.132623 |
| S34 | C(O)F | -661.0766282 | -660.902414 | -660.940391 |
| S35 | C(O)Cl | -1381.765613 | -1381.5947 | -1381.634488 |
| S36 | Ph | -698.0176802 | -697.685074 | -697.727569 |
| S37 | CCH | -388.1873231 | -387.999077 | -388.033376 |
| S38 | CN | -420.3824481 | -420.214744 | -420.248854 |

| Entry | Substituents | | 1,2-Disubstituted cyclohexanes, (Hartree) | | |
|-------|---------------------|---------------------|---|---|-------------------|
| | R | R' | Total Electronic Energy | Sum of Electronic and Zero-Point Energies | Gibbs Free Energy |
| S39 | CH ₃ | NH ₂ | -330.5690585 | -330.353766 | -330.38583 |
| S40 | CH ₃ | OH | -350.437062 | -350.234873 | -350.267031 |
| S41 | CH ₃ | F | -374.4629003 | -374.272461 | -374.304272 |
| S42 | NH ₂ | OH | -366.4729718 | -366.281542 | -366.313537 |
| S43 | NH ₂ | F | -390.4981274 | -390.318554 | -390.350289 |
| S44 | OH | F | -410.3647795 | -410.197931 | -410.229552 |
| S45 | CH ₃ | C(O)CH ₃ | -427.86421 | -427.628777 | -427.664753 |
| S46 | NH ₂ | C(O)CH ₃ | -443.9000962 | -443.675627 | -443.711668 |
| S47 | OH | C(O)CH ₃ | -463.7680628 | -463.556538 | -463.592599 |
| S48 | F | C(O)CH ₃ | -487.7919819 | -487.592573 | -487.628654 |
| S49 | CH ₃ | CN | -367.4602165 | -367.263213 | -367.296351 |
| S50 | NH ₂ | CN | -383.4960639 | -383.310073 | -383.343135 |
| S51 | OH | CN | -403.3629489 | -403.18976 | -403.222828 |
| S52 | F | CN | -427.3865267 | -427.225339 | -427.258174 |
| S53 | C(O)CH ₃ | CN | -480.7885949 | -480.582694 | -480.620282 |
| S54 | F | Cl | -794.7426109 | -794.589151 | -794.621403 |
| S55 | F | Br | -2906.273732 | -2906.120702 | -2906.153955 |
| S56 | Cl | Br | -3266.627892 | -3266.476222 | -3266.510318 |

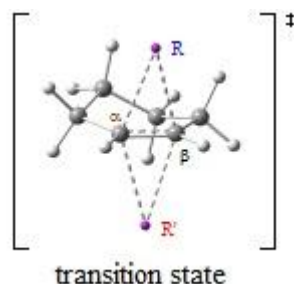


Fig. 3 Generic representation for the transitions states of 1,2-disubstituted cyclohexanes.

Energies for the transition states of 1,2-disubstituted cyclohexanes

| Entry | Substituents (R and R') | Transition states of 1,2-disubstituted cyclohexanes, (Hartree) | | |
|-------|------------------------------------|--|--|-------------------|
| | | Total Electronic Energy | Sum of Electronic and Zero-Point Energies | Gibbs Free Energy |
| TS1 | CH ₃ | -314.3288415 | -314.1138790 | -314.1498570 |
| TS2 | NH ₂ | -346.4534348 | -346.2563820 | -346.2893020 |
| TS3 | OH | -386.2151409 | -386.0415720 | -386.0733900 |
| TS4 | F | -434.2912085 | -434.140499 | -434.172232 |
| TS5 | SiH ₃ | -817.1310973 | -816.9392150 | -816.9797290 |
| TS6 | PH ₂ | -919.6736675 | -919.4944570 | -919.5326070 |
| TS7 | SH | -1032.1901163 | -1032.0255120 | -1032.0602870 |
| TS8 | Cl | -1155.035379 | -1154.886252 | -1154.919981 |
| TS9 | CH ₂ CH ₃ | -392.9612230 | -392.6893100 | -392.7297050 |
| TS10 | CH(CH ₃) ₂ | -471.6000373 | -471.2733120 | -471.3188440 |
| TS11 | C(CH ₃) ₃ | -550.2422946 | -549.8614620 | -549.9128710 |
| TS12 | CH ₂ CHCH ₂ | -469.1732396 | -468.8914810 | -468.9361080 |
| TS13 | Si(CH ₃) ₃ | -1053.1042221 | -1052.7378260 | -1052.7947180 |
| TS14 | P(CH ₃) ₂ | -1076.9560053 | -1076.6599210 | -1076.7087220 |
| TS15 | OCH ₃ | -464.8299248 | -464.6009190 | -464.6379720 |
| TS16 | SCH ₃ | -1110.8212245 | -1110.5973110 | -1110.6380100 |
| TS17 | OC(CH ₃) ₃ | -700.7206532 | -700.3238060 | -700.3694150 |
| TS18 | OCH ₂ Ph | -926.9519426 | -926.5602130 | -926.6134970 |
| TS19 | OCH ₂ OCH ₃ | -693.8824171 | -693.5874490 | -693.6319650 |
| TS20 | OSi(CH ₃) ₃ | -1203.6833691 | -1203.3069210 | -1203.3627570 |
| TS21 | OC(O)CH ₃ | -691.5788691 | -691.3307320 | -691.3768590 |
| TS22 | OPh | -848.3572557 | -848.0228270 | -848.0710370 |
| TS23 | OC(O)Ph | -1075.0650559 | -1074.7099150 | -1074.7648920 |
| TS24 | Br | -5378.10789 | -5377.959205 | -5377.995115 |
| TS25 | CHCH ₂ | -390.4840045 | -390.257552 | -390.295201 |
| TS26 | C(CH ₃)CH ₂ | -469.1293357 | -468.846597 | -468.888237 |
| TS27 | C(O)H | -462.3533134 | -462.177382 | -462.21752 |
| TS28 | C(O)CH ₃ | -541.183833 | -540.783902 | -540.829929 |
| TS29 | C(O)NH ₂ | -573.1428109 | -572.92829 | -572.971812 |
| TS30 | C(O)NHPh | -1035.266837 | -1034.888886 | -1034.947225 |
| TS31 | C(O)OCH ₃ | -691.482772 | -691.235851 | -691.283382 |
| TS32 | C(O)OH | -612.875188 | -612.684406 | -612.726768 |
| TS33 | C(O)OC(O)CH ₃ | -918.1721754 | -917.908328 | -917.964299 |
| TS34 | C(O)F | -660.8951567 | -660.729566 | -660.771831 |
| TS35 | C(O)Cl | -1381.609709 | -1381.447343 | -1381.493517 |

| | | | | |
|------|-----|--------------|-------------|-------------|
| TS36 | Ph | -697.8189253 | -697.494194 | -697.54001 |
| TS37 | CCH | -387.9966093 | -387.815649 | -387.853247 |
| TS38 | CN | -420.2052165 | -420.044392 | -420.081853 |

| Entry | Substituents | | Transition states of 1,2-disubstituted cyclohexanes, (Hartree) | | |
|-------|---------------------|---------------------|--|---|-------------------|
| | R | R' | Total Electronic Energy | Sum of Electronic and Zero-Point Energies | Gibbs Free Energy |
| TS39 | CH ₃ | NH ₂ | -330.38583 | -330.3928581 | -330.186451 |
| TS40 | CH ₃ | OH | -350.267031 | -350.2861224 | -350.090595 |
| TS41 | CH ₃ | F | -374.304272 | -374.334973 | -374.149469 |
| TS42 | NH ₂ | OH | -366.313537 | -366.3523429 | -366.165718 |
| TS43 | NH ₂ | F | -390.350289 | -390.403888 | -390.227241 |
| TS44 | OH | F | -410.229552 | -410.2617874 | -410.099081 |
| TS45 | CH ₃ | C(O)CH ₃ | -427.664753 | -427.6732836 | -427.448369 |
| TS46 | NH ₂ | C(O)CH ₃ | -443.711668 | -443.7332102 | -443.517416 |
| TS47 | OH | C(O)CH ₃ | -463.592599 | -463.622482 | -463.41809 |
| TS48 | F | C(O)CH ₃ | -487.628654 | -487.66876 | -487.474959 |
| TS49 | CH ₃ | CN | -367.296351 | -367.303087 | -367.112227 |
| TS50 | NH ₂ | CN | -383.343135 | -383.3751882 | -383.192912 |
| TS51 | OH | CN | -403.222828 | -403.2200785 | -403.052102 |
| TS52 | F | CN | -427.258174 | -427.2514909 | -427.095521 |
| TS53 | C(O)CH ₃ | CN | -480.620282 | -480.63342 | -480.434449 |
| TS54 | F | Cl | -794.621403 | -794.6632752 | -794.513396 |
| TS55 | F | Br | -2906.153955 | -2906.198305 | -2906.048666 |
| TS56 | Cl | Br | -3266.510318 | -3266.571037 | -3266.42223 |

Bond distances for the transition states of 1,2-disubstituted cyclohexanes

| Entry | Substituents (R and R') | | Bond distance (<i>r</i>), Å | | | | | Average bond distance (<i>r</i>), Å |
|-------|------------------------------------|-----------------|--------------------------------|-------------------|-------------------|--------------------|--------------------|--|
| | | | C ^α -C ^β | C ^α -R | C ^β -R | C ^α -R' | C ^β -R' | C ^α /C ^β -R/R' |
| TS1 | CH ₃ | | 1.368 | 2.431 | 2.404 | 2.430 | 2.434 | 2.425 |
| TS2 | NH ₂ | | 1.445 | 1.639 | 1.611 | 2.495 | 2.513 | 2.065 |
| TS3 | OH | | 1.416 | 1.979 | 1.968 | 1.968 | 1.979 | 1.973 |
| TS4 | F | | 1.423 | 1.915 | 1.904 | 1.904 | 1.915 | 1.909 |
| TS5 | SiH ₃ | | 1.371 | 2.905 | 2.853 | 2.853 | 2.905 | 2.879 |
| TS6 | PH ₂ | | 1.376 | 2.811 | 2.827 | 2.765 | 2.853 | 2.814 |
| TS7 | SH | | 1.418 | 2.505 | 2.480 | 2.480 | 2.505 | 2.492 |
| TS8 | Cl | | 1.434 | 2.398 | 2.369 | 2.369 | 2.398 | 2.384 |
| TS9 | CH ₂ CH ₃ | | 1.362 | 2.538 | 2.558 | 2.558 | 2.510 | 2.541 |
| TS10 | CH(CH ₃) ₂ | | 1.353 | 2.712 | 2.688 | 2.688 | 2.712 | 2.700 |
| TS11 | C(CH ₃) ₃ | | 1.345 | 3.117 | 3.098 | 3.098 | 3.116 | 3.107 |
| TS12 | CH ₂ CHCH ₂ | | 1.353 | 3.172 | 2.949 | 2.975 | 3.059 | 3.039 |
| TS13 | Si(CH ₃) ₃ | | 1.362 | 3.041 | 2.986 | 2.986 | 3.028 | 3.010 |
| TS14 | P(CH ₃) ₂ | | 1.361 | 2.946 | 2.916 | 2.910 | 2.964 | 2.934 |
| TS15 | OCH ₃ | | 1.418 | 1.973 | 1.962 | 1.962 | 1.973 | 1.967 |
| TS16 | SCH ₃ | | 1.417 | 2.475 | 2.447 | 2.447 | 2.475 | 2.461 |
| TS17 | OC(CH ₃) ₃ | | 1.431 | 2.029 | 1.991 | 1.994 | 2.032 | 2.011 |
| TS18 | OCH ₂ Ph | | 1.422 | 2.006 | 1.994 | 1.994 | 2.006 | 2.000 |
| TS19 | OCH ₂ OCH ₃ | | 1.422 | 2.067 | 1.999 | 1.999 | 2.066 | 2.033 |
| TS20 | OSi(CH ₃) ₃ | | 1.424 | 1.976 | 1.973 | 1.973 | 1.976 | 1.975 |
| TS21 | OC(O)CH ₃ | | 1.420 | 2.082 | 2.037 | 2.037 | 2.082 | 2.059 |
| TS22 | OPh | | 1.420 | 2.028 | 2.013 | 2.013 | 2.028 | 2.021 |
| TS23 | OC(O)Ph | | 1.432 | 2.074 | 2.099 | 2.089 | 2.073 | 2.084 |
| TS24 | Br | | 1.428 | 2.524 | 2.488 | 2.488 | 2.524 | 2.506 |
| TS25 | CHCH ₂ | | 1.378 | 2.373 | 2.375 | 2.239 | 2.252 | 2.310 |
| TS26 | C(CH ₃)CH ₂ | | 1.375 | 2.370 | 2.348 | 2.381 | 2.391 | 2.372 |
| TS27 | C(O)H | | 1.364 | 2.569 | 2.556 | 2.585 | 2.617 | 2.582 |
| TS28 | C(O)CH ₃ | | 1.362 | 2.716 | 2.678 | 2.678 | 2.717 | 2.697 |
| TS29 | C(O)NH ₂ | | 1.369 | 2.573 | 2.538 | 2.513 | 2.534 | 2.539 |
| TS30 | C(O)NHPh | | 1.369 | 2.612 | 2.581 | 2.581 | 2.612 | 2.597 |
| TS31 | C(O)OCH ₃ | | 1.378 | 2.427 | 2.414 | 2.415 | 2.427 | 2.421 |
| TS32 | C(O)OH | | 1.380 | 2.417 | 2.403 | 2.403 | 2.417 | 2.410 |
| TS33 | C(O)OC(O)CH ₃ | | 1.381 | 2.417 | 2.413 | 2.411 | 2.429 | 2.417 |
| TS34 | C(O)F | | 1.387 | 2.379 | 2.365 | 2.365 | 2.379 | 2.372 |
| TS35 | C(O)Cl | | 1.385 | 2.426 | 2.410 | 2.407 | 2.424 | 2.417 |
| TS36 | Ph | | 1.379 | 2.329 | 2.327 | 2.327 | 2.329 | 2.328 |
| TS37 | CCH | | 1.431 | 1.717 | 1.643 | 2.778 | 2.648 | 2.197 |
| TS38 | CN | | 1.410 | 2.192 | 2.174 | 2.174 | 2.192 | 2.183 |
| Entry | Substituents | | Bond distance (<i>r</i>), Å | | | | | |
| | R | R' | C ^α -C ^β | C ^α -R | C ^β -R | C ^α -R' | C ^β -R' | |
| TS39 | CH ₃ | NH ₂ | 1.399 | 2.092 | 2.079 | 2.213 | 2.216 | |
| TS40 | CH ₃ | OH | 1.388 | 2.065 | 2.047 | 2.232 | 2.233 | |

| | | | | | | | |
|------|---------------------|---------------------|--------------|-------|-------|-------|-------|
| TS41 | CH ₃ | F | 1.385 | 1.988 | 1.965 | 2.223 | 2.215 |
| TS42 | NH ₂ | OH | 1.449 | 1.613 | 1.574 | 2.426 | 2.513 |
| TS43 | NH ₂ | F | 1.443 | 1.608 | 1.586 | 2.352 | 2.398 |
| TS44 | OH | F | 1.421 | 1.836 | 1.818 | 2.055 | 2.059 |
| TS45 | CH ₃ | C(O)CH ₃ | 1.367 | 2.427 | 2.414 | 2.625 | 2.664 |
| TS46 | NH ₂ | C(O)CH ₃ | 1.404 | 2.392 | 2.404 | 1.942 | 1.965 |
| TS47 | OH | C(O)CH ₃ | 1.389 | 2.187 | 2.171 | 2.217 | 2.226 |
| TS48 | F | C(O)CH ₃ | 1.385 | 2.182 | 2.165 | 2.126 | 2.133 |
| TS49 | CH ₃ | CN | 1.394 | 1.909 | 1.854 | 2.952 | 2.772 |
| TS50 | NH ₂ | CN | 1.463 | 1.735 | 1.509 | 2.516 | 2.867 |
| TS51 | OH | CN | 1.427 | 1.774 | 1.743 | 2.466 | 2.470 |
| TS52 | F | CN | 1.415 | 1.965 | 1.956 | 2.063 | 2.077 |
| TS53 | C(O)CH ₃ | CN | 1.387 | 2.102 | 2.079 | 2.679 | 2.771 |
| TS54 | F | Cl | 1.432 | 1.902 | 1.879 | 2.387 | 2.397 |
| TS55 | F | Br | 1.430 | 1.933 | 1.909 | 2.469 | 2.482 |
| TS56 | Cl | Br | 1.431 | 2.446 | 2.417 | 2.444 | 2.479 |

Bond angles for the transition states of 1,2-disubstituted cyclohexanes

| Entry | Substituents (R and R') | | Bond angle, θ | | Average bond angle, θ |
|-------|------------------------------------|--|----------------------|-----------------------|------------------------------|
| | | | $C^\alpha-R-C^\beta$ | $C^\alpha-R'-C^\beta$ | |
| TS1 | CH ₃ | | 32.86 | 32.67 | 32.77 |
| TS2 | NH ₂ | | 52.77 | 33.53 | 43.15 |
| TS3 | OH | | 42.05 | 42.04 | 42.04 |
| TS4 | F | | 43.77 | 43.78 | 43.77 |
| TS5 | SiH ₃ | | 27.52 | 27.52 | 27.52 |
| TS6 | PH ₂ | | 28.25 | 28.31 | 28.28 |
| TS7 | SH | | 33.04 | 33.04 | 33.04 |
| TS8 | Cl | | 35.00 | 35.00 | 35.00 |
| TS9 | CH ₂ CH ₃ | | 31.00 | 31.55 | 31.28 |
| TS10 | CH(CH ₃) ₂ | | 29.03 | 29.03 | 29.03 |
| TS11 | C(CH ₃) ₃ | | 25.00 | 25.00 | 25.00 |
| TS12 | CH ₂ CHCH ₂ | | 25.21 | 25.87 | 25.54 |
| TS13 | Si(CH ₃) ₃ | | 26.09 | 26.16 | 26.13 |
| TS14 | P(CH ₃) ₂ | | 26.85 | 26.78 | 26.81 |
| TS15 | OCH ₃ | | 42.25 | 42.26 | 42.25 |
| TS16 | SCH ₃ | | 33.45 | 33.45 | 33.45 |
| TS17 | OC(CH ₃) ₃ | | 41.70 | 41.64 | 41.67 |
| TS18 | OCH ₂ Ph | | 41.65 | 41.65 | 41.65 |
| TS19 | OCH ₂ OCH ₃ | | 40.90 | 40.90 | 40.90 |
| TS20 | OSi(CH ₃) ₃ | | 42.27 | 42.26 | 42.27 |
| TS21 | OC(O)CH ₃ | | 40.32 | 40.32 | 40.32 |
| TS22 | OPh | | 41.15 | 41.14 | 41.14 |
| TS23 | OC(O)Ph | | 40.14 | 40.25 | 40.20 |
| TS24 | Br | | 33.11 | 33.11 | 33.11 |
| TS25 | CHCH ₂ | | 33.73 | 35.73 | 34.73 |
| TS26 | C(CH ₃)CH ₂ | | 33.89 | 33.50 | 33.70 |
| TS27 | C(O)H | | 30.88 | 30.40 | 30.64 |
| TS28 | C(O)CH ₃ | | 29.24 | 29.24 | 29.24 |
| TS29 | C(O)NH ₂ | | 31.06 | 31.47 | 31.27 |
| TS30 | C(O)NPh | | 30.57 | 30.57 | 30.57 |
| TS31 | C(O)OCH ₃ | | 33.06 | 33.06 | 33.06 |
| TS32 | C(O)OH | | 33.27 | 33.27 | 33.27 |
| TS33 | C(O)OC(O)CH ₃ | | 33.22 | 33.14 | 33.18 |
| TS34 | C(O)F | | 34.00 | 34.00 | 34.00 |
| TS35 | C(O)Cl | | 33.30 | 33.33 | 33.31 |
| TS36 | Ph | | 34.44 | 34.44 | 34.44 |
| TS37 | CCH | | 50.35 | 30.46 | 40.40 |
| TS38 | CN | | 37.69 | 37.69 | 37.69 |

| Entry | Substituents | | Bond angle, θ | |
|-------|-----------------|-----------------|----------------------|-----------------------|
| | R | R' | $C^\alpha-R-C^\beta$ | $C^\alpha-R'-C^\beta$ |
| TS39 | CH ₃ | NH ₂ | 39.19 | 36.83 |
| TS40 | CH ₃ | OH | 39.46 | 36.24 |

| | | | | |
|------|---------------------|---------------------|-------|-------|
| TS41 | CH ₃ | F | 41.04 | 36.38 |
| TS42 | NH ₂ | OH | 54.07 | 34.07 |
| TS43 | NH ₂ | F | 53.71 | 35.36 |
| TS44 | OH | F | 45.79 | 40.43 |
| TS45 | CH ₃ | C(O)CH ₃ | 32.81 | 29.95 |
| TS46 | NH ₂ | C(O)CH ₃ | 34.04 | 42.11 |
| TS47 | OH | C(O)CH ₃ | 37.18 | 36.44 |
| TS48 | F | C(O)CH ₃ | 37.16 | 37.95 |
| TS49 | CH ₃ | CN | 43.45 | 27.96 |
| TS50 | NH ₂ | CN | 53.07 | 30.66 |
| TS51 | OH | CN | 47.85 | 33.59 |
| TS52 | F | CN | 42.31 | 39.98 |
| TS53 | C(O)CH ₃ | CN | 38.75 | 29.43 |
| TS54 | F | Cl | 44.50 | 34.82 |
| TS55 | F | Br | 43.70 | 33.58 |
| TS56 | Cl | Br | 34.23 | 33.80 |

Cartesian coordinates for 1,2-disubstituted cyclohexanes and corresponding transition states along with IRC

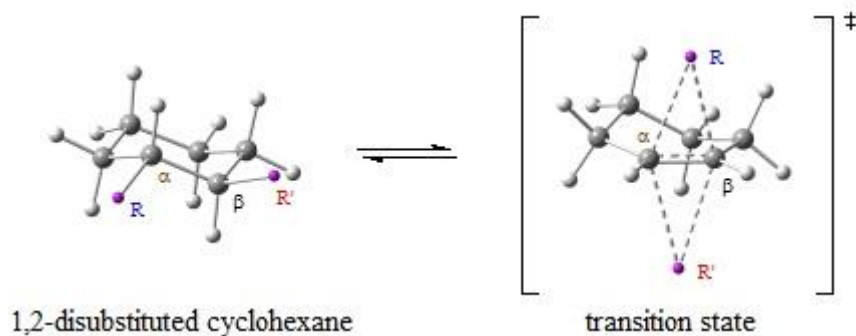


Fig. 4 Generic representation for 1,2-disubstituted cyclohexanes and corresponding transitions states.

Cartesian coordinates for **S1** (R/R' = CH₃)

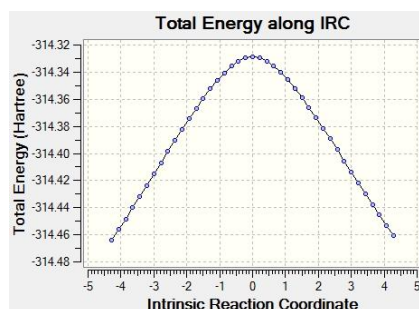
| | | | |
|---|-------------|-------------|-------------|
| C | 0.71278200 | -0.89053700 | -0.31330500 |
| C | -0.71104400 | -0.89194200 | 0.31326400 |
| C | -0.97945600 | 0.40753100 | 1.10857400 |
| C | -0.71312200 | 1.68237700 | 0.29034900 |
| C | 0.70973000 | 1.68385100 | -0.29024200 |
| C | 0.97874100 | 0.40955300 | -1.10845500 |
| H | -2.01392500 | 0.40245300 | 1.47615700 |
| H | -0.75154600 | -1.72745300 | 1.02731600 |
| H | 0.75481700 | -1.72584400 | -1.02750200 |
| H | -1.43960200 | 1.75977900 | -0.53030900 |
| H | -0.86811400 | 2.56714900 | 0.92045400 |
| H | 0.86286800 | 2.56893400 | -0.92036200 |
| H | 1.43605000 | 1.76280100 | 0.53040700 |
| H | 0.33959100 | 0.42392800 | -2.00176300 |
| H | 2.01326500 | 0.40655700 | -1.47590600 |
| H | -0.34021400 | 0.42313600 | 2.00179700 |
| C | 1.80625800 | -1.15497200 | 0.73757000 |
| H | 1.63689900 | -2.11238300 | 1.24386700 |
| H | 2.79559100 | -1.19761500 | 0.26717900 |
| H | 1.84325500 | -0.37834500 | 1.50852800 |
| C | -1.80397500 | -1.15816300 | -0.73771600 |
| H | -1.63277600 | -2.11510500 | -1.24427800 |
| H | -2.79324300 | -1.20280900 | -0.26737800 |
| H | -1.84239700 | -0.38137700 | -1.50844600 |

Cartesian coordinates for **TS1** (R/R' = CH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.09256800 | -0.84808200 | -0.70596700 |
| C | 0.02366600 | -0.88751200 | 0.65639600 |
| C | 0.15545400 | 0.35192600 | 1.50044200 |
| C | 0.50628000 | 1.59672800 | 0.66817600 |
| C | -0.34460300 | 1.68154700 | -0.60825400 |
| C | -0.18370200 | 0.43080300 | -1.49219800 |
| H | -0.14530600 | -1.78286600 | -1.25024100 |
| H | 0.05850300 | -1.85252900 | 1.14687200 |
| H | 0.91602400 | 0.17485900 | 2.26944400 |
| H | 1.56782800 | 1.55778600 | 0.39830000 |
| H | -0.07505300 | 2.57348600 | -1.18493000 |
| H | -1.02182700 | 0.34518100 | -2.19436400 |
| H | 0.71940300 | 0.50484200 | -2.11103900 |
| H | -1.39884600 | 1.79364300 | -0.33055400 |
| H | 0.36441100 | 2.49735200 | 1.27607300 |
| H | -0.79106400 | 0.49899900 | 2.03663400 |
| C | -2.33377300 | -1.04517400 | 0.21503500 |
| H | -2.63483300 | -1.73401600 | -0.57540500 |
| H | -2.48085600 | -1.46972600 | 1.20947000 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.76457800 | -0.04969000 | 0.11011500 |
| C | 2.26940000 | -1.17418400 | -0.23782800 |
| H | 2.69315400 | -0.97856500 | 0.74856600 |
| H | 2.34353700 | -2.22356600 | -0.52533100 |
| H | 2.64857600 | -0.49149700 | -0.99841300 |

IRC for **TS1** (R/R' = CH₃)



Cartesian coordinates for **S2** (R/R' = NH₂)

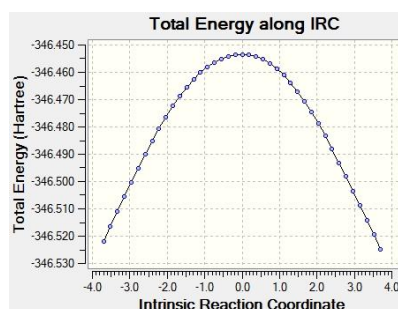
| | | | |
|---|-------------|-------------|-------------|
| C | 0.72252400 | -0.89791900 | -0.27756300 |
| C | -0.72262200 | -0.89784000 | 0.27756400 |
| C | -1.03163600 | 0.39405300 | 1.05505500 |
| C | -0.72768000 | 1.66490700 | 0.24608300 |
| C | 0.72786500 | 1.66482500 | -0.24608600 |
| C | 1.03167500 | 0.39393900 | -1.05506200 |
| H | -2.08386600 | 0.38055300 | 1.37219700 |
| H | -0.79976600 | -1.74361100 | 0.98659000 |
| H | 0.79958200 | -1.74369800 | -0.98658500 |
| H | -1.40394000 | 1.72357800 | -0.61563300 |
| H | -0.91916900 | 2.54981600 | 0.86579000 |
| H | 0.91945700 | 2.54971100 | -0.86579300 |
| H | 1.40413000 | 1.72341500 | 0.61563100 |
| H | 0.42449300 | 0.38994400 | -1.96737200 |
| H | 2.08390200 | 0.38031500 | -1.37220600 |
| H | -0.42446200 | 0.38999600 | 1.96737100 |
| N | 1.66039700 | -1.04426300 | 0.84709800 |
| H | 1.52144700 | -1.92992300 | 1.32749700 |
| H | 2.62208100 | -1.02693200 | 0.51789500 |
| N | -1.66050600 | -1.04410100 | -0.84709400 |
| H | -1.52169300 | -1.92980400 | -1.32745200 |
| H | -2.62219100 | -1.02659500 | -0.51790500 |

Cartesian coordinates for **TS2** (R/R' = NH₂)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.54787100 | 0.78405800 | -0.67418300 |
| C | -0.66791500 | 0.59637900 | 0.75324200 |
| C | 0.23926200 | -0.35171700 | 1.51659500 |
| C | 1.05105500 | -1.27223800 | 0.59041800 |
| C | 1.64022700 | -0.51188000 | -0.60677300 |
| C | 0.52518600 | 0.09062800 | -1.47948800 |
| H | -1.40541300 | 1.17112400 | -1.20748000 |
| H | -1.62019600 | 0.84320500 | 1.20430400 |
| H | -0.40303200 | -0.95391700 | 2.16135700 |
| H | 0.37268400 | -2.04707900 | 0.22066100 |
| H | 2.25044600 | -1.18095500 | -1.22326100 |
| H | 0.93184600 | 0.78092900 | -2.23008300 |
| H | -0.00886400 | -0.70584200 | -2.00393900 |
| H | 2.32981200 | 0.27343100 | -0.25387100 |
| H | 1.84779800 | -1.75883000 | 1.16479300 |
| H | 0.90750600 | 0.23377000 | 2.16734500 |
| N | 0.05714200 | 1.95995000 | 0.29453800 |
| H | -0.44869500 | 2.83460400 | 0.37917800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 1.06187800 | 2.04107200 | 0.41427300 |
| N | -2.07466700 | -1.16384300 | -0.35873100 |
| H | -3.08047900 | -0.95965400 | -0.32263000 |
| H | -2.05228000 | -2.15598800 | -0.62017200 |

IRC for **TS2** (R/R' = NH₂)

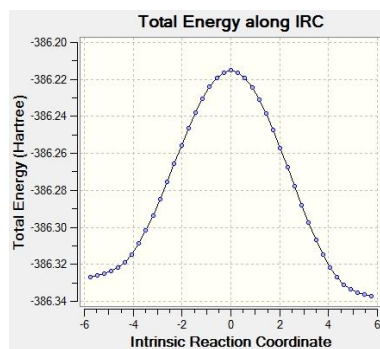


Cartesian coordinates for **S3** (R/R' = OH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68399900 | -0.94317900 | 0.24021400 |
| C | 0.77121700 | -0.87324800 | -0.26602700 |
| C | 1.05075300 | 0.42659500 | -1.02247800 |
| C | 0.66656700 | 1.67265300 | -0.20836500 |
| C | -0.80220000 | 1.60825900 | 0.23975800 |
| C | -1.07977000 | 0.31573300 | 1.02382800 |
| H | 2.11225900 | 0.44853700 | -1.29329100 |
| H | 0.93853000 | -1.72844500 | -0.93552100 |
| H | -0.77769100 | -1.82482000 | 0.89712600 |
| H | 1.31676000 | 1.74617600 | 0.67223000 |
| H | 0.84033800 | 2.57370900 | -0.80883200 |
| H | -1.05207900 | 2.47687900 | 0.86089400 |
| H | -1.45498500 | 1.65014600 | -0.64188100 |
| H | -0.50514700 | 0.32201700 | 1.95873400 |
| H | -2.13976800 | 0.24845900 | 1.30807000 |
| H | 0.47237000 | 0.40045200 | -1.95362000 |
| O | -1.49337300 | -1.14032400 | -0.92788000 |
| O | 1.68141900 | -0.93394800 | 0.84281300 |
| H | -2.42347900 | -1.14774800 | -0.66730300 |
| H | 1.63311200 | -1.81207200 | 1.24234700 |

Cartesian coordinates for **TS3** (R/R' = OH)

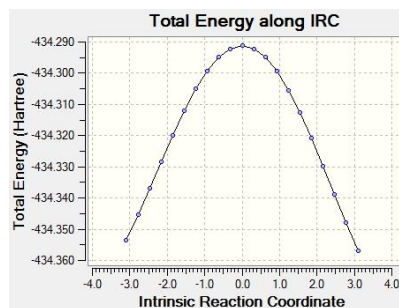
| | | | |
|---|-------------|-------------|-------------|
| C | 0.90993900 | -0.28286000 | -0.64823400 |
| C | 0.90903300 | 0.28684300 | 0.64785300 |
| C | -0.36271600 | 0.64023800 | 1.37326100 |
| C | -1.61262100 | 0.60290600 | 0.47289900 |
| C | -1.61062600 | -0.60880800 | -0.47217600 |
| C | -0.36060000 | -0.64258700 | -1.37261800 |
| H | 1.85851800 | -0.48509900 | -1.12264100 |
| H | 1.85702100 | 0.49366200 | 1.12151800 |
| H | -0.23706500 | 1.63026000 | 1.82413000 |
| H | -1.66893500 | 1.52528300 | -0.11959100 |
| H | -2.50847600 | -0.60067700 | -1.09963500 |
| H | -0.23105300 | -1.63314300 | -1.82125400 |
| H | -0.46867500 | 0.05858500 | -2.20872900 |
| H | -1.66401000 | -1.53128500 | 0.12044900 |
| H | -2.51043800 | 0.59184800 | 1.10036500 |
| H | -0.46803300 | -0.06332200 | 2.20774100 |
| O | 1.14355700 | -1.66434700 | 0.74895400 |
| O | 1.13459200 | 1.66924900 | -0.74993800 |
| H | 0.28505900 | 2.09469000 | -0.94392900 |
| H | 0.29644600 | -2.09439600 | 0.94353600 |

IRC for **TS3** (R/R' = OH)Cartesian coordinates for **S4**, R/R' = F

| | | | |
|---|-------------|-------------|-------------|
| C | -0.91629400 | 0.72875300 | 0.23754800 |
| C | -0.91650600 | -0.72850400 | -0.23755200 |
| C | 0.35760800 | -1.12220400 | -0.97158900 |
| C | 1.62513900 | -0.74586500 | -0.18658300 |
| C | 1.62535200 | 0.74543100 | 0.18655900 |
| C | 0.35793400 | 1.12208600 | 0.97159500 |
| H | 0.32324100 | -2.19699900 | -1.18187200 |
| H | -1.80687600 | -0.91914100 | -0.84519700 |
| H | -1.80660300 | 0.91963600 | 0.84520100 |
| H | 1.68108000 | -1.35410700 | 0.72511600 |
| H | 2.51141900 | -0.98946100 | -0.78351500 |
| H | 2.51170600 | 0.98875700 | 0.78348800 |
| H | 1.68145300 | 1.35368600 | -0.72512000 |
| H | 0.34958800 | 0.60365100 | 1.93919500 |
| H | 0.32387200 | 2.19687800 | 1.18193900 |
| H | 0.34937200 | -0.60382600 | -1.93921800 |
| F | -1.05077700 | 1.52392700 | -0.92988200 |
| F | -1.05118300 | -1.52362200 | 0.92989500 |

Cartesian coordinates for **TS4**, R/R' = F

| | | | |
|---|-------------|-------------|-------------|
| C | -0.90803800 | -0.46832400 | 0.53586200 |
| C | -0.90797200 | 0.46883900 | -0.53560100 |
| C | 0.35241800 | 1.01484000 | -1.11828200 |
| C | 1.59537000 | 0.72211700 | -0.26041500 |
| C | 1.59506600 | -0.72299400 | 0.25989700 |
| C | 0.35221400 | -1.01509400 | 1.11810100 |
| H | -1.86231300 | -0.79764600 | 0.92496300 |
| H | -1.86215900 | 0.79861300 | -0.92448800 |
| H | 0.21563400 | 2.09064900 | -1.27263400 |
| H | 1.61415500 | 1.41869700 | 0.58471500 |
| H | 2.49438200 | -0.91063800 | 0.85593400 |
| H | 0.21484000 | -2.09087000 | 1.27217900 |
| H | 0.44178300 | -0.56116300 | 2.11355100 |
| H | 1.61321200 | -1.41960100 | -0.58523600 |
| H | 2.49459900 | 0.90928300 | -0.85673500 |
| H | 0.44140800 | 0.56051800 | -2.11362800 |
| F | -1.01634000 | -1.32064000 | -1.17538400 |
| F | -1.01475900 | 1.32129100 | 1.17583000 |

IRC for **TS4**, R/R' = FCartesian coordinates for **S5** (R/R' = SiH₃)

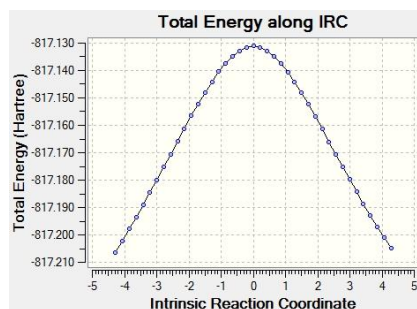
| | | | |
|----|-------------|-------------|-------------|
| C | -0.58664900 | -0.58986900 | 0.51595500 |
| C | 0.58665700 | -0.58985800 | -0.51597200 |
| C | 0.60732200 | 0.71363100 | -1.35410100 |
| C | 0.59458600 | 1.98238500 | -0.48634600 |
| C | -0.59458700 | 1.98237800 | 0.48636800 |
| C | -0.60732500 | 0.71361000 | 1.35410400 |
| H | 1.47932400 | 0.71983000 | -2.02015300 |
| H | 0.44280600 | -1.42976500 | -1.21412000 |
| H | -0.44279400 | -1.42978500 | 1.21409300 |
| H | 1.52980200 | 2.05260200 | 0.08634100 |
| H | 0.55851100 | 2.86970200 | -1.13023400 |
| H | -0.55851000 | 2.86968300 | 1.13027200 |
| H | -1.52980200 | 2.05260600 | -0.08631800 |
| H | 0.27445200 | 0.73291600 | 2.01024900 |
| H | -1.47933100 | 0.71979600 | 2.02015000 |
| H | -0.27446000 | 0.73294400 | -2.01023900 |
| Si | -2.27273700 | -1.00967500 | -0.28066400 |
| H | -2.18476800 | -2.35525800 | -0.91165900 |
| H | -3.32786000 | -1.04523300 | 0.76950600 |
| H | -2.70374500 | -0.04611100 | -1.32909100 |
| Si | 2.27273500 | -1.00967900 | 0.28065800 |
| H | 2.18476700 | -2.35530800 | 0.91155400 |
| H | 3.32789600 | -1.04514500 | -0.76947800 |
| H | 2.70369700 | -0.04618000 | 1.32916400 |

Cartesian coordinates for **TS5** (R/R' = SiH₃)

| | | | |
|----|-------------|-------------|-------------|
| C | 0.01572700 | -0.59024900 | -0.68520700 |
| C | -0.01576800 | -0.59032300 | 0.68508200 |
| C | 0.02798000 | 0.66919900 | 1.50931900 |
| C | 0.36342200 | 1.92028700 | 0.67719200 |
| C | -0.36334400 | 1.92038700 | -0.67705700 |
| C | -0.02799200 | 0.66935800 | -1.50931500 |
| H | 0.02268000 | -1.54033800 | -1.20792700 |
| H | -0.02274200 | -1.54046800 | 1.20770200 |
| H | 0.76312600 | 0.53100800 | 2.31225500 |
| H | 1.44577800 | 1.95682400 | 0.50874100 |
| H | -0.10124400 | 2.81909300 | -1.24600300 |
| H | -0.76317500 | 0.53127200 | -2.31223600 |
| H | 0.94268800 | 0.78176200 | -2.01122600 |
| H | -1.44569900 | 1.95699600 | -0.50861300 |
| H | 0.10139400 | 2.81895600 | 1.24623000 |
| H | -0.94271500 | 0.78159800 | 2.01120200 |
| Si | -2.77263100 | -0.95049100 | 0.04526800 |
| H | -3.63058600 | 0.14420200 | -0.51107900 |
| H | -3.21670800 | -1.18293400 | 1.45665800 |
| H | -3.08604300 | -2.19850400 | -0.71928900 |
| Si | 2.77261500 | -0.95052000 | -0.04528700 |
| H | 3.21668600 | -1.18346800 | -1.45659400 |
| H | 3.63053200 | 0.14442200 | 0.51063200 |

H 3.08610500 -2.19822800 0.71973400

IRC for **TS5** (R/R' = SiH₃)

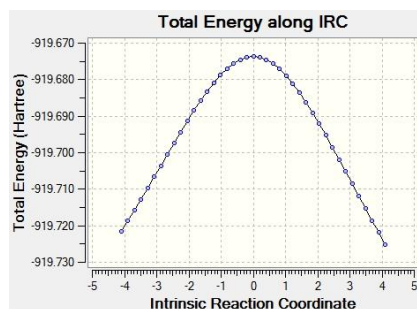


Cartesian coordinates for **S6** (R/R' = PH₂)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.58237100 | -0.61504200 | 0.51336000 |
| C | 0.58237200 | -0.61502900 | -0.51338000 |
| C | 0.62773100 | 0.69063900 | -1.34023200 |
| C | 0.60440400 | 1.96034900 | -0.47383700 |
| C | -0.60439600 | 1.96033900 | 0.47388100 |
| C | -0.62773000 | 0.69060700 | 1.34024400 |
| H | 1.51029600 | 0.68759700 | -1.99202500 |
| H | 0.45305300 | -1.45639400 | -1.20316500 |
| H | -0.45305000 | -1.45642300 | 1.20312500 |
| H | 1.52855300 | 2.02897400 | 0.11569200 |
| H | 0.58050600 | 2.84493100 | -1.12161100 |
| H | -0.58049400 | 2.84490400 | 1.12167800 |
| H | -1.52854400 | 2.02898300 | -0.11564700 |
| H | 0.24445000 | 0.70464200 | 2.00785600 |
| H | -1.51029800 | 0.68755200 | 1.99203300 |
| H | -0.24445200 | 0.70469300 | -2.00783900 |
| P | -2.23822500 | -0.90456600 | -0.38947900 |
| H | -2.02689100 | -2.28529300 | -0.67163200 |
| H | -3.01229800 | -1.17141700 | 0.77677500 |
| P | 2.23821900 | -0.90458200 | 0.38946500 |
| H | 2.02688800 | -2.28532300 | 0.67155200 |
| H | 3.01230800 | -1.17137800 | -0.77679300 |

Cartesian coordinates for **TS6** (R/R' = PH₂)

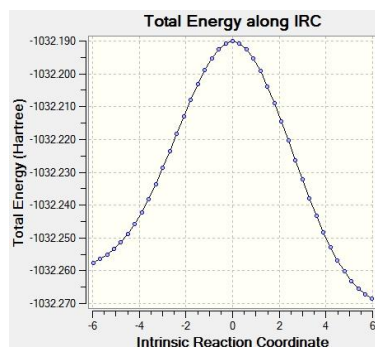
| | | | |
|---|-------------|-------------|-------------|
| C | 0.00235700 | -0.56643500 | -0.67316700 |
| C | 0.00316500 | -0.55392300 | 0.70301500 |
| C | 0.04704500 | 0.72192500 | 1.50310100 |
| C | 0.39751100 | 1.95058200 | 0.64590200 |
| C | -0.36952000 | 1.94252700 | -0.68495100 |
| C | -0.05693900 | 0.68358100 | -1.51162500 |
| H | -0.00231700 | -1.52148800 | -1.18527000 |
| H | 0.00620200 | -1.49641900 | 1.23755900 |
| H | 0.76490900 | 0.59842000 | 2.32232400 |
| H | 1.47577100 | 1.95728900 | 0.44556900 |
| H | -0.12495100 | 2.83544400 | -1.27044400 |
| H | -0.81218100 | 0.53826400 | -2.29262200 |
| H | 0.90459000 | 0.78593300 | -2.02984800 |
| H | -1.44700400 | 1.97906500 | -0.48354900 |
| H | 0.17533500 | 2.86375300 | 1.20874300 |
| H | -0.93088800 | 0.85840300 | 1.98341200 |
| P | -2.70669500 | -0.92458600 | -0.01326100 |
| P | 2.69001000 | -0.96767700 | -0.16130100 |
| H | 2.83384700 | -0.51931600 | 1.18617100 |
| H | 2.44446300 | -2.31356700 | 0.24856200 |
| H | -2.46072500 | -2.33105400 | -0.06026700 |
| H | -2.71850100 | -0.92031800 | 1.41443100 |

IRC for **TS6** (R/R' = PH₂)Cartesian coordinates for **S7** (R/R' = SH)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.55703300 | -0.65151000 | -0.51837900 |
| C | -0.58000200 | -0.63308100 | 0.52914600 |
| C | -0.59112900 | 0.66156800 | 1.36020100 |
| C | -0.56171400 | 1.93307800 | 0.49909400 |
| C | 0.61942800 | 1.91410500 | -0.48426800 |
| C | 0.60082000 | 0.64410900 | -1.35027700 |
| H | -1.46293600 | 0.66492000 | 2.02453300 |
| H | -0.46753400 | -1.49601000 | 1.19065500 |
| H | 0.42365800 | -1.50507400 | -1.18804800 |
| H | -1.50132800 | 2.01660400 | -0.06136200 |
| H | -0.50031100 | 2.81321000 | 1.14996200 |
| H | 0.58761100 | 2.79686300 | -1.13369900 |
| H | 1.56430900 | 1.97155400 | 0.07266100 |
| H | -0.29354800 | 0.65893600 | -1.98687400 |
| H | 1.46479800 | 0.61550400 | -2.02285600 |
| H | 0.29652700 | 0.64001700 | 2.00637500 |
| S | 2.21843500 | -0.89822700 | 0.29537400 |
| H | 2.01867800 | -2.18305500 | 0.65256300 |
| S | -2.18395500 | -0.92120700 | -0.39647500 |
| H | -2.94822200 | -1.09213600 | 0.70059900 |

Cartesian coordinates for **TS7** (R/R' = SH)

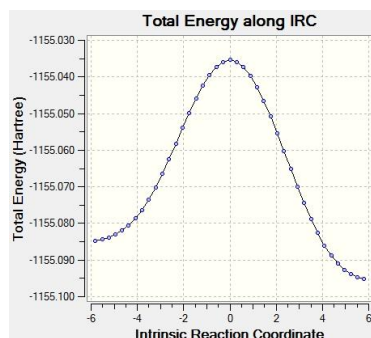
| | | | |
|---|-------------|-------------|-------------|
| C | -0.00811800 | -0.62329600 | -0.70877200 |
| C | 0.00810200 | -0.62330000 | 0.70876700 |
| C | 0.06383400 | 0.65219300 | 1.51719000 |
| C | 0.37163000 | 1.90344400 | 0.67258700 |
| C | -0.37163500 | 1.90345200 | -0.67257800 |
| C | -0.06385500 | 0.65220100 | -1.51719000 |
| H | -0.02491200 | -1.56668500 | -1.23484900 |
| H | 0.02492000 | -1.56669000 | 1.23484100 |
| H | 0.81352300 | 0.52206100 | 2.30417900 |
| H | 1.45118600 | 1.96515400 | 0.49200300 |
| H | -0.10579800 | 2.79730200 | -1.24708400 |
| H | -0.81354600 | 0.52207500 | -2.30417700 |
| H | 0.89711400 | 0.76179100 | -2.03165300 |
| H | -1.45119100 | 1.96517700 | -0.49199200 |
| H | 0.10580200 | 2.79729400 | 1.24709400 |
| H | -0.89713700 | 0.76178900 | 2.03164900 |
| H | -2.74059800 | 0.26960400 | 0.12572600 |
| H | 2.74065200 | 0.26960500 | -0.12573800 |
| S | -2.35502700 | -1.02146300 | 0.07163800 |
| S | 2.35504200 | -1.02145200 | -0.07163900 |

IRC for **TS7** (R/R' = SH)Cartesian coordinates for **S8** (R/R' = Cl)

| | | | |
|----|-------------|-------------|-------------|
| C | 0.54808300 | -0.65416600 | -0.53838200 |
| C | -0.54807300 | -0.65417600 | 0.53838200 |
| C | -0.59242400 | 0.63460800 | 1.36064400 |
| C | -0.58890400 | 1.90286000 | 0.49402700 |
| C | 0.58887900 | 1.90287400 | -0.49402100 |
| C | 0.59241500 | 0.63462200 | -1.36064000 |
| H | -1.46375600 | 0.60898700 | 2.02236700 |
| H | -0.44292800 | -1.52931500 | 1.17956900 |
| H | 0.44294600 | -1.52930200 | -1.17957400 |
| H | -1.53482300 | 1.97037500 | -0.05779300 |
| H | -0.53959100 | 2.78407000 | 1.14371200 |
| H | 0.53954200 | 2.78408500 | -1.14370200 |
| H | 1.53479900 | 1.97040500 | 0.05779300 |
| H | -0.29755000 | 0.62609600 | -2.00356800 |
| H | 1.46373900 | 0.60901200 | -2.02237400 |
| H | 0.29753200 | 0.62609100 | 2.00358300 |
| Cl | -2.15885200 | -0.92707300 | -0.32063500 |
| Cl | 2.15886600 | -0.92705800 | 0.32063000 |

Cartesian coordinates for **TS8** (R/R' = Cl)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.01162500 | -0.63733800 | -0.71684400 |
| C | 0.01161400 | -0.63734100 | 0.71684100 |
| C | 0.07680100 | 0.63320600 | 1.51418200 |
| C | 0.39159400 | 1.87496600 | 0.66082200 |
| C | -0.39157400 | 1.87497500 | -0.66081600 |
| C | -0.07680000 | 0.63321400 | -1.51417900 |
| H | -0.02649900 | -1.58937200 | -1.22886100 |
| H | 0.02648200 | -1.58937800 | 1.22885300 |
| H | 0.82280900 | 0.49382000 | 2.30354100 |
| H | 1.46671900 | 1.90087300 | 0.45340200 |
| H | -0.15270700 | 2.77298300 | -1.23976500 |
| H | -0.82281100 | 0.49384100 | -2.30353700 |
| Cl | 2.25463200 | -0.91424800 | -0.08570000 |
| Cl | -2.25463800 | -0.91423600 | 0.08569700 |
| H | 0.89023400 | 0.73874700 | -2.01954500 |
| H | -1.46669900 | 1.90090500 | -0.45339800 |
| H | 0.15274600 | 2.77297600 | 1.23977500 |
| H | -0.89023300 | 0.73874900 | 2.01954400 |

IRC for **TS8** (R/R' = Cl)Cartesian coordinates for **S9** (R/R' = CH₂CH₃)

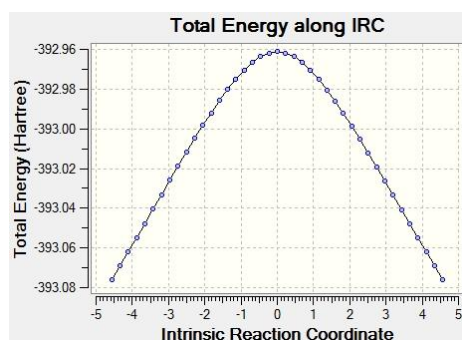
| | | | |
|---|-------------|-------------|-------------|
| C | 0.70376300 | -0.59073200 | -0.33282300 |
| C | -0.70374500 | -0.59075700 | 0.33280000 |
| C | -0.92910800 | 0.70529400 | 1.14865800 |
| C | -0.69598700 | 1.98352200 | 0.32553700 |
| C | 0.69594600 | 1.98354600 | -0.32548500 |
| C | 0.92909200 | 0.70534800 | -1.14864400 |
| H | -1.93835500 | 0.71115600 | 1.57662400 |
| H | -0.72685600 | -1.43331300 | 1.04105400 |
| H | 0.72688900 | -1.43326900 | -1.04110000 |
| H | -1.46162200 | 2.06965100 | -0.45793700 |
| H | -0.81586700 | 2.86527800 | 0.96754600 |
| H | 0.81580700 | 2.86532400 | -0.96746800 |
| H | 1.46158000 | 2.06966700 | 0.45799100 |
| H | 0.24367700 | 0.70884400 | -2.00687200 |
| H | 1.93833300 | 0.71124700 | -1.57662200 |
| H | -0.24370200 | 0.70878100 | 2.00689300 |
| C | 1.82497500 | -0.86423000 | 0.69663400 |
| H | 1.52660000 | -1.73338000 | 1.29868500 |
| H | 1.91274900 | -0.02844700 | 1.40170300 |
| C | -1.82495700 | -0.86424000 | -0.69666100 |
| H | -1.52658700 | -1.73337800 | -1.29873100 |
| H | -1.91273500 | -0.02844100 | -1.40170800 |
| C | -3.20187400 | -1.14764400 | -0.08095900 |
| C | 3.20189700 | -1.14763000 | 0.08094100 |
| H | 3.92658100 | -1.42133400 | 0.85565400 |
| H | 3.15151400 | -1.97762500 | -0.63452800 |
| H | 3.60545200 | -0.27831000 | -0.44876800 |
| H | -3.60540700 | -0.27833800 | 0.44879000 |
| H | -3.92657400 | -1.42130700 | -0.85567200 |
| H | -3.15149100 | -1.97766700 | 0.63447600 |

Cartesian coordinates for **TS9** (R/R' = CH₂CH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.20799300 | -0.57020800 | 0.37791900 |
| C | 0.27267000 | -0.21765500 | -0.93596000 |
| C | -0.11336300 | 1.14671600 | -1.43853000 |
| C | -0.89979100 | 1.95764000 | -0.39588900 |
| C | -0.25829700 | 1.84408000 | 0.99482400 |
| C | -0.19451600 | 0.38126800 | 1.46759900 |
| H | 0.46906400 | -1.58417400 | 0.66055200 |
| H | 0.59388900 | -0.95818500 | -1.66072500 |
| H | -0.69500000 | 1.03322000 | -2.36106500 |
| H | -1.92940500 | 1.58280000 | -0.35362300 |
| H | -0.81581200 | 2.44367100 | 1.72325400 |
| H | 0.50678100 | 0.27583400 | 2.30472200 |
| H | -1.16998000 | 0.05826500 | 1.85546000 |
| H | 0.75751300 | 2.25634400 | 0.95668500 |
| H | -0.95403900 | 3.00717300 | -0.70663200 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.80459500 | 1.67874100 | -1.72437800 |
| C | 2.60805900 | 0.00748200 | -0.07387300 |
| H | 2.67000200 | 0.71574900 | 0.75328300 |
| H | 2.82353400 | 0.47696400 | -1.03493200 |
| C | -1.94131000 | -1.43611800 | -0.70465300 |
| H | -2.27065800 | -0.87517400 | -1.58154600 |
| H | -1.51043700 | -2.40219500 | -0.97436800 |
| C | -2.92280500 | -1.46694600 | 0.43861900 |
| C | 3.24775400 | -1.33726300 | 0.14744800 |
| H | -3.84850500 | -2.02013700 | 0.19580800 |
| H | -2.50377100 | -1.95393600 | 1.32956400 |
| H | -3.24151500 | -0.45841000 | 0.73388800 |
| H | 2.95188600 | -2.06166100 | -0.62539800 |
| H | 4.35086300 | -1.30233100 | 0.12500500 |
| H | 2.97264000 | -1.76653800 | 1.11942600 |

IRC for **TS9** (R/R' = CH₂CH₃)



Cartesian coordinates for **S10** (R/R' = CH(CH₃)₂)

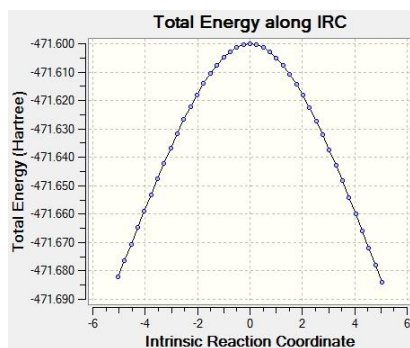
| | | | |
|---|-------------|-------------|-------------|
| C | -0.64018000 | -0.25926300 | 0.65998000 |
| C | 0.51477300 | -0.21855900 | -0.39601700 |
| C | 0.53525200 | 1.12481800 | -1.16756400 |
| C | 0.57239400 | 2.36006500 | -0.25755700 |
| C | -0.64782400 | 2.36815500 | 0.67164300 |
| C | -0.72750900 | 1.06121800 | 1.47622600 |
| H | 1.37541600 | 1.13872500 | -1.86899200 |
| H | 0.32514100 | -1.00341400 | -1.14316500 |
| H | -0.35912900 | -1.01712500 | 1.40147800 |
| H | 1.49164600 | 2.36198700 | 0.34551200 |
| H | 0.59807400 | 3.27299000 | -0.86580500 |
| H | -0.60094400 | 3.21853000 | 1.36397100 |
| H | -1.55536100 | 2.51047900 | 0.07144900 |
| H | 0.10393100 | 1.06918200 | 2.19508100 |
| H | -1.64241700 | 1.04458100 | 2.08320500 |
| H | -0.36622200 | 1.18756700 | -1.78712000 |
| C | -2.02064000 | -0.77797800 | 0.14102800 |
| C | 1.88476900 | -0.58882800 | 0.26537100 |
| C | -1.97806900 | -2.29221300 | -0.13934400 |
| C | -2.64200500 | -0.05345900 | -1.06646900 |
| C | 3.11139200 | -0.22487100 | -0.58989800 |
| C | 1.95238100 | -2.09168600 | 0.59946800 |
| H | -2.74660500 | 1.02250500 | -0.90431000 |
| H | -2.05076400 | -0.20357300 | -1.97676800 |
| H | -3.64336100 | -0.45404800 | -1.26357900 |
| H | -2.97592300 | -2.66704000 | -0.39418500 |
| H | -1.31629900 | -2.53186500 | -0.97991800 |
| H | -1.62412700 | -2.85312800 | 0.73299600 |
| H | 3.22403100 | 0.85373000 | -0.73080000 |
| H | 4.02715300 | -0.58828400 | -0.10997800 |
| H | 3.05478900 | -0.69055200 | -1.58239100 |
| H | 1.94543500 | -2.68915100 | -0.32133800 |
| H | 2.87528900 | -2.32888500 | 1.14057900 |

| | | | |
|---|-------------|-------------|------------|
| H | 1.11522700 | -2.42843800 | 1.21757800 |
| H | -2.71258900 | -0.63631300 | 0.98511900 |
| H | 1.96921100 | -0.03285200 | 1.21017800 |

Cartesian coordinates for **TS10** (R/R' = CH(CH₃)₂)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.00388500 | -0.14302600 | 0.67674900 |
| C | 0.00393800 | -0.14315300 | -0.67666700 |
| C | -0.02190100 | 1.11400400 | -1.50110900 |
| C | -0.36701400 | 2.36493500 | -0.67451000 |
| C | 0.36654800 | 2.36516700 | 0.67414900 |
| C | 0.02180800 | 1.11427300 | 1.50097800 |
| H | -0.00981500 | -1.09100500 | 1.20500000 |
| H | 0.00997100 | -1.09122500 | -1.20474400 |
| H | -0.73798800 | 0.98785400 | -2.32319700 |
| H | -1.44926700 | 2.39228800 | -0.49701300 |
| H | 0.11811400 | 3.26783700 | 1.24411800 |
| H | 0.73804100 | 0.98839300 | 2.32298100 |
| H | -0.96076800 | 1.23179700 | 1.98139700 |
| H | 1.44879600 | 2.39282500 | 0.49665900 |
| H | -0.11885100 | 3.26757900 | -1.24463900 |
| H | 0.96072400 | 1.23167700 | -1.98139400 |
| C | 2.58480900 | -0.53068400 | -0.03328500 |
| C | -2.58470400 | -0.53086600 | 0.03330200 |
| C | -2.84650700 | -1.26597300 | 1.31321500 |
| C | -2.86860800 | -1.27478900 | -1.23679100 |
| C | 2.86885100 | -1.27428100 | 1.23696000 |
| C | 2.84664200 | -1.26606200 | -1.31303000 |
| H | -3.93180100 | -1.57795800 | -1.31464000 |
| H | -2.64396500 | -0.68167200 | -2.13040800 |
| H | -2.29043700 | -2.20966100 | -1.29925900 |
| H | -3.91109500 | -1.55594200 | 1.41706800 |
| H | -2.27775800 | -2.20707100 | 1.36633600 |
| H | -2.59491800 | -0.67240800 | 2.19982000 |
| H | 2.29074200 | -2.20917400 | 1.29967200 |
| H | 3.93207000 | -1.57736200 | 1.31480900 |
| H | 2.64422500 | -0.68098600 | 2.13046200 |
| H | 2.59492100 | -0.67277700 | -2.19978400 |
| H | 3.91126400 | -1.55590500 | -1.41688000 |
| H | 2.27802200 | -2.20725500 | -1.36588000 |
| H | -2.84894700 | 0.52632600 | 0.03283000 |
| H | 2.84885900 | 0.52655400 | -0.03309200 |

IRC for **TS10** [R/R' = CH(CH₃)₂]



Cartesian coordinates for **S11** [R/R' = C(CH₃)₃]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.60701800 | -0.10517100 | 0.50041000 |
| C | 0.60701400 | -0.10518800 | -0.50040600 |
| C | 0.74173300 | 1.24916900 | -1.25703700 |
| C | 0.64832800 | 2.52373800 | -0.40700900 |
| C | -0.64827800 | 2.52372100 | 0.40702500 |

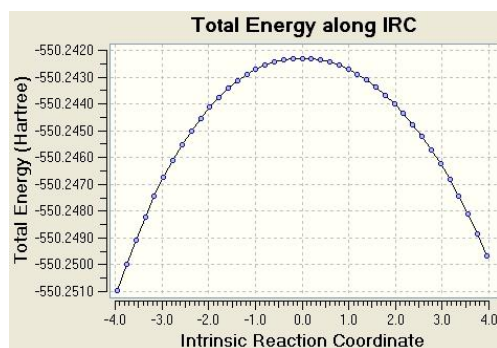
| | | | |
|---|-------------|-------------|-------------|
| C | -0.74172600 | 1.24916000 | 1.25705600 |
| H | 1.66291300 | 1.25711900 | -1.84581500 |
| H | 0.37039000 | -0.83078200 | -1.28861900 |
| H | -0.37041600 | -0.83077500 | 1.28861200 |
| H | 1.50576400 | 2.60567500 | 0.27270000 |
| H | 0.69148600 | 3.40167200 | -1.06436800 |
| H | -0.69147200 | 3.40164100 | 1.06439900 |
| H | -1.50570900 | 2.60565100 | -0.27270900 |
| H | 0.06937900 | 1.29756800 | 1.99337900 |
| H | -1.66292300 | 1.25716900 | 1.84580100 |
| H | -0.06938900 | 1.29762600 | -1.99332900 |
| C | -1.95272300 | -0.68660400 | -0.10484500 |
| C | 1.95269600 | -0.68662600 | 0.10483800 |
| C | -1.76742900 | -2.19534900 | -0.39582400 |
| C | -3.09678900 | -0.57409100 | 0.92976600 |
| C | -2.42298400 | -0.00797300 | -1.40989400 |
| C | 3.09673700 | -0.57401500 | -0.92977500 |
| C | 1.76750400 | -2.19539500 | 0.39577600 |
| C | 2.42294200 | -0.00802300 | 1.40992300 |
| H | -3.96401700 | -1.15304300 | 0.59192600 |
| H | -2.79569300 | -0.96963900 | 1.90748900 |
| H | -3.43330900 | 0.45748800 | 1.07110200 |
| H | -2.59899800 | 1.06350100 | -1.27939000 |
| H | -1.70369400 | -0.13847800 | -2.22441400 |
| H | -3.36778600 | -0.45666200 | -1.74000400 |
| H | -2.69805800 | -2.62078300 | -0.78846600 |
| H | -0.98526700 | -2.38877200 | -1.13581800 |
| H | -1.50897800 | -2.74696600 | 0.51540600 |
| H | 3.43311400 | 0.45759700 | -1.07114700 |
| H | 3.96402800 | -1.15285000 | -0.59190500 |
| H | 2.79568500 | -0.96963900 | -1.90748100 |
| H | 1.50896500 | -2.74699300 | -0.51543600 |
| H | 2.69819800 | -2.62080000 | 0.78829300 |
| H | 0.98544800 | -2.38886100 | 1.13586500 |
| H | 1.70332500 | -0.13799000 | 2.22424700 |
| H | 3.36742400 | -0.45713400 | 1.74036300 |
| H | 2.59954900 | 1.06333600 | 1.27929700 |

Cartesian coordinates for **TS11** [R/R' = C(CH₃)₃]

| | | | |
|---|-------------|-------------|-------------|
| C | 0.00528100 | 0.00663000 | -0.67338300 |
| C | -0.00539600 | 0.00591000 | 0.67191000 |
| C | 0.00086700 | 1.26324600 | 1.50132500 |
| C | 0.36208600 | 2.51132900 | 0.67789500 |
| C | -0.36100700 | 2.51226000 | -0.67666600 |
| C | -0.00069200 | 1.26482400 | -1.50148600 |
| H | 0.01668900 | -0.93905200 | -1.20695000 |
| H | -0.01700800 | -0.94032700 | 1.20448100 |
| H | 0.70031900 | 1.14429000 | 2.33962100 |
| H | 1.44591100 | 2.52836900 | 0.50699600 |
| H | -0.11615100 | 3.41949300 | -1.24158600 |
| H | -0.70050400 | 1.14706300 | -2.33965600 |
| H | 0.99119200 | 1.38902400 | -1.96387500 |
| H | -1.44478400 | 2.52980200 | -0.50548600 |
| H | 0.11767500 | 3.41811700 | 1.24372500 |
| H | -0.99113200 | 1.38748200 | 1.96345500 |
| C | -2.91535800 | -0.83231000 | 0.01851800 |
| C | 2.91518500 | -0.83265500 | -0.01861300 |
| C | 3.67174400 | 0.45366400 | -0.01886600 |
| C | 2.87924800 | -1.60896700 | -1.29270500 |
| C | 2.88402400 | -1.61619400 | 1.25122300 |
| C | -2.88370000 | -1.61944900 | -1.24907100 |
| C | -2.88061200 | -1.60515100 | 1.29476000 |
| C | -3.67156000 | 0.45421700 | 0.01483500 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.84379300 | -2.15061100 | 1.42453000 |
| H | 2.72475200 | -0.97915000 | 2.12961800 |
| H | 2.10661100 | -2.39140000 | 1.24031700 |
| H | 3.84082100 | -2.13711100 | -1.47491000 |
| H | 2.10575100 | -2.38802600 | -1.28183400 |
| H | 2.71190900 | -0.96770400 | -2.16667300 |
| H | 4.77067100 | 0.28089400 | -0.04624500 |
| H | 3.44134700 | 1.07004400 | -0.89678800 |
| H | 3.47930500 | 1.04719000 | 0.88269100 |
| H | -2.10602900 | -2.39437900 | -1.23577400 |
| H | -3.84324100 | -2.15472100 | -1.42099500 |
| H | -2.72445600 | -0.98489600 | -2.12925800 |
| H | -2.71360000 | -0.96158800 | 2.16709600 |
| H | -3.84254800 | -2.13237100 | 1.47772500 |
| H | -2.10744800 | -2.38457000 | 1.28655500 |
| H | -3.47900400 | 1.04496700 | -0.88852400 |
| H | -4.77053200 | 0.28182100 | 0.04282900 |
| H | -3.44096900 | 1.07322400 | 0.89085800 |

IRC for **TS11** [R/R' = C(CH₃)₃]



Cartesian coordinates for **S12** (R/R' = CH₂CHCH₂)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68669900 | -0.55396200 | 0.36402900 |
| C | 0.68670200 | -0.55396000 | -0.36402400 |
| C | 0.89355500 | 0.74242100 | -1.18115700 |
| C | 0.68502800 | 2.01819800 | -0.34775000 |
| C | -0.68503900 | 2.01819400 | 0.34775000 |
| C | -0.89355700 | 0.74241800 | 1.18116000 |
| H | 1.89649500 | 0.74060800 | -1.62366700 |
| H | 0.68019900 | -1.39589000 | -1.07295100 |
| H | -0.68019300 | -1.39589200 | 1.07295600 |
| H | 1.47627000 | 2.10328500 | 0.40967600 |
| H | 0.78508900 | 2.90044700 | -0.99218700 |
| H | -0.78510500 | 2.90044400 | 0.99218500 |
| H | -1.47628200 | 2.10327400 | -0.40967600 |
| H | -0.18799000 | 0.75002300 | 2.02294800 |
| H | -1.89649600 | 0.74060000 | 1.62367200 |
| H | 0.18799000 | 0.75002200 | -2.02294600 |
| C | -1.85495100 | -0.82784800 | -0.62008200 |
| C | 1.85495600 | -0.82784100 | 0.62008500 |
| C | -3.16605600 | -1.10705100 | 0.06368100 |
| C | 3.16605800 | -1.10705100 | -0.06367900 |
| C | 4.31355000 | -0.45702900 | 0.15441700 |
| C | -4.31354800 | -0.45703300 | -0.15442900 |
| H | -1.98196500 | 0.00231600 | -1.32423600 |
| H | -1.58303700 | -1.70724200 | -1.22312100 |
| H | -3.15565000 | -1.92061900 | 0.79210700 |
| H | -5.22797700 | -0.72292600 | 0.36830000 |
| H | -4.37810400 | 0.36162800 | -0.86825100 |
| H | 1.58304300 | -1.70723000 | 1.22313100 |
| H | 1.98197400 | 0.00232800 | 1.32423300 |

| | | | |
|---|------------|-------------|-------------|
| H | 3.15565000 | -1.92063000 | -0.79209400 |
| H | 4.37811000 | 0.36164100 | 0.86822900 |
| H | 5.22797800 | -0.72292900 | -0.36831300 |

Cartesian coordinates for **TS12** (R/R' = CH₂CHCH₂)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.06991900 | -0.38048600 | -0.54761900 |
| C | 0.11116100 | 0.82639500 | -1.15844700 |
| C | -0.06972100 | 2.12961300 | -0.42552500 |
| C | -0.58129600 | 1.92647700 | 1.01157900 |
| C | 0.14546200 | 0.76309700 | 1.70247600 |
| C | -0.04744000 | -0.55533500 | 0.93291500 |
| H | 0.19305100 | -1.27755500 | -1.14790900 |
| H | 0.23287900 | 0.87078900 | -2.23808700 |
| H | -0.76128500 | 2.76946300 | -0.99027800 |
| H | -1.65598900 | 1.70900400 | 0.98193900 |
| H | -0.20945800 | 0.64953200 | 2.73315100 |
| H | 0.68825100 | -1.30385800 | 1.25995900 |
| H | -1.03900500 | -0.99067600 | 1.15896800 |
| H | 1.21768400 | 0.99281100 | 1.76255000 |
| H | -0.45974800 | 2.85231800 | 1.58579000 |
| H | 0.88789500 | 2.67303600 | -0.41805100 |
| C | 3.02935700 | 0.29503200 | -0.92694900 |
| H | 2.95759400 | 0.57131800 | -1.97184300 |
| H | 2.97356900 | 1.09515800 | -0.19631300 |
| C | -2.72439100 | -0.55908900 | -1.47279700 |
| H | -2.73876000 | 0.29808200 | -2.13509600 |
| H | -2.28380400 | -1.47346200 | -1.85676200 |
| C | 3.37290500 | -1.00521900 | -0.54425500 |
| H | 3.46436500 | -1.74480400 | -1.34076300 |
| C | 3.58938300 | -1.43854900 | 0.74610000 |
| H | 3.85735900 | -2.46755700 | 0.95883500 |
| H | 3.53227700 | -0.75536300 | 1.58913400 |
| C | -3.39677400 | -0.54217300 | -0.25142700 |
| H | -3.87307500 | 0.39571000 | 0.03670700 |
| C | -3.48312800 | -1.59329700 | 0.64073200 |
| H | -3.04722500 | -2.56265200 | 0.41449000 |
| H | -4.02919800 | -1.50009700 | 1.57288800 |

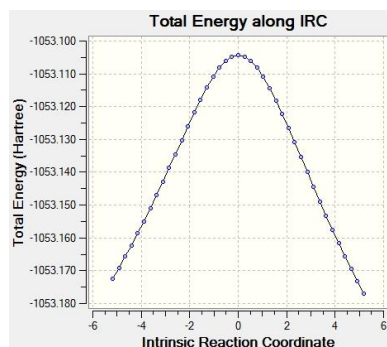
Cartesian coordinates for **S13** [R/R' = Si(CH₃)₃]

| | | | |
|----|-------------|-------------|-------------|
| C | -0.55627900 | -0.00255200 | 0.55174800 |
| C | 0.55629000 | -0.00252200 | -0.55182700 |
| C | 0.55451700 | 1.31464000 | -1.37090700 |
| C | 0.58013000 | 2.58134200 | -0.50253100 |
| C | -0.57997100 | 2.58132900 | 0.50271200 |
| C | -0.55442400 | 1.31453600 | 1.37096000 |
| H | 1.39702400 | 1.32303100 | -2.07303300 |
| H | 0.32415700 | -0.80912200 | -1.26829300 |
| H | -0.32418100 | -0.80922400 | 1.26814500 |
| H | 1.53095700 | 2.64576300 | 0.04450200 |
| H | 0.53034500 | 3.47061000 | -1.14360900 |
| H | -0.53012000 | 3.47052800 | 1.14388200 |
| H | -1.53080000 | 2.64586500 | -0.04429800 |
| H | 0.35111900 | 1.35255000 | 1.99178500 |
| H | -1.39691400 | 1.32290500 | 2.07310400 |
| H | -0.35100800 | 1.35276400 | -1.99175300 |
| Si | -2.28483400 | -0.58475800 | -0.06241800 |
| Si | 2.28478600 | -0.58489800 | 0.06236400 |
| C | -3.53188600 | -0.44412700 | 1.36248900 |
| C | -2.13486700 | -2.41561900 | -0.54386100 |
| C | -2.98658800 | 0.34597400 | -1.56187100 |
| C | 2.13458200 | -2.41576900 | 0.54366900 |
| C | 2.98662500 | 0.34563900 | 1.56190300 |

| | | | |
|---|-------------|-------------|-------------|
| C | 3.53196300 | -0.44402400 | -1.36241100 |
| H | -3.75105300 | 0.59942400 | 1.61480100 |
| H | -4.48001500 | -0.92204200 | 1.08815600 |
| H | -3.16555900 | -0.93631000 | 2.27130200 |
| H | -1.78811000 | -3.02620300 | 0.29805400 |
| H | -3.10736800 | -2.81057800 | -0.86098500 |
| H | -1.43447600 | -2.56676900 | -1.37333500 |
| H | -2.34452600 | 0.24670000 | -2.44386300 |
| H | -3.96755800 | -0.07027600 | -1.82329400 |
| H | -3.12365800 | 1.41470200 | -1.36628800 |
| H | 3.96756600 | -0.07074700 | 1.82323300 |
| H | 3.12383600 | 1.41435200 | 1.36632300 |
| H | 2.34463500 | 0.24644600 | 2.44395200 |
| H | 3.10705400 | -2.81095900 | 0.86058900 |
| H | 1.43433600 | -2.56673600 | 1.37330500 |
| H | 1.78748100 | -3.02627700 | -0.29815600 |
| H | 4.48008200 | -0.92197600 | -1.08811100 |
| H | 3.16576600 | -0.93593700 | -2.27141900 |
| H | 3.75112100 | 0.59961600 | -1.61438000 |

Cartesian coordinates for **TS13** [R/R' = Si(CH₃)₃]

| | | | |
|----|-------------|-------------|-------------|
| C | -0.01933600 | -0.06540000 | 0.66312900 |
| C | 0.02552100 | -0.05263700 | -0.69762600 |
| C | -0.01553800 | 1.21251300 | -1.51259100 |
| C | -0.36221100 | 2.45326700 | -0.67013000 |
| C | 0.36364900 | 2.44203400 | 0.68420000 |
| C | 0.02186600 | 1.18377500 | 1.50231700 |
| H | -0.03187000 | -1.01950500 | 1.17921600 |
| H | 0.03552500 | -0.99668300 | -1.23151200 |
| H | -0.74786600 | 1.08192900 | -2.32003200 |
| H | -1.44489600 | 2.47581500 | -0.49967300 |
| H | 0.10506800 | 3.33799700 | 1.26026000 |
| H | 0.75544200 | 1.03949500 | 2.30649000 |
| H | -0.95074400 | 1.29781400 | 2.00045900 |
| H | 1.44592000 | 2.47432800 | 0.51403200 |
| H | -0.10908400 | 3.36160900 | -1.22889800 |
| H | 0.95768100 | 1.33954500 | -2.00688500 |
| Si | 2.89415200 | -0.52869300 | -0.01845200 |
| Si | -2.89449200 | -0.53003100 | 0.00666500 |
| C | 4.14686900 | 0.84919200 | 0.42386300 |
| C | 3.39676500 | -1.23032200 | -1.72692900 |
| C | 3.11798200 | -1.93915000 | 1.25527600 |
| C | -3.01804000 | -2.32343400 | -0.64843000 |
| C | -3.58929600 | -0.53347800 | 1.79054300 |
| C | -4.06380900 | 0.54943800 | -1.05780500 |
| H | 2.46604000 | -2.79139700 | 1.03150100 |
| H | 4.15530200 | -2.30519300 | 1.24861000 |
| H | 2.89119000 | -1.60398000 | 2.27380400 |
| H | 3.34011500 | -0.46724800 | -2.51137400 |
| H | 4.43160000 | -1.60270100 | -1.69934100 |
| H | 2.75285900 | -2.06512800 | -2.02627800 |
| H | 3.95157700 | 1.26987200 | 1.41646500 |
| H | 5.17134900 | 0.44733900 | 0.42732900 |
| H | 4.11437600 | 1.67071900 | -0.30029000 |
| H | -4.05506100 | -2.68550600 | -0.58951600 |
| H | -2.70143700 | -2.39331400 | -1.69535000 |
| H | -2.39504900 | -3.01109400 | -0.06496400 |
| H | -4.61663000 | -0.92733000 | 1.80069900 |
| H | -2.98791000 | -1.16051400 | 2.45858000 |
| H | -3.61814900 | 0.47595200 | 2.21606900 |
| H | -5.09346500 | 0.16482500 | -1.00348200 |
| H | -4.07934000 | 1.58961700 | -0.71406300 |
| H | -3.76432200 | 0.55007200 | -2.11174500 |

IRC for **TS13** [R/R' = Si(CH₃)₃]Cartesian coordinates for **S14** [R/R' = P(CH₃)₂]

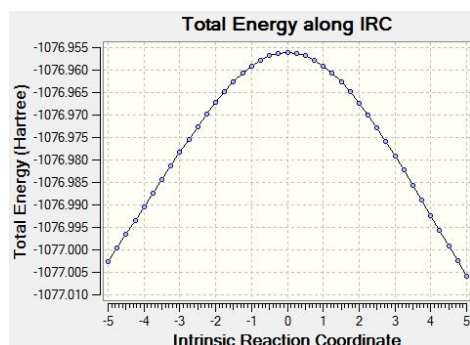
| | | | |
|---|-------------|-------------|-------------|
| C | 0.71509900 | 0.01124200 | -0.48654500 |
| C | -0.53808700 | -0.33462700 | 0.36851100 |
| C | -0.82271700 | 0.73220600 | 1.45334000 |
| C | -0.78594200 | 2.18707800 | 0.95201000 |
| C | 0.49222600 | 2.48614300 | 0.15691500 |
| C | 0.67450900 | 1.47271400 | -0.98270800 |
| H | -1.78477700 | 0.52812200 | 1.93978400 |
| H | -0.33025200 | -1.27559100 | 0.89741200 |
| H | 0.72902000 | -0.64907600 | -1.36502400 |
| H | -1.65518400 | 2.39407000 | 0.31734200 |
| H | -0.86443600 | 2.86396700 | 1.81204900 |
| H | 0.45362000 | 3.50397100 | -0.25067900 |
| H | -0.16299300 | 1.57474000 | -1.68864000 |
| H | 1.57648500 | 1.70320400 | -1.56066000 |
| H | -0.06036000 | 0.62324100 | 2.23677900 |
| P | 2.31175100 | -0.37510400 | 0.47746700 |
| P | -1.97947500 | -0.92765100 | -0.73263200 |
| C | 3.58616300 | -0.05842700 | -0.85198400 |
| C | 2.28557300 | -2.24130200 | 0.37400800 |
| C | -2.96960500 | -1.86507400 | 0.54535800 |
| C | -3.13830400 | 0.52373400 | -0.94119600 |
| H | 3.24764800 | -2.62488600 | 0.72880200 |
| H | 1.51120600 | -2.65203400 | 1.02821700 |
| H | 2.11643600 | -2.60590000 | -0.64676200 |
| H | 4.53507900 | -0.50443900 | -0.53662100 |
| H | 3.30225300 | -0.48947900 | -1.82032100 |
| H | 3.75454800 | 1.01476200 | -0.97689300 |
| H | -2.69117400 | 1.28742900 | -1.58310100 |
| H | -4.03590200 | 0.15262100 | -1.44774300 |
| H | -3.44255500 | 0.98346600 | 0.00542500 |
| H | -3.19785300 | -1.26654800 | 1.43530600 |
| H | -3.91361100 | -2.18801400 | 0.09473400 |
| H | -2.42503400 | -2.76306100 | 0.85331900 |
| H | 1.36019400 | 2.44862200 | 0.82848900 |

Cartesian coordinates for **TS14** [R/R' = P(CH₃)₂]

| | | | |
|---|-------------|-------------|-------------|
| C | 0.01325000 | 0.11844800 | -0.91742500 |
| C | -0.02105300 | 0.08600200 | 0.44313000 |
| C | 0.01668800 | 1.32776300 | 1.29186300 |
| C | 0.38939600 | 2.58293200 | 0.48464500 |
| C | -0.35710100 | 2.62065700 | -0.85690700 |
| C | -0.02046900 | 1.39064400 | -1.71622100 |
| H | 0.02196200 | -0.81975600 | -1.46338500 |
| H | -0.03122500 | -0.87591400 | 0.94920900 |
| H | 0.72472100 | 1.17290000 | 2.11542700 |
| H | 1.47022700 | 2.58298000 | 0.29760400 |
| H | -0.11023800 | 3.53543500 | -1.40707800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.75280900 | 1.27401200 | -2.52488600 |
| H | 0.95710100 | 1.51126100 | -2.20359900 |
| H | -1.43827500 | 2.63926900 | -0.67183300 |
| H | 0.16653000 | 3.47997000 | 1.07325600 |
| H | -0.96552900 | 1.45610600 | 1.76771000 |
| P | -2.81026100 | -0.40051700 | -0.25571700 |
| P | 2.80831200 | -0.40015200 | -0.29472600 |
| C | -2.47063700 | -2.20114100 | -0.63858800 |
| C | -3.12750300 | -0.58172900 | 1.58386000 |
| C | 2.48551400 | -2.20006300 | -0.69479200 |
| C | 3.09834300 | -0.59516700 | 1.54782700 |
| H | 1.61423700 | -2.60770300 | -0.16078400 |
| H | 2.31571800 | -2.31692600 | -1.76975600 |
| H | 3.35279700 | -2.81548700 | -0.42517700 |
| H | 3.25899600 | 0.38615500 | 2.00470300 |
| H | 2.26855900 | -1.09233400 | 2.06768200 |
| H | 4.00140800 | -1.19467900 | 1.72102800 |
| H | -1.60294200 | -2.60027700 | -0.09224000 |
| H | -3.33713800 | -2.82032200 | -0.37531700 |
| H | -2.28761800 | -2.32394600 | -1.71069600 |
| H | -3.31496800 | 0.40129400 | 2.02653500 |
| H | -4.02247200 | -1.19559400 | 1.74865600 |
| H | -2.29837900 | -1.05647300 | 2.12524200 |

IRC for **TS14** [R/R' = P(CH₃)₂]



Cartesian coordinates for **S15** (R/R' = OCH₃)

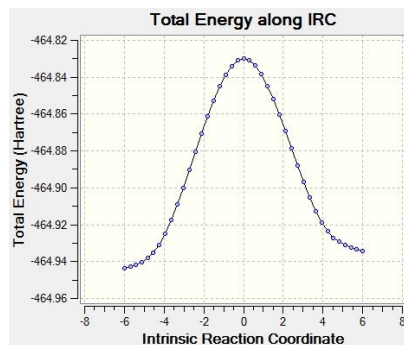
| | | | |
|---|-------------|-------------|-------------|
| C | -0.47189700 | -0.62164400 | 0.24651900 |
| C | 0.78449500 | -0.30531100 | -0.59617400 |
| C | 0.70173600 | 1.08721900 | -1.22775100 |
| C | 0.42960400 | 2.18636200 | -0.18837900 |
| C | -0.83724500 | 1.87597900 | 0.62446400 |
| C | -0.74793800 | 0.48652000 | 1.27515100 |
| H | 1.63657100 | 1.28124700 | -1.76583100 |
| H | 0.86456500 | -1.06455000 | -1.38852100 |
| H | -0.31971900 | -1.57863900 | 0.77200000 |
| H | 1.28985900 | 2.26623400 | 0.48804900 |
| H | 0.33001300 | 3.15525800 | -0.69272100 |
| H | -0.99075600 | 2.63781200 | 1.39854000 |
| H | -1.71354200 | 1.91237200 | -0.03583100 |
| H | 0.07567800 | 0.47135300 | 2.00023400 |
| H | -1.66192400 | 0.25867600 | 1.83686600 |
| H | -0.10818500 | 1.06963000 | -1.96694700 |
| O | 1.95747400 | -0.35116900 | 0.22518900 |
| O | -1.53733000 | -0.78798000 | -0.69619800 |
| C | 2.51202200 | -1.64334900 | 0.39974200 |
| H | 1.83101700 | -2.32675700 | 0.92755200 |
| H | 2.78211600 | -2.09503100 | -0.56683400 |
| H | 3.41683800 | -1.52124600 | 1.00005300 |
| C | -2.67631300 | -1.46607000 | -0.19817600 |
| H | -3.19583700 | -0.89513800 | 0.58402100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.35724200 | -1.60208600 | -1.04182500 |
| H | -2.40738600 | -2.45417000 | 0.20688400 |

Cartesian coordinates for **TS15** (R/R' = OCH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.08232800 | -0.38445600 | -0.70984400 |
| C | -0.02532800 | -0.39434400 | 0.70721300 |
| C | 0.20227000 | 0.85409000 | 1.50891300 |
| C | 0.69058000 | 2.03485000 | 0.65288700 |
| C | -0.11723800 | 2.14933800 | -0.64821000 |
| C | 0.02820500 | 0.88188800 | -1.50855700 |
| H | -0.22738100 | -1.32299200 | -1.23345700 |
| H | -0.13290400 | -1.33971000 | 1.22751800 |
| H | 0.91711600 | 0.62642200 | 2.30694200 |
| H | 1.75017800 | 1.88812500 | 0.41621900 |
| H | 0.21426000 | 3.01823300 | -1.22774000 |
| H | -0.72796400 | 0.85651700 | -2.30053500 |
| H | 1.01078700 | 0.85845800 | -1.99538900 |
| H | -1.17655700 | 2.29814300 | -0.41114500 |
| H | 0.60891500 | 2.96004400 | 1.23427000 |
| H | -0.75447200 | 1.09619000 | 1.98743700 |
| O | -1.88065000 | -0.23835700 | 0.08874900 |
| O | 1.74796400 | -0.72499500 | -0.09127000 |
| C | 2.10200900 | -2.08432400 | -0.10261600 |
| C | -2.57992800 | -1.45652900 | 0.10252600 |
| H | -3.25465400 | -1.52986200 | -0.76407700 |
| H | -1.90699100 | -2.33609000 | 0.06656900 |
| H | -3.18416600 | -1.54895000 | 1.01810000 |
| H | 2.72895300 | -2.33214800 | 0.76756900 |
| H | 1.22119900 | -2.75579500 | -0.07104500 |
| H | 2.66572000 | -2.33284500 | -1.01494400 |

IRC for **TS15** (R/R' = OCH₃)



Cartesian coordinates for **S16** (R/R' = SCH₃)

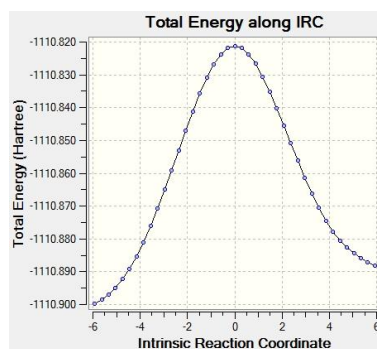
| | | | |
|---|-------------|-------------|-------------|
| C | -0.49023100 | -0.34581600 | 0.28566900 |
| C | 0.71789000 | -0.10279300 | -0.64873600 |
| C | 0.71107800 | 1.32232200 | -1.23374600 |
| C | 0.58797000 | 2.40992500 | -0.15473600 |
| C | -0.64619800 | 2.17605500 | 0.73066100 |
| C | -0.63903500 | 0.76625700 | 1.34079800 |
| H | 1.61261600 | 1.47143300 | -1.83730300 |
| H | 0.69101100 | -0.82824800 | -1.46840700 |
| H | -0.36411100 | -1.31107800 | 0.78785100 |
| H | 1.49305400 | 2.41795200 | 0.46762400 |
| H | 0.53084500 | 3.39503500 | -0.63306500 |
| H | -0.68561100 | 2.92243000 | 1.53314800 |
| H | -1.55543400 | 2.30692400 | 0.12998200 |
| H | 0.20629100 | 0.67513300 | 2.03606100 |
| H | -1.54714900 | 0.59908100 | 1.93130500 |
| H | -0.14520300 | 1.39809900 | -1.91782300 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.38740800 | -2.22923900 | 0.19372400 |
| H | 1.58044100 | -2.67246800 | 0.78350300 |
| H | 2.34786800 | -2.60815000 | -0.83158400 |
| H | 3.34148600 | -2.51989200 | 0.63997800 |
| C | -3.08354800 | -1.47376800 | 0.38629000 |
| H | -3.33035800 | -0.87515700 | 1.26687100 |
| H | -4.00729400 | -1.69789400 | -0.15244200 |
| H | -2.61956600 | -2.41517900 | 0.69528700 |
| S | -2.00943100 | -0.55925600 | -0.77493300 |
| S | 2.33312600 | -0.40297400 | 0.22302500 |

Cartesian coordinates for **TS16** (R/R' = SCH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.01260200 | -0.10414700 | -0.70832800 |
| C | 0.01258900 | -0.10416800 | 0.70830000 |
| C | 0.07308200 | 1.17400000 | 1.51351500 |
| C | 0.40105000 | 2.40740000 | 0.65478800 |
| C | -0.40090000 | 2.40745300 | -0.65473200 |
| C | -0.07305500 | 1.17404700 | -1.51350500 |
| H | -0.03118500 | -1.04668600 | -1.23990900 |
| H | 0.03110100 | -1.04672600 | 1.23985100 |
| H | 0.81439900 | 1.04402900 | 2.30803600 |
| H | 1.47460000 | 2.41869700 | 0.42841400 |
| H | -0.18997900 | 3.31431300 | -1.23188000 |
| H | -0.81442900 | 1.04413800 | -2.30798200 |
| H | 0.89734700 | 1.30237000 | -2.00632200 |
| H | -1.47444700 | 2.41883100 | -0.42834700 |
| H | 0.19019800 | 3.31426200 | 1.23195900 |
| H | -0.89734200 | 1.30237700 | 2.00627400 |
| S | -2.33529100 | -0.41167100 | 0.09075500 |
| S | 2.33523800 | -0.41174800 | -0.09079200 |
| C | 2.31875600 | -2.23964100 | 0.00028200 |
| C | -2.31880300 | -2.23956600 | -0.00025500 |
| H | 2.76656000 | -2.58229200 | 0.93649000 |
| H | 1.29169300 | -2.62838400 | -0.05024800 |
| H | 2.87796100 | -2.66102700 | -0.83878700 |
| H | -1.29171900 | -2.62828100 | 0.05003800 |
| H | -2.87779900 | -2.66094300 | 0.83895700 |
| H | -2.76681900 | -2.58225900 | -0.93634700 |

IRC for **TS16** (R/R' = SCH₃)



Cartesian coordinates for **S17** [R/R' = OC(CH₃)₃]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.60777700 | 0.28244400 | 0.47824000 |
| C | 0.60777100 | 0.28244700 | -0.47822400 |
| C | 0.63670600 | 1.55815100 | -1.33359800 |
| C | 0.60635600 | 2.83119500 | -0.47239800 |
| C | -0.60640500 | 2.83118700 | 0.47239300 |
| C | -0.63672800 | 1.55815300 | 1.33361100 |
| H | 1.52734500 | 1.54327800 | -1.97178800 |
| H | 0.52034100 | -0.59361800 | -1.12998500 |

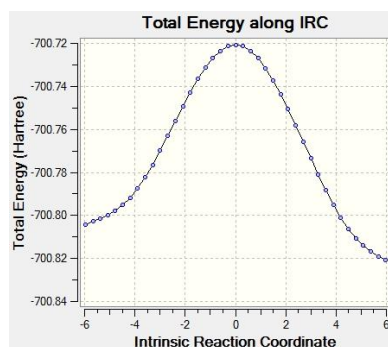
| | | | |
|---|-------------|-------------|-------------|
| H | -0.52033200 | -0.59362100 | 1.12999600 |
| H | 1.53013300 | 2.88944900 | 0.11716100 |
| H | 0.58434400 | 3.71626300 | -1.12014200 |
| H | -0.58441500 | 3.71626200 | 1.12012800 |
| H | -1.53018400 | 2.88940900 | -0.11716600 |
| H | 0.24002000 | 1.53975300 | 1.99340900 |
| H | -1.52738600 | 1.54326100 | 1.97177600 |
| H | -0.24005400 | 1.53972200 | -1.99338200 |
| O | 1.79533300 | 0.20067900 | 0.32698500 |
| O | -1.79536600 | 0.20070600 | -0.32692400 |
| C | 2.74237600 | -0.86711300 | 0.09480400 |
| C | -2.74236300 | -0.86712900 | -0.09481700 |
| C | -2.10943900 | -2.23820500 | -0.39075700 |
| C | -3.86203700 | -0.58052400 | -1.10205500 |
| C | -3.29777700 | -0.81786800 | 1.33909900 |
| C | 2.10944600 | -2.23825400 | 0.39044000 |
| C | 3.86191100 | -0.58066200 | 1.10223800 |
| C | 3.29798200 | -0.81758500 | -1.33902700 |
| H | -3.75482300 | 0.15634900 | 1.53818000 |
| H | -4.06219300 | -1.59034500 | 1.47615300 |
| H | -2.51710200 | -0.99189200 | 2.08643300 |
| H | -3.46520400 | -0.58742300 | -2.12189100 |
| H | -4.65173700 | -1.33552600 | -1.02908700 |
| H | -4.30023200 | 0.40396100 | -0.91240900 |
| H | -1.29417800 | -2.47105000 | 0.30142900 |
| H | -2.85777400 | -3.03224300 | -0.29431200 |
| H | -1.71515700 | -2.26132000 | -1.41176300 |
| H | 2.85784500 | -3.03224000 | 0.29405000 |
| H | 1.71497200 | -2.26151600 | 1.41136700 |
| H | 1.29433700 | -2.47106700 | -0.30193400 |
| H | 4.06246700 | -1.58999200 | -1.47610200 |
| H | 2.51742400 | -0.99153600 | -2.08649700 |
| H | 3.75499800 | 0.15669200 | -1.53787300 |
| H | 4.30009600 | 0.40387500 | 0.91283500 |
| H | 3.46494700 | -0.58776900 | 2.12202000 |
| H | 4.65164900 | -1.33561900 | 1.02922400 |

Cartesian coordinates for **TS17** [R/R' = OC(CH₃)₃]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.00704900 | -0.48060000 | 0.71537300 |
| C | 0.00447100 | -0.48015300 | -0.71578400 |
| C | -0.03647800 | 0.78926000 | -1.51211700 |
| C | -0.35257100 | 2.04680600 | -0.68183900 |
| C | 0.35269000 | 2.04592600 | 0.68250000 |
| C | 0.03452000 | 0.78855000 | 1.51220800 |
| H | -0.00047700 | -1.42489600 | 1.23272600 |
| H | 0.00093300 | -1.42418100 | -1.23364800 |
| H | -0.76606900 | 0.65982300 | -2.31798200 |
| H | -1.43367500 | 2.11573400 | -0.52933400 |
| H | 0.06418600 | 2.93635700 | 1.25245500 |
| H | 0.76367200 | 0.65787800 | 2.31825700 |
| H | -0.93732600 | 0.88545100 | 2.00510200 |
| H | 1.43387800 | 2.11302400 | 0.53002400 |
| H | -0.06263500 | 2.93701000 | -1.25141200 |
| H | 0.93543200 | 0.88463000 | -2.00515600 |
| O | 1.82213900 | -0.94268400 | -0.03928600 |
| O | -1.82129300 | -0.94299000 | 0.03784200 |
| C | -3.16771500 | -0.46004400 | 0.01707600 |
| C | 3.16814100 | -0.46005600 | -0.01714000 |
| C | -3.45630800 | 0.58459900 | 1.11114600 |
| C | -3.53417000 | 0.10297800 | -1.36941300 |
| C | -4.02366200 | -1.71648600 | 0.29158500 |
| C | 4.02492000 | -1.71618400 | -0.29086600 |
| C | 3.45757000 | 0.58471800 | -1.11110200 |

| | | | |
|---|-------------|-------------|-------------|
| C | 3.53385700 | 0.10328100 | 1.36952900 |
| H | -5.09444200 | -1.47625700 | 0.28985600 |
| H | -3.83203200 | -2.47373400 | -0.47450000 |
| H | -3.76138600 | -2.14307400 | 1.26466100 |
| H | -4.60693500 | 0.32053100 | -1.43349300 |
| H | -2.99764300 | 1.03169500 | -1.58557300 |
| H | -3.28691000 | -0.62823800 | -2.14601800 |
| H | -4.52215200 | 0.83987700 | 1.12481400 |
| H | -3.19424900 | 0.18900200 | 2.09854300 |
| H | -2.90114000 | 1.51361200 | 0.94977900 |
| H | 2.90063700 | 1.51296400 | -0.95133600 |
| H | 4.52304500 | 0.84164300 | -1.12311200 |
| H | 3.19751300 | 0.18769000 | -2.09840100 |
| H | 3.28838900 | -0.62869500 | 2.14600100 |
| H | 4.60611800 | 0.32337400 | 1.43349000 |
| H | 2.99515200 | 1.03065100 | 1.58611100 |
| H | 3.76494600 | -2.14190700 | -1.26495100 |
| H | 5.09573100 | -1.47604000 | -0.28637500 |
| H | 3.83138300 | -2.47410600 | 0.47408000 |

IRC for **TS17** [R/R' = OC(CH₃)₃]



Cartesian coordinates for **S18** (R/R' = OCH₂Ph)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.37982400 | 0.35940800 | 0.50930800 |
| C | 0.44537500 | 0.41305100 | -0.79621000 |
| C | 0.18978200 | 1.70768100 | -1.57291800 |
| C | 0.41199700 | 2.96155200 | -0.71177000 |
| C | -0.43987900 | 2.91027100 | 0.56604300 |
| C | -0.16507700 | 1.62260100 | 1.35855800 |
| H | 0.84024500 | 1.71876100 | -2.45494700 |
| H | 0.15936500 | -0.44950500 | -1.41626100 |
| H | -0.07432800 | -0.52628300 | 1.09010200 |
| H | 1.47341500 | 3.03382500 | -0.44317100 |
| H | 0.16886800 | 3.85768900 | -1.29548800 |
| H | -0.23456400 | 3.78369600 | 1.19682700 |
| H | -1.50345500 | 2.95377300 | 0.29750800 |
| H | 0.87893300 | 1.61463800 | 1.69644600 |
| H | -0.78555800 | 1.57867900 | 2.26171800 |
| H | -0.84779100 | 1.68261600 | -1.92756300 |
| O | 1.84640900 | 0.34142900 | -0.49661600 |
| O | -1.74183100 | 0.18305500 | 0.09875800 |
| C | 2.36116500 | -0.98396000 | -0.36295500 |
| H | 1.87223200 | -1.51531600 | 0.46658900 |
| H | 2.15184300 | -1.54697600 | -1.28687100 |
| C | -2.62244900 | -0.28490500 | 1.11930800 |
| H | -2.74471600 | 0.46986600 | 1.90871100 |
| H | -2.18967300 | -1.18635800 | 1.58420000 |
| C | 3.84807200 | -0.91406200 | -0.11622900 |
| C | 4.71936900 | -0.54432500 | -1.15106500 |
| C | 4.38300600 | -1.20976400 | 1.14315900 |
| C | 6.09530500 | -0.47135100 | -0.93068300 |

| | | | |
|---|-------------|-------------|-------------|
| H | 4.31281600 | -0.30850000 | -2.13096600 |
| C | 5.76141100 | -1.14192700 | 1.36808200 |
| H | 3.71724700 | -1.49528400 | 1.95406900 |
| C | 6.62026300 | -0.77196200 | 0.33095700 |
| H | 6.75881500 | -0.18431600 | -1.74158300 |
| H | 6.16154600 | -1.37614000 | 2.35051400 |
| H | 7.69163800 | -0.71923000 | 0.50237700 |
| C | -3.96466100 | -0.60258300 | 0.50679000 |
| C | -5.07676300 | 0.21046000 | 0.75480800 |
| C | -4.11624400 | -1.71938200 | -0.32790500 |
| C | -6.31916200 | -0.08439400 | 0.18487100 |
| H | -4.96995300 | 1.08135200 | 1.39686700 |
| C | -5.35294500 | -2.01591600 | -0.90200600 |
| H | -3.25773000 | -2.35459600 | -0.52960400 |
| C | -6.45923400 | -1.19853500 | -0.64513000 |
| H | -7.17314300 | 0.55561000 | 0.38782400 |
| H | -5.45649400 | -2.88484000 | -1.54580400 |
| H | -7.42323400 | -1.43078300 | -1.08871900 |

Cartesian coordinates for **TS18** (R/R' = OCH₂Ph)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.07963600 | 0.12178000 | 0.70618400 |
| C | 0.07955800 | 0.12145900 | -0.70683800 |
| C | 0.15730700 | 1.38791600 | -1.50194000 |
| C | -0.25548400 | 2.65475900 | -0.72546900 |
| C | 0.25525800 | 2.65510800 | 0.72364200 |
| C | -0.15741600 | 1.38859400 | 1.50071900 |
| H | -0.13638200 | -0.82545400 | 1.21953300 |
| H | 0.13643200 | -0.82601000 | -1.21974200 |
| H | -0.45376000 | 1.26706000 | -2.40398100 |
| H | -1.34549500 | 2.74321800 | -0.72658600 |
| H | -0.12574200 | 3.53753400 | 1.24951100 |
| H | 0.45374500 | 1.26817100 | 2.40275300 |
| H | -1.19321300 | 1.47622000 | 1.85683300 |
| H | 1.34526400 | 2.74363000 | 0.72469900 |
| H | 0.12547300 | 3.53696400 | -1.25174200 |
| H | 1.19313800 | 1.47543900 | -1.85798300 |
| O | 1.82534700 | -0.23272000 | 0.18839000 |
| O | -1.82531100 | -0.23293100 | -0.18879400 |
| C | -2.91656700 | 0.65490200 | -0.28142400 |
| H | -2.92538300 | 1.17543200 | -1.25426700 |
| H | -2.88112900 | 1.43231200 | 0.50338200 |
| C | 2.91656200 | 0.65520800 | 0.28042800 |
| H | 2.88125500 | 1.43189500 | -0.50511300 |
| H | 2.92522800 | 1.17664800 | 1.25278400 |
| C | 4.20616600 | -0.12903400 | 0.12880800 |
| C | 4.79804400 | -0.74440900 | 1.24040100 |
| C | 4.80827500 | -0.28617100 | -1.12657300 |
| C | 5.96551600 | -1.49819200 | 1.10250400 |
| H | 4.33735500 | -0.63259100 | 2.21887200 |
| C | 5.97639300 | -1.03899800 | -1.27088700 |
| H | 4.35780800 | 0.18462100 | -1.99733400 |
| C | 6.55823100 | -1.64764400 | -0.15517400 |
| H | 6.41364900 | -1.96689800 | 1.97434900 |
| H | 6.43259400 | -1.14865100 | -2.25094200 |
| H | 7.46742200 | -2.23210100 | -0.26421400 |
| C | -4.20613100 | -0.12921200 | -0.12881000 |
| C | -4.79737400 | -0.74693900 | -1.23944300 |
| C | -4.80884300 | -0.28386100 | 1.12658400 |
| C | -5.96480600 | -1.50059500 | -1.10058200 |
| H | -4.33619900 | -0.63707300 | -2.21790500 |
| C | -5.97694000 | -1.03655000 | 1.27186000 |
| H | -4.35888700 | 0.18878300 | 1.99660800 |
| C | -6.55813200 | -1.64755600 | 0.15710900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -6.41244200 | -1.97114800 | -1.97168600 |
| H | -6.43361100 | -1.14425800 | 2.25191100 |
| H | -7.46729700 | -2.23191400 | 0.26689000 |

Cartesian coordinates for **S19** (R/R' = OCH₂OCH₃)

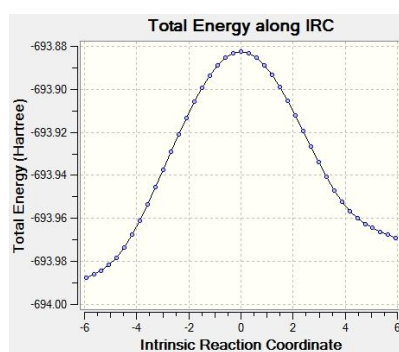
| | | | |
|---|-------------|-------------|-------------|
| C | -0.48062900 | -0.38969900 | 0.64012800 |
| C | -0.56265500 | 0.33402700 | -0.72440500 |
| C | -1.85979500 | -0.00470100 | -1.46306800 |
| C | -3.10862600 | 0.25495700 | -0.60346400 |
| C | -3.02443800 | -0.49281600 | 0.73713200 |
| C | -1.73022800 | -0.13942800 | 1.48771800 |
| H | -1.89721000 | 0.57466900 | -2.39286500 |
| H | 0.30625300 | 0.04396400 | -1.32695800 |
| H | 0.41401900 | -0.04407800 | 1.16859000 |
| H | -3.20204700 | 1.33259100 | -0.41782100 |
| H | -4.00594800 | -0.05142000 | -1.15491000 |
| H | -3.89254100 | -0.25070200 | 1.36234900 |
| H | -3.05441800 | -1.57501200 | 0.55689600 |
| H | -1.73825800 | 0.92327600 | 1.75880800 |
| H | -1.64815700 | -0.71430700 | 2.41759600 |
| H | -1.81534800 | -1.06533300 | -1.73848800 |
| O | -0.53415500 | 1.76471900 | -0.51454400 |
| O | -0.37191700 | -1.81353700 | 0.40351200 |
| C | 0.70552300 | 2.37603600 | -0.57686100 |
| C | 0.89672600 | -2.35446800 | 0.51041900 |
| O | 1.44794200 | 2.12484500 | 0.61139400 |
| C | 2.71659800 | 2.75655100 | 0.60138500 |
| H | 1.40154900 | -2.01765800 | 1.43595700 |
| H | 0.52086800 | 3.45563200 | -0.67679200 |
| H | 1.28858100 | 2.01402700 | -1.44479300 |
| H | 3.20479000 | 2.50935700 | 1.54609100 |
| H | 3.34218500 | 2.39805100 | -0.23071200 |
| H | 2.62234200 | 3.85086800 | 0.52475900 |
| H | 0.77343400 | -3.44704000 | 0.53157700 |
| O | 1.69289700 | -1.97847200 | -0.60713400 |
| C | 3.01379900 | -2.48600400 | -0.52683300 |
| H | 3.54184800 | -2.14815000 | -1.42059700 |
| H | 3.53871900 | -2.10923800 | 0.36469000 |
| H | 3.02355400 | -3.58666700 | -0.50210100 |

Cartesian coordinates for **TS19** (R/R' = OCH₂OCH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.14257400 | -1.05505300 | -0.69655600 |
| C | -0.14236000 | -1.05535800 | 0.69644300 |
| C | -0.21089700 | 0.20635400 | 1.49570000 |
| C | 0.24308300 | 1.46490300 | 0.72828300 |
| C | -0.24390900 | 1.46501300 | -0.72748800 |
| C | 0.21086300 | 0.20701200 | -1.49523500 |
| H | 0.24450500 | -2.00387200 | -1.20031600 |
| H | -0.24424600 | -2.00440600 | 1.19975000 |
| H | 0.38858800 | 0.05943800 | 2.40332000 |
| H | 1.33419200 | 1.53440200 | 0.73665700 |
| H | 0.13475900 | 2.35244300 | -1.24612400 |
| H | -0.38820300 | 0.06025000 | -2.40315100 |
| H | 1.25199900 | 0.30445100 | -1.82102000 |
| H | -1.33507100 | 1.53381900 | -0.73589600 |
| H | -0.13611800 | 2.35193600 | 1.24720400 |
| H | -1.25195600 | 0.30326400 | 1.82197400 |
| O | -1.83897700 | -1.46613400 | -0.27802000 |
| O | 1.83910700 | -1.46605100 | 0.27779200 |
| C | 2.88210200 | -0.64975800 | 0.61656400 |
| H | 2.67024800 | -0.00795000 | 1.49783200 |
| H | 3.75078000 | -1.29045900 | 0.86736700 |

| | | | |
|---|-------------|-------------|-------------|
| C | -2.88208900 | -0.65001100 | -0.61662600 |
| H | -2.67065900 | -0.00849900 | -1.49822200 |
| H | -3.75081800 | -1.29086000 | -0.86687600 |
| O | -3.25046400 | 0.20636000 | 0.47441300 |
| O | 3.25079900 | 0.20620100 | -0.47464100 |
| C | -4.41183400 | 0.96714400 | 0.19859700 |
| C | 4.41207200 | 0.96725000 | -0.19915800 |
| H | -5.28193200 | 0.32020100 | 0.00689200 |
| H | -4.61475100 | 1.58105100 | 1.07898600 |
| H | -4.27092200 | 1.62752500 | -0.67236200 |
| H | 5.28217200 | 0.32049600 | -0.00681000 |
| H | 4.61512200 | 1.58051000 | -1.07996800 |
| H | 4.27094900 | 1.62826900 | 0.67127800 |

IRC for **TS19** (R/R' = OCH₂OCH₃)



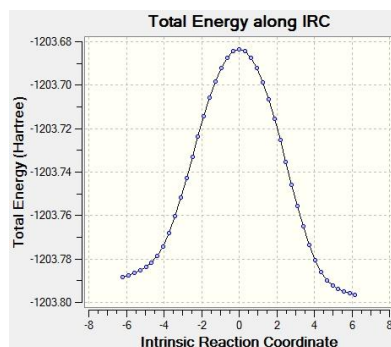
Cartesian coordinates for **S20** [R/R' = OSi(CH₃)₃]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.74793200 | 1.19210800 | 0.22517500 |
| C | 0.70570100 | 1.47597700 | -0.20284300 |
| C | 0.86628000 | 2.86200700 | -0.82710400 |
| C | 0.28736800 | 3.97705600 | 0.05999400 |
| C | -1.18172800 | 3.69778000 | 0.41652000 |
| C | -1.33891300 | 2.31902500 | 1.07712300 |
| H | 1.92827000 | 3.03841600 | -1.03334600 |
| H | 1.02254500 | 0.69822100 | -0.90239700 |
| H | -0.78496300 | 0.24588800 | 0.77201400 |
| H | 0.88206600 | 4.05694500 | 0.97833700 |
| H | 0.37504100 | 4.93743300 | -0.46082600 |
| H | -1.56025900 | 4.47182200 | 1.09377700 |
| H | -1.79648900 | 3.73906200 | -0.49074900 |
| H | -0.81703300 | 2.30317300 | 2.04175800 |
| H | -2.39356300 | 2.09883100 | 1.28107200 |
| H | 0.34531100 | 2.84709600 | -1.79170800 |
| O | 1.51729500 | 1.42293600 | 1.00095400 |
| O | -1.48092200 | 1.06821800 | -1.02555300 |
| C | 2.13579800 | 0.28083600 | 1.42100200 |
| C | -2.66548700 | 0.39143400 | -1.10423800 |
| C | 2.82213000 | -0.58008100 | 0.40338900 |
| C | 2.88835100 | -1.96099400 | 0.64375000 |
| C | 3.47387200 | -0.04108900 | -0.71655200 |
| C | 3.57091000 | -2.79532800 | -0.24116600 |
| H | 2.40943900 | -2.36262400 | 1.53086900 |
| C | 4.17442200 | -0.87599300 | -1.58866900 |
| H | 3.45589600 | 1.02991100 | -0.89130300 |
| C | 4.21561200 | -2.25411200 | -1.35821000 |
| H | 3.61028300 | -3.86440800 | -0.05456700 |
| H | 4.68921100 | -0.45089800 | -2.44505300 |
| H | 4.75510100 | -2.90282400 | -2.04207100 |
| C | -2.76950500 | -0.94133300 | -0.42808200 |
| C | -1.69206200 | -1.83975400 | -0.38838400 |
| C | -4.01299800 | -1.32818200 | 0.09325300 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.85715900 | -3.10656600 | 0.17361600 |
| H | -0.73616600 | -1.56067800 | -0.82085600 |
| C | -4.16831200 | -2.58616300 | 0.67505300 |
| H | -4.84758200 | -0.63743600 | 0.03092900 |
| C | -3.09150400 | -3.47762000 | 0.71465000 |
| H | -1.02414600 | -3.80298800 | 0.18714100 |
| H | -5.12997500 | -2.87489600 | 1.08850500 |
| H | -3.21564000 | -4.46058400 | 1.15956900 |
| O | -3.56550900 | 0.85182800 | -1.77224000 |
| O | 2.17208400 | 0.03158000 | 2.60674500 |

Cartesian coordinates for **TS20** [R/R' = OSi(CH₃)₃]

| | | | |
|---|-------------|-------------|-------------|
| C | 0.01748800 | 0.21845100 | -0.74540100 |
| C | -0.02874800 | 0.16944500 | 0.68519000 |
| C | -0.05527300 | 1.40091500 | 1.51548300 |
| C | 0.32758200 | 2.68786000 | 0.75873600 |
| C | -0.28983900 | 2.74624300 | -0.64877600 |
| C | 0.05021200 | 1.50160100 | -1.49241700 |
| H | 0.03239400 | -0.71867400 | -1.28290000 |
| H | -0.04278800 | -0.80163900 | 1.15824200 |
| H | 0.58101800 | 1.23275000 | 2.39220700 |
| H | 1.41533900 | 2.74409000 | 0.67971300 |
| H | 0.08153300 | 3.63222400 | -1.17348300 |
| H | -0.60759800 | 1.40133900 | -2.36394800 |
| H | 1.07393800 | 1.57499800 | -1.88591100 |
| H | -1.37521000 | 2.83283300 | -0.56507000 |
| H | -0.01377400 | 3.54821200 | 1.34323800 |
| H | -1.08612700 | 1.47212900 | 1.89054400 |
| O | -1.89335600 | -0.29994900 | -0.13139800 |
| O | 1.88700700 | -0.30791800 | 0.05046400 |
| C | 2.98392600 | 0.39085700 | -0.19550700 |
| C | -2.98375100 | 0.39526600 | 0.15308100 |
| C | -4.25547400 | -0.40863800 | 0.03219500 |
| C | -4.25153000 | -1.75731800 | -0.35193500 |
| C | -5.47298400 | 0.22725800 | 0.31691500 |
| C | -5.45334600 | -2.46121400 | -0.44969200 |
| H | -3.30717900 | -2.24303400 | -0.56975700 |
| C | -6.67219100 | -0.47832500 | 0.21860100 |
| H | -5.45713900 | 1.27075500 | 0.61271200 |
| C | -6.66461200 | -1.82368000 | -0.16465400 |
| H | -5.44513700 | -3.50582000 | -0.74748500 |
| H | -7.61190300 | 0.01925300 | 0.44057500 |
| H | -7.59898800 | -2.37273900 | -0.24060700 |
| C | 4.25277300 | -0.41412900 | -0.04983500 |
| C | 5.47658000 | 0.22188100 | -0.30570300 |
| C | 4.24000300 | -1.76307400 | 0.33301400 |
| C | 6.67329000 | -0.48353400 | -0.17916000 |
| H | 5.46747400 | 1.26562400 | -0.60091900 |
| C | 5.43929200 | -2.46666800 | 0.45984200 |
| H | 3.29072600 | -2.24906900 | 0.52757400 |
| C | 6.65691300 | -1.82880900 | 0.20408000 |
| H | 7.61793400 | 0.01423200 | -0.37871000 |
| H | 5.42424600 | -3.51122900 | 0.75757500 |
| H | 7.58936400 | -2.37752900 | 0.30283100 |
| O | 3.01706100 | 1.57429700 | -0.52703900 |
| O | -3.00695800 | 1.57419100 | 0.50037800 |

IRC for **TS20** [R/R' = OSi(CH₃)₃]Cartesian coordinates for **S21** [R/R' = OC(O)CH₃]

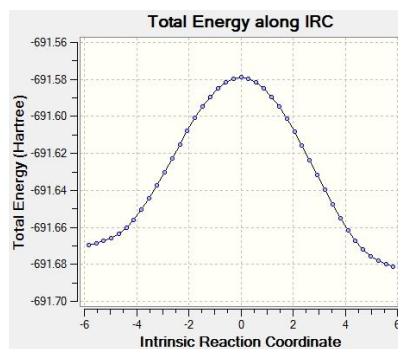
| | | | |
|----|-------------|-------------|-------------|
| C | 0.58871000 | 0.47599200 | -0.50050700 |
| C | -0.58835500 | 0.47567200 | 0.50018600 |
| C | -0.59308200 | 1.75019100 | 1.35403500 |
| C | -0.59128100 | 3.02267100 | 0.49187700 |
| C | 0.59090000 | 3.02298500 | -0.49150200 |
| C | 0.59306900 | 1.75074800 | -1.35401300 |
| H | -1.46509100 | 1.73021500 | 2.01832300 |
| H | -0.46976500 | -0.40013800 | 1.15508900 |
| H | 0.47036000 | -0.39965500 | -1.15566900 |
| H | -1.53339500 | 3.08068100 | -0.06782700 |
| H | -0.54913500 | 3.90772100 | 1.13846600 |
| H | 0.54849200 | 3.90820800 | -1.13783600 |
| H | 1.53299800 | 3.08110600 | 0.06821400 |
| H | -0.30213100 | 1.73273000 | -1.98803000 |
| H | 1.46509900 | 1.73118900 | -2.01828700 |
| H | 0.30212800 | 1.73225200 | 1.98804100 |
| O | -1.80383200 | 0.38140600 | -0.25200900 |
| O | 1.80427500 | 0.38190400 | 0.25157800 |
| Si | 2.98761900 | -0.79749900 | 0.07592100 |
| Si | -2.98761900 | -0.79748300 | -0.07594200 |
| C | -3.68372700 | -0.78103400 | 1.68078700 |
| H | -2.90453600 | -0.97137400 | 2.42811700 |
| H | -4.14320000 | 0.18570400 | 1.91545800 |
| H | -4.45087000 | -1.55528100 | 1.80316800 |
| C | -4.31028800 | -0.33955700 | -1.33055900 |
| H | -3.89960300 | -0.32986300 | -2.34614300 |
| H | -5.14151000 | -1.05409300 | -1.30903200 |
| H | -4.71596200 | 0.65688400 | -1.12423100 |
| C | -2.26903400 | -2.50653100 | -0.44538000 |
| H | -3.03548500 | -3.28384300 | -0.33919800 |
| H | -1.88077000 | -2.55839600 | -1.46896500 |
| H | -1.45032800 | -2.76050700 | 0.23793100 |
| C | 4.31031400 | -0.33989100 | 1.33062900 |
| H | 3.89960600 | -0.32990900 | 2.34620000 |
| H | 5.14132800 | -1.05467000 | 1.30923300 |
| H | 4.71628600 | 0.65640200 | 1.12415400 |
| C | 3.68415300 | -0.78142200 | -1.68064100 |
| H | 2.90511600 | -0.97131000 | -2.42824200 |
| H | 4.14420700 | 0.18509100 | -1.91510100 |
| H | 4.45093800 | -1.55606200 | -1.80279500 |
| C | 2.26826900 | -2.50620300 | 0.44544700 |
| H | 3.03437500 | -3.28386200 | 0.33933500 |
| H | 1.87999000 | -2.55780000 | 1.46904200 |
| H | 1.44944700 | -2.75986900 | -0.23783600 |

Cartesian coordinates for **TS21** [R/R' = OC(O)CH₃]

| | | | |
|---|-------------|------------|------------|
| C | -0.00995400 | 0.52558600 | 0.71175500 |
|---|-------------|------------|------------|

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00981400 | 0.52566500 | -0.71191900 |
| C | -0.00255700 | 1.79316000 | -1.51475200 |
| C | -0.36246000 | 3.03259400 | -0.67713600 |
| C | 0.36245200 | 3.03250200 | 0.67723600 |
| C | 0.00249400 | 1.79299800 | 1.51472500 |
| H | -0.01811500 | -0.42446500 | 1.22846500 |
| H | 0.01798900 | -0.42434000 | -1.22873400 |
| H | -0.70521000 | 1.66425900 | -2.34474400 |
| H | -1.44501100 | 3.04474900 | -0.51457400 |
| H | 0.10344900 | 3.93407800 | 1.24360600 |
| H | 0.70516300 | 1.66397100 | 2.34468300 |
| H | -0.99887300 | 1.89408100 | 1.94843300 |
| H | 1.44500200 | 3.04461400 | 0.51467000 |
| H | -0.10340800 | 3.93421500 | -1.24341000 |
| H | 0.99883000 | 1.89422700 | -1.94841900 |
| O | 1.84131600 | 0.49062200 | 0.02106600 |
| O | -1.84135500 | 0.49065200 | -0.02126600 |
| Si | 2.91717700 | -0.78315200 | -0.01448700 |
| Si | -2.91715200 | -0.78318900 | 0.01449400 |
| C | 4.37551500 | -0.36117900 | 1.11214900 |
| H | 5.12968700 | -1.15788600 | 1.10949200 |
| H | 4.86205100 | 0.56532600 | 0.78710400 |
| H | 4.04296600 | -0.21653100 | 2.14655900 |
| C | 3.53408900 | -1.04630500 | -1.78558900 |
| H | 3.99200300 | -0.13111300 | -2.17832800 |
| H | 4.28586700 | -1.84372300 | -1.83390800 |
| H | 2.71491400 | -1.32381100 | -2.46008900 |
| C | 2.12248300 | -2.39844000 | 0.59142500 |
| H | 1.77357700 | -2.31806000 | 1.62833600 |
| H | 1.27018500 | -2.70033300 | -0.02923900 |
| H | 2.84995400 | -3.21888000 | 0.55837900 |
| C | -2.12270500 | -2.39828900 | -0.59221600 |
| H | -1.77426500 | -2.31759100 | -1.62925900 |
| H | -1.27013100 | -2.70039600 | 0.02796400 |
| H | -2.85017400 | -3.21872900 | -0.55910000 |
| C | -3.53322500 | -1.04676400 | 1.78582300 |
| H | -3.99096800 | -0.13166700 | 2.17898100 |
| H | -4.28497900 | -1.84419400 | 1.83430000 |
| H | -2.71374400 | -1.32442400 | 2.45989000 |
| C | -4.37599900 | -0.36095100 | -1.11136900 |
| H | -5.13015200 | -1.15767700 | -1.10857600 |
| H | -4.86241800 | 0.56546300 | -0.78588800 |
| H | -4.04390600 | -0.21604800 | -2.14588900 |

IRC for **TS21** [R/R' = OC(O)CH₃]



Cartesian coordinates for **S22** (R/R' = OPh)

| | | | |
|---|-------------|------------|-------------|
| C | -0.65540600 | 0.24113500 | 0.40504800 |
| C | 0.65549200 | 0.24105300 | -0.40500900 |
| C | 0.82146200 | 1.52039100 | -1.23636900 |
| C | 0.66631800 | 2.78958900 | -0.38271700 |

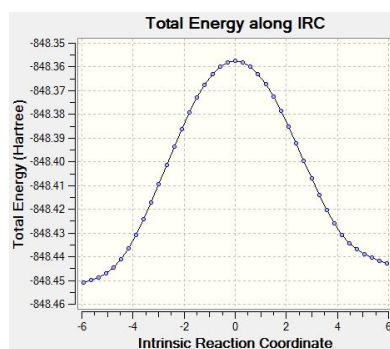
| | | | |
|---|-------------|-------------|-------------|
| C | -0.66644300 | 2.78965100 | 0.38193100 |
| C | -0.82142000 | 1.52071700 | 1.23602000 |
| H | 1.79474400 | 1.50959700 | -1.73828600 |
| H | 0.64460100 | -0.64585200 | -1.04846700 |
| H | -0.64444300 | -0.64554600 | 1.04880300 |
| H | 1.49852100 | 2.85212500 | 0.32997000 |
| H | 0.73506500 | 3.67416800 | -1.02667400 |
| H | -0.73525900 | 3.67444400 | 1.02558200 |
| H | -1.49867600 | 2.85184200 | -0.33075100 |
| H | -0.05423800 | 1.50348500 | 2.02001300 |
| H | -1.79465600 | 1.51001200 | 1.73801600 |
| H | 0.05437100 | 1.50286900 | -2.02044300 |
| O | 1.69349200 | 0.11017300 | 0.58221000 |
| O | -1.69339100 | 0.10986600 | -0.58216100 |
| C | 2.92534900 | -0.38281600 | 0.23993400 |
| C | 3.86519600 | -0.42024200 | 1.28221800 |
| C | 3.28255000 | -0.84545700 | -1.03364400 |
| C | 5.14463200 | -0.91858100 | 1.05258700 |
| H | 3.56858600 | -0.05785900 | 2.26137200 |
| C | 4.57311200 | -1.34466200 | -1.24826400 |
| H | 2.58017400 | -0.82176500 | -1.85787600 |
| C | 5.50984300 | -1.38577100 | -0.21611400 |
| H | 5.86065000 | -0.94294800 | 1.86926400 |
| H | 4.83952200 | -1.70089900 | -2.23949900 |
| H | 6.50817000 | -1.77288300 | -0.39407600 |
| C | -2.92529600 | -0.38301600 | -0.23980100 |
| C | -3.28271300 | -0.84495400 | 1.03396000 |
| C | -3.86500100 | -0.42095200 | -1.28220500 |
| C | -4.57335300 | -1.34396300 | 1.24865300 |
| H | -2.58046500 | -0.82092300 | 1.85828700 |
| C | -5.14449600 | -0.91908300 | -1.05251100 |
| H | -3.56819500 | -0.05912100 | -2.26150600 |
| C | -5.50993300 | -1.38555600 | 0.21639800 |
| H | -4.83993300 | -1.69963200 | 2.24004700 |
| H | -5.86038600 | -0.94384800 | -1.86928800 |
| H | -6.50831800 | -1.77248000 | 0.39444000 |

Cartesian coordinates for **TS22** (R/R' = OPh)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.03248100 | 1.10729300 | 0.70926400 |
| C | -0.03253500 | 1.10730600 | -0.70931000 |
| C | -0.09299400 | 2.37268700 | -1.50700400 |
| C | -0.40915500 | 3.61041800 | -0.64959500 |
| C | 0.40921400 | 3.61038500 | 0.64959900 |
| C | 0.09298700 | 2.37265600 | 1.50698500 |
| H | 0.05736100 | 0.15214500 | 1.22151900 |
| H | -0.05741800 | 0.15217000 | -1.22159400 |
| H | -0.83098100 | 2.24307300 | -2.30598200 |
| H | -1.47872200 | 3.61557300 | -0.41192700 |
| H | 0.19976000 | 4.51432600 | 1.23161900 |
| H | 0.83096100 | 2.24299400 | 2.30596800 |
| H | -0.88613400 | 2.47971200 | 1.99086300 |
| H | 1.47878100 | 3.61548400 | 0.41192800 |
| H | -0.19965200 | 4.51435700 | -1.23160000 |
| H | 0.88612700 | 2.47970400 | -1.99088900 |
| O | 1.88563400 | 1.00250800 | -0.10852300 |
| O | -1.88566100 | 1.00255100 | 0.10849500 |
| C | -2.44321300 | -0.22514800 | 0.08566600 |
| C | -2.63758200 | -0.95505100 | 1.27680500 |
| C | -2.87314500 | -0.79328200 | -1.13190200 |
| C | -3.25692500 | -2.20522100 | 1.24736700 |
| H | -2.31877900 | -0.51806300 | 2.21904800 |
| C | -3.49306900 | -2.04283700 | -1.15055600 |
| H | -2.73446500 | -0.22900000 | -2.04992300 |

| | | | |
|---|-------------|-------------|-------------|
| C | -3.68696600 | -2.75800200 | 0.03643600 |
| H | -3.40561600 | -2.75039200 | 2.17567000 |
| H | -3.82687400 | -2.46080600 | -2.09659900 |
| H | -4.16690000 | -3.73171500 | 0.01793000 |
| C | 2.44319600 | -0.22515900 | -0.08566000 |
| C | 2.87324100 | -0.79322500 | 1.13190000 |
| C | 2.63746900 | -0.95512300 | -1.27677800 |
| C | 3.49318700 | -2.04277000 | 1.15056100 |
| H | 2.73461900 | -0.22890600 | 2.04990700 |
| C | 3.25683400 | -2.20528000 | -1.24733300 |
| H | 2.31858300 | -0.51817400 | -2.21901400 |
| C | 3.68699100 | -2.75799200 | -0.03641100 |
| H | 3.82708000 | -2.46068700 | 2.09659600 |
| H | 3.40545400 | -2.75049700 | -2.17562100 |
| H | 4.16694100 | -3.73169700 | -0.01789700 |

IRC for **TS22** (R/R' = OPh)

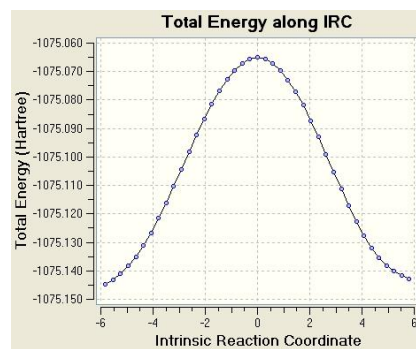


Cartesian coordinates for **S23** [R/R' = OC(O)Ph]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.42346100 | -0.09131100 | 0.33942300 |
| C | 0.65879700 | 0.17843100 | -0.72050900 |
| C | 0.55754000 | 1.57567200 | -1.33208900 |
| C | 0.47394200 | 2.68507700 | -0.27118900 |
| C | -0.67180800 | 2.42129600 | 0.71896200 |
| C | -0.53718600 | 1.03555900 | 1.37053700 |
| H | 1.41225200 | 1.73177800 | -1.99984400 |
| H | 0.60703600 | -0.59739400 | -1.48697000 |
| H | -0.23207700 | -1.04769400 | 0.83126600 |
| H | 1.42472200 | 2.74033100 | 0.27437800 |
| H | 0.33619500 | 3.65451700 | -0.76427600 |
| H | -0.68713300 | 3.19297200 | 1.49740800 |
| H | -1.63310700 | 2.48725100 | 0.19255200 |
| H | 0.37085100 | 1.00641000 | 1.98657100 |
| H | -1.37798400 | 0.82138600 | 2.03758900 |
| H | -0.34474600 | 1.59273700 | -1.95613100 |
| O | 1.95433800 | 0.08070000 | -0.06207400 |
| O | -1.66096700 | -0.21996200 | -0.41902500 |
| C | 2.59039600 | -1.11903300 | -0.08801800 |
| C | -2.63516300 | -1.00698100 | 0.10304900 |
| O | -2.54037200 | -1.57918000 | 1.16880200 |
| O | 2.13974800 | -2.11200100 | -0.62018300 |
| C | -3.82684100 | -1.07520800 | -0.82029000 |
| C | 3.91540400 | -1.04058100 | 0.62968300 |
| H | -3.54172000 | -1.57120000 | -1.75362700 |
| H | -4.62727400 | -1.63512700 | -0.33720500 |
| H | -4.17019800 | -0.06842800 | -1.07502300 |
| H | 4.52563000 | -0.23412700 | 0.21288400 |
| H | 3.75067600 | -0.81371800 | 1.68785900 |
| H | 4.43517700 | -1.99366400 | 0.53505600 |

Cartesian coordinates for **TS23** [R/R' = OC(O)Ph₂]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.01463300 | 0.09937300 | -0.70986900 |
| C | 0.01459300 | 0.09933600 | 0.70982000 |
| C | 0.07048600 | 1.36007400 | 1.50898700 |
| C | 0.38878400 | 2.60585700 | 0.66266900 |
| C | -0.38874300 | 2.60590500 | -0.66258200 |
| C | -0.07048300 | 1.36015700 | -1.50896800 |
| H | -0.04017700 | -0.87237300 | -1.19124000 |
| H | 0.04012500 | -0.87243700 | 1.19113600 |
| H | 0.80131500 | 1.22275400 | 2.31328100 |
| H | 1.46438900 | 2.62821600 | 0.45779800 |
| H | -0.14880000 | 3.50461100 | -1.24057100 |
| H | -0.80131000 | 1.22290500 | -2.31327400 |
| H | 0.91042800 | 1.45334800 | -1.99288900 |
| H | -1.46434700 | 2.62828600 | -0.45771200 |
| H | 0.14886900 | 3.50454000 | 1.24070400 |
| H | -0.91041700 | 1.45327400 | 1.99292100 |
| O | -1.93042800 | 0.08633700 | 0.10424400 |
| O | 1.93043400 | 0.08630800 | -0.10432300 |
| C | -2.51258400 | -1.09966100 | -0.06154500 |
| C | 2.51258000 | -1.09967700 | 0.06153100 |
| C | 4.00825800 | -1.05813300 | -0.21627400 |
| H | 4.18126400 | -0.79670300 | -1.26518400 |
| H | 4.48448600 | -0.28592200 | 0.39514500 |
| H | 4.44799100 | -2.03273400 | -0.00095500 |
| O | 1.92941100 | -2.11963700 | 0.40286700 |
| C | -4.00827100 | -1.05812200 | 0.21626000 |
| H | -4.48450400 | -0.28590500 | -0.39514600 |
| H | -4.44799100 | -2.03272500 | 0.00092400 |
| H | -4.18128300 | -0.79671700 | 1.26517500 |
| O | -1.92941300 | -2.11964200 | -0.40282300 |

IRC for **TS23** [R/R' = OC(O)Ph]Cartesian coordinates for **S24** (R/R' = Br)

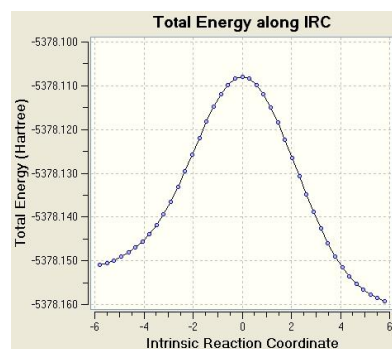
| | | | |
|---|-------------|-------------|-------------|
| C | -0.47270200 | -0.32355700 | 0.59808500 |
| C | 0.47271000 | -0.32355400 | -0.59809100 |
| C | 0.44660300 | 0.96493300 | -1.41692100 |
| C | 0.53547600 | 2.23104100 | -0.55186900 |
| C | -0.53553600 | 2.23103600 | 0.55187100 |
| C | -0.44659900 | 0.96492700 | 1.41692600 |
| H | 1.24701500 | 0.93656500 | -2.16209100 |
| H | 0.30475700 | -1.19770900 | -1.22382300 |
| H | -0.30474000 | -1.19771300 | 1.22381400 |
| H | 1.53268400 | 2.29600500 | -0.09882400 |
| H | 0.42028200 | 3.11333800 | -1.19142500 |
| H | -0.42036800 | 3.11334400 | 1.19141500 |
| H | -1.53275000 | 2.29594900 | 0.09883500 |
| H | 0.50371600 | 0.96499200 | 1.96797700 |
| H | -1.24696900 | 0.93652700 | 2.16213800 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.50367800 | 0.96497000 | -1.96803100 |
| Br | 2.31312700 | -0.66706700 | 0.12347400 |
| Br | -2.31311800 | -0.66708200 | -0.12347400 |

Cartesian coordinates for **TS24** (R/R' = Br)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.00987800 | -0.31792200 | 0.71410300 |
| C | 0.00986200 | -0.31790900 | -0.71412300 |
| C | -0.02910400 | 0.95170900 | -1.51934200 |
| C | -0.36587500 | 2.19503800 | -0.67595300 |
| C | 0.36632900 | 2.19492000 | 0.67599400 |
| C | 0.02916900 | 0.95168200 | 1.51934100 |
| H | -0.00404600 | -1.26909900 | 1.22684600 |
| H | 0.00392900 | -1.26907700 | -1.22688400 |
| H | -0.75539200 | 0.81405300 | -2.32701200 |
| H | -1.44768700 | 2.23120300 | -0.50793400 |
| H | 0.10011800 | 3.09158300 | 1.24523800 |
| H | 0.75527100 | 0.81391500 | 2.32716000 |
| H | -0.94918400 | 1.05952900 | 2.00003500 |
| H | 1.44815400 | 2.23077800 | 0.50799900 |
| H | -0.09941900 | 3.09163400 | -1.24518600 |
| H | 0.94916700 | 1.05935600 | -2.00024600 |
| Br | 2.37817500 | -0.65433700 | -0.02910200 |
| Br | -2.37828700 | -0.65420500 | 0.02909800 |

IRC for **TS24** (R/R' = Br)



Cartesian coordinates for **S25** (R/R' = CHCH₂)

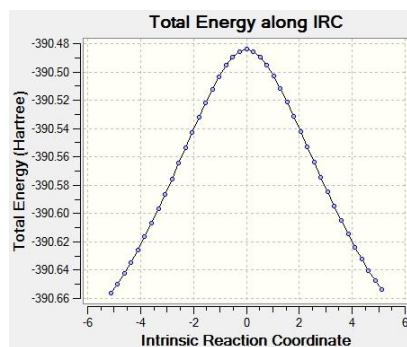
| | | | |
|---|-------------|-------------|-------------|
| C | 0.64739000 | -0.49777900 | -0.44323000 |
| C | -0.64739000 | -0.49777900 | 0.44323000 |
| C | -0.75838700 | 0.80917400 | 1.27198800 |
| C | -0.64453600 | 2.08269900 | 0.41797100 |
| C | 0.64453600 | 2.08269900 | -0.41797100 |
| C | 0.75838700 | 0.80917400 | -1.27198800 |
| H | -1.70471100 | 0.80357700 | 1.82568900 |
| H | -0.56239000 | -1.33687500 | 1.14542200 |
| H | 0.56239000 | -1.33687500 | -1.14542200 |
| H | -1.51248100 | 2.16393600 | -0.25078900 |
| H | -0.67611400 | 2.96598500 | 1.06768600 |
| H | 0.67611400 | 2.96598600 | -1.06768600 |
| H | 1.51248100 | 2.16393700 | 0.25078900 |
| H | -0.04042600 | 0.81566300 | -2.02592400 |
| H | 1.70471100 | 0.80357800 | -1.82568900 |
| H | 0.04042600 | 0.81566300 | 2.02592400 |
| C | 1.88192600 | -0.74184800 | 0.39099300 |
| C | -1.88192600 | -0.74184900 | -0.39099300 |
| C | 2.68562200 | -1.80319500 | 0.26574500 |
| C | -2.68562200 | -1.80319600 | -0.26574500 |
| H | 2.49208000 | -2.58122600 | -0.47019900 |
| H | -2.49207900 | -2.58122700 | 0.47019900 |
| H | 3.56373800 | -1.93079700 | 0.89257000 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.56373700 | -1.93079700 | -0.89257000 |
| H | 2.12689700 | 0.00543700 | 1.14576300 |
| H | -2.12689800 | 0.00543700 | -1.14576300 |

Cartesian coordinates for **TS25** (R/R' = CHCH₂)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.26359800 | -0.58317400 | 0.64446400 |
| C | 0.32492200 | -0.54285500 | -0.73122900 |
| C | -0.09159000 | 0.65647100 | -1.53945500 |
| C | -0.86617000 | 1.69889500 | -0.71548100 |
| C | -0.24751400 | 1.90613800 | 0.67556900 |
| C | -0.17582500 | 0.59171400 | 1.47275500 |
| H | 0.53402100 | -1.50142100 | 1.15144600 |
| H | 0.65015600 | -1.43020400 | -1.26096100 |
| H | -0.69807500 | 0.30323100 | -2.38042100 |
| H | -1.90273000 | 1.36163400 | -0.60805300 |
| H | -0.82950300 | 2.64201000 | 1.24163700 |
| H | 0.50134300 | 0.69074900 | 2.32867700 |
| H | -1.15824800 | 0.33688700 | 1.88897600 |
| H | 0.76131700 | 2.32195500 | 0.56859600 |
| H | -0.89442200 | 2.64881500 | -1.26097100 |
| H | 0.81397300 | 1.09623400 | -1.97750800 |
| C | 2.36976800 | -0.06039400 | 0.04209500 |
| C | -1.71942800 | -1.60805400 | -0.16796000 |
| H | 2.70832400 | 0.97781100 | 0.09581700 |
| C | 3.22147100 | -1.08444200 | 0.04990400 |
| H | 2.87443000 | -2.12011600 | -0.00600800 |
| H | -1.56831200 | -2.62765800 | -0.54469500 |
| C | -2.93664100 | -1.23886400 | 0.23788000 |
| H | -3.14297400 | -0.24642200 | 0.64714700 |
| H | 4.30773000 | -0.96930600 | 0.10843500 |
| H | -3.81257700 | -1.89681600 | 0.19663600 |

IRC for **TS25** (R/R' = CHCH₂)



Cartesian coordinates for **S26** [R/R' = C(CH₃)CH₂]

| | | | |
|---|-------------|-------------|-------------|
| C | 0.54269700 | -0.33979100 | -0.57557300 |
| C | -0.54266500 | -0.33982900 | 0.57559100 |
| C | -0.70214100 | 1.02405600 | 1.31022900 |
| C | -0.63815300 | 2.27651700 | 0.42377300 |
| C | 0.63796800 | 2.27657300 | -0.42377500 |
| C | 0.70208000 | 1.02410400 | -1.31021300 |
| H | -1.63759800 | 1.00599400 | 1.88286900 |
| H | -0.18335100 | -1.04910100 | 1.32918300 |
| H | 0.18341700 | -1.04907800 | -1.32916600 |
| H | -1.51161900 | 2.33247400 | -0.23778700 |
| H | -0.67553900 | 3.16991800 | 1.05962800 |
| H | 0.67526700 | 3.16996800 | -1.05964200 |
| H | 1.51142700 | 2.33262500 | 0.23778600 |
| H | -0.10210100 | 1.10620700 | -2.05340800 |
| H | 1.63754700 | 1.00611500 | -1.88284000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.10204500 | 1.10623100 | 2.05341000 |
| C | 1.86984000 | -0.92377700 | -0.09764800 |
| C | -1.86977100 | -0.92387200 | 0.09764300 |
| C | 2.31367300 | -2.08247600 | -0.60818100 |
| C | -2.31355600 | -2.08260100 | 0.60815000 |
| C | -2.67428200 | -0.19219500 | -0.95236100 |
| C | 2.67432800 | -0.19209300 | 0.95236900 |
| H | -3.02666600 | 0.77838400 | -0.58433500 |
| H | -2.08070400 | 0.00774600 | -1.85188000 |
| H | -3.55093000 | -0.77461300 | -1.24982200 |
| H | 2.08074700 | 0.00780900 | 1.85189400 |
| H | 3.55099600 | -0.77448800 | 1.24981400 |
| H | 3.02667900 | 0.77850300 | 0.58436100 |
| H | -3.25134900 | -2.52607600 | 0.28305700 |
| H | -1.75338800 | -2.62525700 | 1.36497000 |
| H | 1.75352300 | -2.62514200 | -1.36500800 |
| H | 3.25148800 | -2.52591500 | -0.28310500 |

Cartesian coordinates for **TS26** [R/R' = C(CH₃)CH₂]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.03919500 | 0.32090600 | -0.72976200 |
| C | -0.03762400 | 0.44423600 | 0.63998000 |
| C | 0.04748400 | -0.73452600 | 1.56963800 |
| C | -0.22025200 | -2.07507300 | 0.86726900 |
| C | 0.49571800 | -2.15798100 | -0.48953600 |
| C | 0.10079000 | -1.00215300 | -1.42826900 |
| H | -0.13564600 | 1.21309900 | -1.33650000 |
| H | -0.12712100 | 1.43218500 | 1.07396100 |
| H | -0.66137700 | -0.58036100 | 2.39086500 |
| H | -1.29981000 | -2.18846900 | 0.72459700 |
| H | 0.27291400 | -3.11373400 | -0.97711900 |
| H | 0.83423000 | -0.89111100 | -2.23588400 |
| H | -0.85717200 | -1.20960600 | -1.92112000 |
| H | 1.57814600 | -2.13595200 | -0.32537000 |
| H | 0.10349100 | -2.89882400 | 1.51342600 |
| H | 1.04688300 | -0.72639700 | 2.02521400 |
| C | 2.15014200 | 0.93231400 | -0.05927300 |
| C | -2.31618700 | 0.55426900 | -0.07471200 |
| C | 2.24180700 | 2.25767800 | -0.16166600 |
| H | 1.36316500 | 2.90416900 | -0.21921000 |
| C | -3.17206100 | -0.38895900 | -0.46414000 |
| H | -2.86967300 | -1.40403700 | -0.71944700 |
| H | 3.20382000 | 2.78369100 | -0.19419400 |
| H | -4.24928800 | -0.19359400 | -0.55564900 |
| C | 3.32158600 | 0.00275100 | 0.01535600 |
| C | -2.69560000 | 1.96518600 | 0.25233300 |
| H | 4.27925700 | 0.55043500 | 0.04066200 |
| H | 3.28233200 | -0.63390000 | 0.90902700 |
| H | 3.35353700 | -0.67419500 | -0.84804000 |
| H | -2.07778500 | 2.68950400 | -0.29794100 |
| H | -3.74869900 | 2.18111300 | 0.01030500 |
| H | -2.55085200 | 2.18409800 | 1.31911500 |

Cartesian coordinates for **S27** [R/R' = C(O)H]

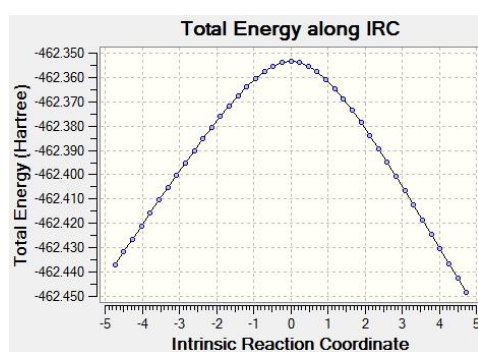
| | | | |
|---|-------------|-------------|-------------|
| C | -0.37956600 | -0.83149600 | 0.25228800 |
| C | 0.73651900 | -0.43345100 | -0.74290600 |
| C | 0.56924000 | 1.00295100 | -1.29109100 |
| C | 0.37470900 | 2.03175800 | -0.16672000 |
| C | -0.80961200 | 1.64946300 | 0.73315700 |
| C | -0.63526700 | 0.24152100 | 1.32543100 |
| H | 1.43882600 | 1.26160200 | -1.90949500 |
| H | 0.71747200 | -1.12292400 | -1.60683300 |
| H | -0.03780000 | -1.75623800 | 0.74657800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 1.29100600 | 2.09531500 | 0.43884900 |
| H | 0.22088800 | 3.02626400 | -0.60175400 |
| H | -0.91611700 | 2.37724800 | 1.54605300 |
| H | -1.73937600 | 1.68993400 | 0.15190900 |
| H | 0.21368600 | 0.23840000 | 2.01928600 |
| H | -1.52385200 | -0.03670400 | 1.90059200 |
| H | -0.30117700 | 1.02623700 | -1.95934600 |
| C | -1.62538200 | -1.24678700 | -0.50592800 |
| C | 2.12687600 | -0.64139200 | -0.16164100 |
| O | -2.75881000 | -0.89407400 | -0.25518900 |
| O | 2.38149200 | -1.26700000 | 0.84560800 |
| H | -1.43831300 | -1.95834600 | -1.34431600 |
| H | 2.94819300 | -0.18759700 | -0.76040800 |

Cartesian coordinates for **TS27** [R/R' = C(O)H]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.19365100 | -0.64798600 | -0.59085100 |
| C | -0.30121800 | -0.54924200 | 0.76572800 |
| C | 0.05261900 | 0.69164300 | 1.53249000 |
| C | 0.82773200 | 1.71945400 | 0.68956800 |
| C | 0.24755500 | 1.83535200 | -0.72764300 |
| C | 0.28141100 | 0.47938500 | -1.45427000 |
| H | -0.45643900 | -1.58984700 | -1.06389700 |
| H | -0.65945400 | -1.41076000 | 1.32177800 |
| H | 0.62511700 | 0.40698500 | 2.42450400 |
| H | 1.87708800 | 1.41159500 | 0.62113500 |
| H | 0.80758000 | 2.57710700 | -1.30727400 |
| H | -0.31300400 | 0.50958200 | -2.37598900 |
| H | 1.31147600 | 0.24140700 | -1.76294000 |
| H | -0.78824200 | 2.19503500 | -0.67279800 |
| H | 0.81191200 | 2.69385300 | 1.19018600 |
| H | -0.88407700 | 1.12742400 | 1.91337200 |
| C | 2.07367100 | -1.53448000 | 0.27886300 |
| O | 2.98897200 | -1.08075900 | -0.34962100 |
| H | 2.21010400 | -2.50303400 | 0.85707600 |
| C | -2.67105700 | -0.16755100 | -0.11242800 |
| O | -3.41058400 | -1.10438600 | -0.03197200 |
| H | -3.07154200 | 0.86235300 | -0.38115900 |

IRC for **TS27** [R/R' = C(O)H]



Cartesian coordinates for **S28** [R/R' = C(O)CH₃]

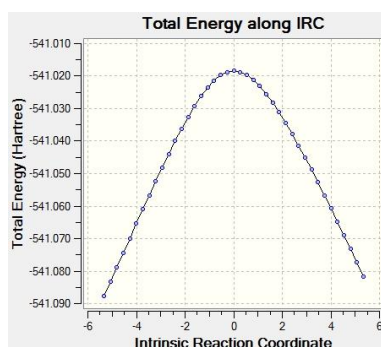
| | | | |
|---|-------------|-------------|-------------|
| C | 0.53850800 | -0.40200000 | -0.56469400 |
| C | -0.53870000 | -0.40186900 | 0.56470700 |
| C | -0.46303900 | 0.88405700 | 1.40938500 |
| C | -0.53087500 | 2.16082700 | 0.55476500 |
| C | 0.53145600 | 2.16065800 | -0.55469500 |
| C | 0.46308000 | 0.88394500 | -1.40935400 |
| H | -1.27380000 | 0.87929900 | 2.14393500 |
| H | -0.34967100 | -1.26840500 | 1.21676200 |
| H | 0.34931600 | -1.26851600 | -1.21671600 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.53196000 | 2.24173100 | 0.11570300 |
| H | -0.39962100 | 3.03737600 | 1.20056300 |
| H | 0.40049500 | 3.03726900 | -1.20047000 |
| H | 1.53259100 | 2.24118500 | -0.11567600 |
| H | -0.48160000 | 0.87392500 | -1.97101600 |
| H | 1.27375000 | 0.87892600 | -2.14399300 |
| H | 0.48155100 | 0.87368600 | 1.97118400 |
| C | 1.95357500 | -0.67345400 | -0.02662400 |
| C | -1.95370800 | -0.67316700 | 0.02654100 |
| O | 2.90526900 | 0.01451900 | -0.35305500 |
| O | -2.90533500 | 0.01505900 | 0.35258700 |
| C | 2.15311600 | -1.87035300 | 0.89180200 |
| C | -2.15334700 | -1.87036700 | -0.89148400 |
| H | 3.20249600 | -2.16864400 | 0.86109300 |
| H | 1.90801700 | -1.59089400 | 1.92377800 |
| H | 1.51391000 | -2.71663500 | 0.61978600 |
| H | -1.51410800 | -2.71656000 | -0.61922900 |
| H | -3.20270900 | -2.16873300 | -0.86043300 |
| H | -1.90852700 | -1.59129600 | -1.92361800 |

Cartesian coordinates for **TS28** [R/R' = C(O)CH₃]

| | | | |
|---|-------------|-------------|-------------|
| C | 0.01346200 | -0.46025900 | 0.68143700 |
| C | -0.01311100 | -0.46070300 | -0.68067200 |
| C | 0.01781700 | 0.79316100 | -1.49989100 |
| C | -0.34871100 | 2.04595500 | -0.68543700 |
| C | 0.34780900 | 2.04658200 | 0.68464200 |
| C | -0.01796800 | 0.79408300 | 1.49990400 |
| H | 0.01051800 | -1.41196700 | 1.20468500 |
| H | -0.00984500 | -1.41273900 | -1.20332400 |
| H | -0.64314100 | 0.68291700 | -2.36849700 |
| H | -1.43480000 | 2.07911300 | -0.53882800 |
| H | 0.07248100 | 2.94464000 | 1.24893000 |
| H | 0.64319900 | 0.68468600 | 2.36846300 |
| H | -1.03936200 | 0.88609300 | 1.90188300 |
| H | 1.43389000 | 2.08024700 | 0.53800100 |
| H | -0.07387000 | 2.94381400 | -1.25028000 |
| H | 1.03921500 | 0.88550500 | -1.90167000 |
| C | 2.60091300 | -0.63927300 | -0.12641000 |
| C | -2.60059000 | -0.63965200 | 0.12656700 |
| O | -3.17686600 | 0.07138100 | 0.90368700 |
| O | 3.17697900 | 0.07171900 | -0.90370900 |
| C | -3.28796000 | -1.71133600 | -0.71273600 |
| H | -2.82113000 | -2.67907500 | -0.50100200 |
| H | -4.36545400 | -1.75350900 | -0.50329300 |
| H | -3.11579600 | -1.49392900 | -1.77218600 |
| C | 3.28829500 | -1.71106900 | 0.71271700 |
| H | 3.11767300 | -1.49263300 | 1.77221500 |
| H | 2.82028800 | -2.67852800 | 0.50235900 |
| H | 4.36549700 | -1.75438600 | 0.50200600 |

IRC for **TS28** [R/R' = C(O)CH₃]

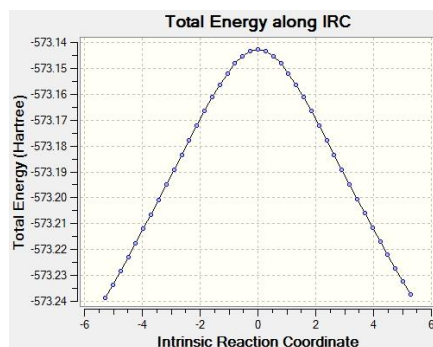


Cartesian coordinates for **S29** [R/R' = C(O)NH₂]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.60683900 | -0.46981500 | 0.47798800 |
| C | 0.60694900 | -0.47011900 | -0.47756500 |
| C | 0.68114300 | 0.83501100 | -1.31151000 |
| C | 0.62648800 | 2.10078300 | -0.44456800 |
| C | -0.62685500 | 2.10104900 | 0.44276400 |
| C | -0.68132000 | 0.83600700 | 1.31079600 |
| H | 1.58273600 | 0.84351200 | -1.93497800 |
| H | 0.46900300 | -1.29689300 | -1.18628200 |
| H | -0.46877900 | -1.29595600 | 1.18741800 |
| H | 1.52247900 | 2.16082100 | 0.18950700 |
| H | 0.63801600 | 2.98811400 | -1.08898500 |
| H | -0.63850600 | 2.98892600 | 1.08642100 |
| H | -1.52284800 | 2.16042700 | -0.19137200 |
| H | 0.17033200 | 0.82744800 | 1.99948200 |
| H | -1.58294200 | 0.84485300 | 1.93422700 |
| H | -0.17054500 | 0.82571900 | -2.00015100 |
| C | 1.89787900 | -0.78171100 | 0.29610600 |
| C | -1.89771500 | -0.78236000 | -0.29542300 |
| O | 1.92831800 | -1.01608800 | 1.50191600 |
| O | -1.92797000 | -1.01876900 | -1.50086800 |
| N | 3.04296100 | -0.80726400 | -0.45310400 |
| N | -3.04296200 | -0.80635500 | 0.45360400 |
| H | -3.89370900 | -1.10609800 | 0.00003500 |
| H | 3.03240800 | -0.73811300 | -1.45823700 |
| H | 3.89375600 | -1.10624200 | 0.00088200 |
| H | -3.03255400 | -0.73540800 | 1.45861800 |

Cartesian coordinates for **TS29** [R/R' = C(O)NH₂]

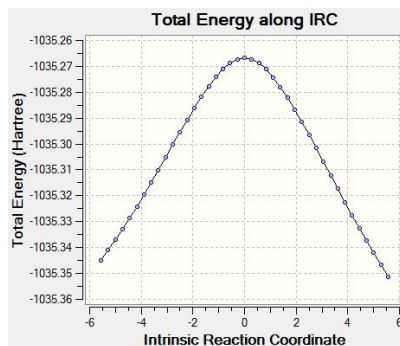
| | | | |
|---|-------------|-------------|-------------|
| C | -0.04056900 | -0.41883200 | 0.64896800 |
| C | -0.03072000 | -0.33658300 | -0.71737400 |
| C | 0.08386900 | 0.96478400 | -1.45362000 |
| C | -0.17824400 | 2.18443100 | -0.55304200 |
| C | 0.53966400 | 2.04601400 | 0.79746900 |
| C | 0.09454200 | 0.77780600 | 1.54697300 |
| H | -0.16328100 | -1.39409000 | 1.10821600 |
| H | -0.13121700 | -1.25170600 | -1.29115700 |
| H | -0.59981500 | 0.95057800 | -2.31091400 |
| H | -1.25940800 | 2.29091700 | -0.38912500 |
| H | 0.35193600 | 2.92689800 | 1.42150400 |
| H | 0.79981100 | 0.53715700 | 2.35195400 |
| H | -0.87703700 | 0.92873000 | 2.04049000 |
| H | 1.61910100 | 1.99589900 | 0.62108100 |
| H | 0.14905200 | 3.09556800 | -1.06537300 |
| H | 1.09956800 | 1.01972900 | -1.87082300 |
| C | -2.45493300 | -0.83281400 | -0.01378000 |
| C | 2.36747900 | -0.72929800 | -0.07755000 |
| N | 2.67259300 | -2.03753600 | 0.10088900 |
| O | 3.17611600 | 0.15244800 | -0.28667800 |
| H | 1.94598600 | -2.72051800 | 0.24337700 |
| H | 3.63774300 | -2.35984400 | 0.04745600 |
| O | -2.62751900 | -2.03733400 | -0.03939200 |
| N | -3.46446300 | 0.07845400 | -0.00770900 |
| H | -4.43801300 | -0.22473500 | -0.02825700 |
| H | -3.26663300 | 1.06502800 | 0.00961000 |

IRC for **TS29** [R/R' = C(O)NH₂]Cartesian coordinates for **S30** [R/R' = C(O)NHPH]

| | | | |
|---|-------------|-------------|-------------|
| C | 0.32467500 | 0.78290900 | -0.64012100 |
| C | -0.23757200 | 0.77832000 | 0.81626900 |
| C | -0.05020900 | 2.16111900 | 1.48439300 |
| C | -0.67632800 | 3.28913900 | 0.65338500 |
| C | -0.07060300 | 3.33820700 | -0.75600400 |
| C | -0.18608300 | 1.98216500 | -1.47353400 |
| H | -0.48703700 | 2.12009700 | 2.48510900 |
| H | 0.33430400 | 0.05219300 | 1.40990700 |
| H | 0.02251400 | -0.14853300 | -1.14326600 |
| H | -1.76417600 | 3.14034000 | 0.59431700 |
| H | -0.52379900 | 4.24808400 | 1.16231300 |
| H | -0.57131800 | 4.10411500 | -1.36056500 |
| H | 0.98564900 | 3.61671700 | -0.69126300 |
| H | -1.24206600 | 1.80829800 | -1.72071100 |
| H | 0.35869000 | 2.01251000 | -2.42256500 |
| H | 1.02443100 | 2.34805100 | 1.60104900 |
| C | -1.69592200 | 0.30081300 | 1.02231600 |
| C | 1.86804800 | 0.72857600 | -0.62442400 |
| O | -2.18869400 | 0.35055900 | 2.14500900 |
| O | 2.57361000 | 1.67966100 | -0.93847200 |
| N | -2.36109400 | -0.21259400 | -0.06426700 |
| N | 2.37194900 | -0.49447600 | -0.23944300 |
| H | -1.87903700 | -0.17237100 | -0.94906400 |
| C | -3.66452600 | -0.75970900 | -0.14092500 |
| C | -4.52333500 | -0.88374500 | 0.96254100 |
| C | -4.09503900 | -1.19726800 | -1.40561300 |
| C | -5.79172300 | -1.44188300 | 0.78118800 |
| H | -4.19624700 | -0.54564500 | 1.93520000 |
| C | -5.36286100 | -1.75074000 | -1.56946800 |
| H | -3.43320800 | -1.10268200 | -2.26418700 |
| C | -6.22181400 | -1.87730100 | -0.47375500 |
| H | -6.44929500 | -1.53321900 | 1.64095900 |
| H | -5.67728200 | -2.08219500 | -2.55476900 |
| H | -7.21051100 | -2.30797800 | -0.59841400 |
| H | 1.68975200 | -1.21018100 | -0.02913000 |
| C | 3.71618400 | -0.90934100 | -0.08985700 |
| C | 3.93190700 | -2.23305300 | 0.33057100 |
| C | 4.81707100 | -0.07517600 | -0.34098900 |
| C | 5.22647600 | -2.71984600 | 0.49716500 |
| H | 3.08166900 | -2.88264500 | 0.52822500 |
| C | 6.10902400 | -0.57891800 | -0.16794900 |
| H | 4.65473500 | 0.94233200 | -0.66637200 |
| C | 6.32652000 | -1.89381300 | 0.24838900 |
| H | 5.37282400 | -3.74555300 | 0.82272700 |
| H | 6.95445900 | 0.07405400 | -0.36497800 |
| H | 7.33629500 | -2.27077700 | 0.37767600 |

Cartesian coordinates for **TS30** [R/R' = C(O)NHPH]

| | | | |
|---|-------------|-------------|-------------|
| C | 0.11235000 | 0.64002500 | 0.67540300 |
| C | -0.11226600 | 0.64003200 | -0.67545500 |
| C | -0.19017700 | 1.89376400 | -1.48797300 |
| C | -0.44021400 | 3.14637800 | -0.62957500 |
| C | 0.44022500 | 3.14637400 | 0.62957500 |
| C | 0.19019600 | 1.89374200 | 1.48795000 |
| H | 0.17342300 | -0.31303000 | 1.19339700 |
| H | -0.17331000 | -0.31301300 | -1.19347200 |
| H | -0.95817500 | 1.78267500 | -2.26268500 |
| H | -1.49519400 | 3.18094200 | -0.33565300 |
| H | 0.24115800 | 4.04158500 | 1.22870600 |
| H | 0.95816400 | 1.78266400 | 2.26269200 |
| H | -0.77425900 | 1.97887500 | 2.01337400 |
| H | 1.49520500 | 3.18095800 | 0.33565500 |
| H | -0.24115900 | 4.04160100 | -1.22869100 |
| H | 0.77424700 | 1.97893800 | -2.01344500 |
| C | 2.45707200 | 0.50865400 | -0.46864600 |
| C | -2.45705900 | 0.50863600 | 0.46865200 |
| O | -2.96507200 | 1.29689200 | 1.24529200 |
| O | 2.96517400 | 1.29705700 | -1.24508600 |
| N | -3.12044500 | -0.50064700 | -0.17987200 |
| N | 3.12039400 | -0.50075200 | 0.17974900 |
| H | -2.54509600 | -1.06332900 | -0.78977300 |
| H | 2.54499200 | -1.06352700 | 0.78951400 |
| C | 4.49225200 | -0.87186900 | 0.13380600 |
| C | 4.89694700 | -1.96392700 | 0.91902500 |
| C | 5.43649000 | -0.19546500 | -0.65276300 |
| C | 6.22808600 | -2.37704800 | 0.91890400 |
| H | 4.16691200 | -2.48951000 | 1.53102600 |
| C | 6.76715200 | -0.62183100 | -0.64265700 |
| H | 5.12657700 | 0.64623900 | -1.25750100 |
| C | 7.17362500 | -1.70743800 | 0.13652300 |
| H | 6.52441800 | -3.22323400 | 1.53217400 |
| H | 7.49157000 | -0.09227700 | -1.25484400 |
| H | 8.21088900 | -2.02777400 | 0.13561700 |
| C | -4.49229300 | -0.87180500 | -0.13385800 |
| C | -5.43650100 | -0.19547200 | 0.65280800 |
| C | -4.89700900 | -1.96381700 | -0.91913000 |
| C | -6.76715100 | -0.62187600 | 0.64275800 |
| H | -5.12657200 | 0.64620000 | 1.25758000 |
| C | -6.22813700 | -2.37697200 | -0.91895700 |
| H | -4.16699700 | -2.48933900 | -1.53121200 |
| C | -7.17364500 | -1.70744100 | -0.13647000 |
| H | -7.49154600 | -0.09238100 | 1.25502200 |
| H | -6.52448600 | -3.22312400 | -1.53226700 |
| H | -8.21090000 | -2.02780200 | -0.13552300 |

IRC for **TS30** [R/R' = C(O)NHPH]

Cartesian coordinates for **S31** [R/R' = C(O)OCH₃]

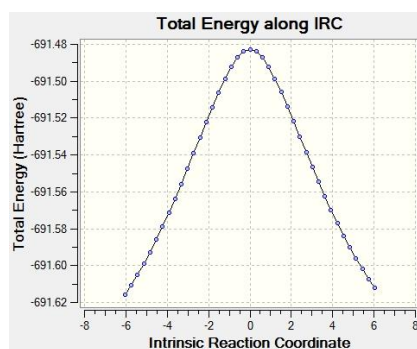
| | | | |
|---|-------------|-------------|-------------|
| C | 0.41808200 | -0.13535400 | -0.65581600 |
| C | -0.41814400 | -0.13528700 | 0.65559100 |
| C | -0.19285400 | 1.15272600 | 1.47117300 |
| C | -0.42297200 | 2.42589100 | 0.64061000 |
| C | 0.42382200 | 2.42578000 | -0.64061600 |
| C | 0.19320400 | 1.15276700 | -1.47126300 |
| H | -0.84690800 | 1.14551300 | 2.34787300 |
| H | -0.09988100 | -0.99785600 | 1.25413900 |
| H | 0.09959800 | -0.99778600 | -1.25443700 |
| H | -1.48739300 | 2.49853200 | 0.38431500 |
| H | -0.18766200 | 3.30712200 | 1.24949800 |
| H | 0.18882000 | 3.30712000 | -1.24946500 |
| H | 1.48827100 | 2.49800200 | -0.38432000 |
| H | -0.84110900 | 1.14017000 | -1.84080600 |
| H | 0.84723400 | 1.14540100 | -2.34797800 |
| H | 0.84143500 | 1.13979100 | 1.84076300 |
| C | 1.90376300 | -0.38354200 | -0.40176600 |
| C | -1.90393900 | -0.38310000 | 0.40172100 |
| O | 2.81712900 | 0.18228300 | -0.96823000 |
| O | -2.81705000 | 0.18246200 | 0.96884100 |
| O | -2.10757600 | -1.37448200 | -0.49844300 |
| O | 2.10710700 | -1.37532700 | 0.49797300 |
| C | -3.48170400 | -1.73559600 | -0.73976900 |
| H | -4.03945400 | -0.87842100 | -1.12404100 |
| H | -3.44535300 | -2.53519500 | -1.47919000 |
| H | -3.95097700 | -2.08364700 | 0.18349500 |
| C | 3.48112400 | -1.73597600 | 0.73990000 |
| H | 3.44480800 | -2.53495000 | 1.47999000 |
| H | 3.95066800 | -2.08479200 | -0.18297500 |
| H | 4.03873700 | -0.87835300 | 1.12342200 |

Cartesian coordinates for **TS31** [R/R' = C(O)OCH₃]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.02232400 | -0.07026900 | -0.68885300 |
| C | 0.02237800 | -0.07079000 | 0.68806800 |
| C | 0.05855100 | 1.18751300 | 1.50241700 |
| C | 0.38695100 | 2.43560200 | 0.66396500 |
| C | -0.38711800 | 2.43605300 | -0.66289800 |
| C | -0.05846100 | 1.18864100 | -1.50226300 |
| H | -0.04099000 | -1.02838100 | -1.19693800 |
| H | 0.04108600 | -1.02930900 | 1.19540100 |
| H | 0.77965300 | 1.05639700 | 2.31796900 |
| H | 1.46306600 | 2.45769900 | 0.46064300 |
| H | -0.14633700 | 3.33473100 | -1.24092500 |
| H | -0.77936700 | 1.05808000 | -2.31807700 |
| H | 0.92685100 | 1.29019600 | -1.97896900 |
| H | -1.46326300 | 2.45779800 | -0.45966100 |
| H | 0.14605300 | 3.33380400 | 1.24268000 |
| H | -0.92663600 | 1.28863400 | 1.97941400 |
| C | -2.30949600 | -0.27860800 | 0.09735700 |
| C | 2.30956100 | -0.27852600 | -0.09780300 |
| O | 3.16699000 | 0.53840100 | -0.34486700 |
| O | -3.16681500 | 0.53845500 | 0.34450300 |
| O | 2.56013600 | -1.58686400 | 0.15025700 |
| O | -2.56021600 | -1.58695700 | -0.15038200 |
| C | -3.95555500 | -2.00435000 | -0.11024000 |
| C | 3.95543200 | -2.00437700 | 0.11048600 |
| H | -3.94487900 | -3.07238000 | -0.32541400 |
| H | -4.37686100 | -1.81072700 | 0.87886000 |
| H | -4.53168600 | -1.46145100 | -0.86303000 |
| H | 3.94465000 | -3.07232600 | 0.32605100 |
| H | 4.37687900 | -1.81115200 | -0.87864000 |

H 4.53150900 -1.46123200 0.86314000

IRC for **TS31** [R/R' = C(O)OCH₃]



Cartesian coordinates for **S32** [R/R' = C(O)OH]

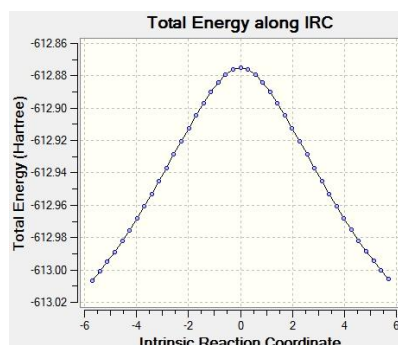
| | | | |
|---|-------------|-------------|-------------|
| C | 0.54799500 | -0.44856000 | -0.55271300 |
| C | -0.54803900 | -0.44853300 | 0.55274700 |
| C | -0.50072700 | 0.83844600 | 1.39804800 |
| C | -0.54770600 | 2.11248900 | 0.53897100 |
| C | 0.54772500 | 2.11246400 | -0.53895100 |
| C | 0.50068500 | 0.83842800 | -1.39805000 |
| H | -1.32745200 | 0.83097400 | 2.11406600 |
| H | -0.37006600 | -1.31454300 | 1.20274900 |
| H | 0.37003900 | -1.31459300 | -1.20268400 |
| H | -1.53525200 | 2.19072800 | 0.06741200 |
| H | -0.44092800 | 2.99167200 | 1.18538200 |
| H | 0.44100500 | 2.99168100 | -1.18532600 |
| H | 1.53528000 | 2.19064400 | -0.06739100 |
| H | -0.42975000 | 0.82323800 | -1.98114700 |
| H | 1.32738800 | 0.83092100 | -2.11409800 |
| H | 0.42969300 | 0.82322800 | 1.98118100 |
| C | 1.93960900 | -0.69397800 | 0.01831100 |
| C | -1.93959100 | -0.69398700 | -0.01836100 |
| O | 2.95760500 | -0.13083700 | -0.32483900 |
| O | -2.95757000 | -0.13052800 | 0.32439400 |
| O | -1.95460200 | -1.68962300 | -0.94538800 |
| O | 1.95460300 | -1.68921600 | 0.94578100 |
| H | 2.88124700 | -1.81127300 | 1.21356600 |
| H | -2.88120200 | -1.81166400 | -1.21331300 |

Cartesian coordinates for **TS32** [R/R' = C(O)OH]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.00579400 | -0.42941700 | -0.69024600 |
| C | 0.00555700 | -0.43001000 | 0.68971000 |
| C | 0.02249300 | 0.82815500 | 1.50370300 |
| C | 0.37019500 | 2.07682700 | 0.67404500 |
| C | -0.36957500 | 2.07753800 | -0.67244400 |
| C | -0.02238100 | 0.82943100 | -1.50317700 |
| H | -0.01122300 | -1.38765000 | -1.19901200 |
| H | 0.01078100 | -1.38867900 | 1.19766000 |
| H | 0.72248200 | 0.69587700 | 2.33710100 |
| H | 1.45116600 | 2.10178700 | 0.49897000 |
| H | -0.11221900 | 2.97506000 | -1.24469700 |
| H | -0.72251200 | 0.69809100 | -2.33660300 |
| H | 0.97409800 | 0.92895100 | -1.95654300 |
| H | -1.45053800 | 2.10275000 | -0.49733900 |
| H | 0.11317000 | 2.97396500 | 1.24705000 |
| H | -0.97399300 | 0.92768100 | 1.95706100 |
| C | -2.29935100 | -0.63774100 | 0.04220300 |
| C | 2.29916700 | -0.63796100 | -0.04298500 |
| O | 3.16809000 | 0.16337600 | -0.28773300 |

| | | | |
|---|-------------|-------------|-------------|
| O | -3.16829300 | 0.16387100 | 0.28593600 |
| O | 2.55341400 | -1.94570400 | 0.23462000 |
| O | -2.55357500 | -1.94580700 | -0.23397600 |
| H | 3.52385100 | -2.08730900 | 0.19690900 |
| H | -3.52402000 | -2.08734300 | -0.19618800 |

IRC for **TS32** [R/R' = C(O)OH]



Cartesian coordinates for **S33** [R/R' = C(O)OC(O)CH₃]

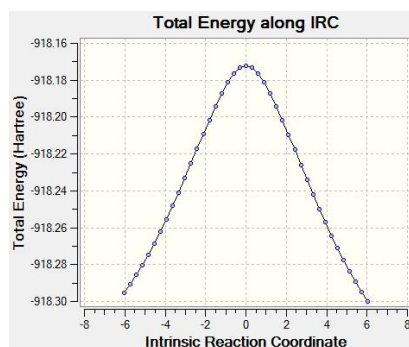
| | | | |
|---|-------------|-------------|-------------|
| C | 0.28715400 | 0.23621400 | -0.72276900 |
| C | -0.28711100 | 0.23575100 | 0.72262700 |
| C | 0.08965900 | 1.52193900 | 1.48304200 |
| C | -0.29051800 | 2.79660800 | 0.71205600 |
| C | 0.29085800 | 2.79707300 | -0.71042200 |
| C | -0.08945700 | 1.52297600 | -1.48229900 |
| H | -0.38563700 | 1.51444200 | 2.46783600 |
| H | 0.12741900 | -0.63412800 | 1.24802500 |
| H | -0.12750800 | -0.63325500 | -1.24875100 |
| H | -1.38393600 | 2.87588100 | 0.66750400 |
| H | 0.06160100 | 3.67575100 | 1.26422500 |
| H | -0.06115400 | 3.67664100 | -1.26197900 |
| H | 1.38428500 | 2.87617900 | -0.66581700 |
| H | -1.17452600 | 1.50774100 | -1.65269800 |
| H | 0.38582100 | 1.51610900 | -2.46710700 |
| H | 1.17472400 | 1.50645300 | 1.65345400 |
| C | 1.79347400 | -0.00386800 | -0.75281400 |
| C | -1.79346200 | -0.00411900 | 0.75245900 |
| O | 2.57813100 | 0.55604000 | -1.48127300 |
| O | -2.57812800 | 0.55557900 | 1.48107700 |
| O | -2.14373500 | -1.02817900 | -0.09664600 |
| O | 2.14363100 | -1.02840100 | 0.09581000 |
| C | 3.47178300 | -1.45133000 | 0.33281300 |
| O | 3.62764500 | -2.61710300 | 0.56584000 |
| C | 4.54538900 | -0.39946900 | 0.36073600 |
| H | 5.40872700 | -0.81415800 | 0.88203000 |
| H | 4.82038500 | -0.12999900 | -0.66185100 |
| H | 4.20093000 | 0.51291900 | 0.85369700 |
| C | -3.47203500 | -1.45109900 | -0.33304300 |
| C | -4.54507000 | -0.39872400 | -0.36272300 |
| H | -4.19993300 | 0.51280900 | -0.85679100 |
| H | -5.40855400 | -0.81356300 | -0.88365200 |
| H | -4.82016900 | -0.12769100 | 0.65943500 |
| O | -3.62835200 | -2.61716700 | -0.56424900 |

Cartesian coordinates for **TS33** [R/R' = C(O)OC(O)CH₃]

| | | | |
|---|-------------|------------|-------------|
| C | 0.04752300 | 0.39522400 | 0.70062400 |
| C | -0.07939100 | 0.46256700 | -0.67245100 |
| C | -0.13995800 | 1.75983300 | -1.41962600 |
| C | -0.42556800 | 2.96612300 | -0.50681800 |
| C | 0.40760500 | 2.90288100 | 0.78226700 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.12531000 | 1.61154300 | 1.57022900 |
| H | 0.09463100 | -0.58622800 | 1.16163000 |
| H | -0.13702900 | -0.47072200 | -1.22293800 |
| H | -0.88816400 | 1.67499900 | -2.21642900 |
| H | -1.49118600 | 2.98172400 | -0.25279800 |
| H | 0.18883300 | 3.76832100 | 1.41628200 |
| H | 0.88094700 | 1.44046700 | 2.34598100 |
| H | -0.83614600 | 1.68281900 | 2.09946200 |
| H | 1.47309100 | 2.94806000 | 0.53193900 |
| H | -0.20951900 | 3.89081900 | -1.05205100 |
| H | 0.82955700 | 1.87908700 | -1.92459600 |
| C | 2.28132400 | 0.23205600 | -0.23817300 |
| C | -2.30905700 | 0.19715900 | 0.22124200 |
| O | -3.13714600 | 0.95266200 | 0.65797500 |
| O | 3.08011300 | 1.01945700 | -0.67555000 |
| O | -2.55608600 | -1.12108300 | -0.13770300 |
| O | 2.60989800 | -1.01747700 | 0.26289600 |
| C | 3.91429200 | -1.58473300 | 0.23037100 |
| C | -3.82883300 | -1.75176100 | -0.15548300 |
| O | -3.84066600 | -2.94015500 | 0.01173500 |
| O | 4.24301900 | -2.24711300 | 1.17482000 |
| C | -5.03031100 | -0.89706500 | -0.45011300 |
| C | 4.72251300 | -1.36437100 | -1.01758000 |
| H | 4.10573700 | -1.49274500 | -1.91101000 |
| H | 5.10300500 | -0.33968600 | -1.03119100 |
| H | 5.55175300 | -2.07279200 | -1.02023800 |
| H | -5.27285800 | -0.28496300 | 0.42229700 |
| H | -4.83329500 | -0.20952900 | -1.27647300 |
| H | -5.86509800 | -1.55669500 | -0.69019300 |

IRC for **TS33** [R/R' = C(O)OC(O)CH₃]



Cartesian coordinates for **S34** [R/R' = C(O)F]

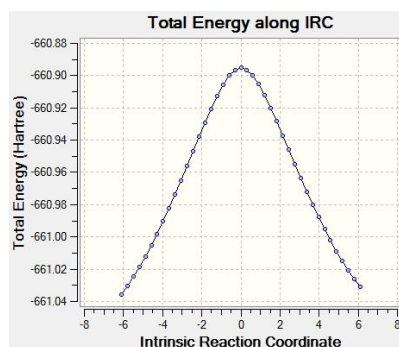
| | | | |
|---|-------------|-------------|-------------|
| C | 0.54517100 | -0.43817600 | -0.55752100 |
| C | -0.54519100 | -0.43821500 | 0.55753800 |
| C | -0.50037900 | 0.85110100 | 1.40069200 |
| C | -0.54701400 | 2.12426000 | 0.53976400 |
| C | 0.54709400 | 2.12427500 | -0.53964000 |
| C | 0.50036800 | 0.85120200 | -1.40066200 |
| H | -1.32594000 | 0.84298600 | 2.11846800 |
| H | -0.37043700 | -1.31008200 | 1.20089700 |
| H | 0.37048700 | -1.31003900 | -1.20091900 |
| H | -1.53472700 | 2.20661300 | 0.07005500 |
| H | -0.43645000 | 3.00158200 | 1.18703200 |
| H | 0.43658700 | 3.00168000 | -1.18681000 |
| H | 1.53482200 | 2.20654900 | -0.06994100 |
| H | -0.42870100 | 0.83537900 | -1.98555100 |
| H | 1.32591300 | 0.84305700 | -2.11844400 |
| H | 0.42867100 | 0.83518500 | 1.98561100 |
| C | -1.92411800 | -0.67803100 | -0.02272000 |
| C | 1.92411900 | -0.67799400 | 0.02260700 |

| | | | |
|---|-------------|-------------|-------------|
| O | -2.94324000 | -0.10064200 | 0.18648900 |
| O | 2.94334200 | -0.10089200 | -0.18676400 |
| F | 1.92535100 | -1.76947500 | 0.86345400 |
| F | -1.92550000 | -1.76954300 | -0.86329300 |

Cartesian coordinates for **TS34** [R/R' = C(O)F]

| | | | |
|---|-------------|-------------|-------------|
| C | -0.00728700 | -0.40360100 | -0.69346000 |
| C | 0.00724900 | -0.40379500 | 0.69325500 |
| C | 0.03826200 | 0.85436700 | 1.50483500 |
| C | 0.37374100 | 2.10421000 | 0.67141500 |
| C | -0.37377400 | 2.10438800 | -0.67090200 |
| C | -0.03823900 | 0.85479100 | -1.50467500 |
| H | -0.01264600 | -1.36379700 | -1.19949200 |
| H | 0.01257600 | -1.36413900 | 1.19901500 |
| H | 0.75041800 | 0.71747500 | 2.32714300 |
| H | 1.45380100 | 2.13610000 | 0.49198300 |
| H | -0.11704800 | 2.99971900 | -1.24585500 |
| H | -0.75033400 | 0.71815000 | -2.32707700 |
| H | 0.94827500 | 0.95232300 | -1.97951400 |
| H | -1.45384600 | 2.13617600 | -0.49146800 |
| H | 0.11697900 | 2.99936800 | 1.24662200 |
| H | -0.94821100 | 0.95177300 | 1.97978800 |
| C | -2.25653300 | -0.62795200 | 0.04685200 |
| C | 2.25652700 | -0.62794900 | -0.04706100 |
| O | 3.16451300 | 0.11667100 | -0.21554900 |
| O | -3.16457500 | 0.11665000 | 0.21498500 |
| F | -2.50567500 | -1.99318400 | -0.15332500 |
| F | 2.50577000 | -1.99309100 | 0.15352700 |

IRC for **TS34** [R/R' = C(O)F]



Cartesian coordinates for **S35** [R/R' = C(O)Cl]

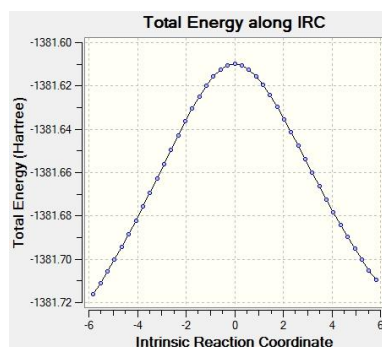
| | | | |
|---|-------------|-------------|-------------|
| C | 0.45735900 | -0.04203100 | -0.63031900 |
| C | -0.45711700 | -0.04218500 | 0.63007300 |
| C | -0.29374300 | 1.25261800 | 1.45382300 |
| C | -0.46253800 | 2.52880100 | 0.61283000 |
| C | 0.46266100 | 2.52903600 | -0.61243800 |
| C | 0.29395400 | 1.25305700 | -1.45379200 |
| H | -1.00367200 | 1.24381800 | 2.28621900 |
| H | -0.18904900 | -0.91115800 | 1.24304500 |
| H | 0.18922800 | -0.91088300 | -1.24344900 |
| H | -1.50740500 | 2.61570200 | 0.29284100 |
| H | -0.25447000 | 3.40267800 | 1.24052800 |
| H | 0.25450500 | 3.40312000 | -1.23983900 |
| H | 1.50752600 | 2.61595700 | -0.29249000 |
| H | -0.71129600 | 1.23331700 | -1.89544000 |
| H | 1.00386500 | 1.24451500 | -2.28621500 |
| H | 0.71151200 | 1.23268400 | 1.89552900 |
| C | -1.91950600 | -0.28286600 | 0.27027200 |
| C | 1.91973100 | -0.28304200 | -0.27058800 |

| | | | |
|----|-------------|-------------|-------------|
| O | -2.85647500 | 0.38975800 | 0.56157900 |
| O | 2.85708300 | 0.38913200 | -0.56164200 |
| Cl | -2.19998200 | -1.84929700 | -0.63859900 |
| Cl | 2.19937000 | -1.84959700 | 0.63863500 |

Cartesian coordinates for **TS35** [R/R' = C(O)Cl]

| | | | |
|----|-------------|-------------|-------------|
| C | -0.03989900 | 0.06411900 | -0.69138700 |
| C | 0.04101800 | 0.06409600 | 0.69172000 |
| C | 0.10417700 | 1.32152600 | 1.50066900 |
| C | 0.40408000 | 2.57270700 | 0.65499500 |
| C | -0.39855200 | 2.57332200 | -0.65469000 |
| C | -0.10071500 | 1.32163800 | -1.50038300 |
| H | -0.07504200 | -0.89627000 | -1.19696900 |
| H | 0.07313000 | -0.89631500 | 1.19747800 |
| H | 0.84542200 | 1.18661600 | 2.29766900 |
| H | 1.47570400 | 2.60661900 | 0.42923100 |
| H | -0.16676100 | 3.46855100 | -1.24020100 |
| H | -0.84235600 | 1.18789000 | -2.29720100 |
| H | 0.86611300 | 1.41970500 | -2.01615100 |
| H | -1.47012400 | 2.60888000 | -0.42889600 |
| H | 0.17366400 | 3.46830200 | 1.24049000 |
| H | -0.86259600 | 1.42112100 | 2.01626700 |
| C | -2.29403500 | -0.20797700 | 0.16290500 |
| C | 2.29232500 | -0.21232700 | -0.16297900 |
| O | 3.12027000 | 0.56832300 | -0.44575000 |
| O | -3.12240600 | 0.57254700 | 0.44426100 |
| Cl | -2.72926500 | -2.04862900 | -0.20599000 |
| Cl | 2.72629600 | -2.05047000 | 0.20629000 |

IRC for **TS35** [R/R' = C(O)Cl]



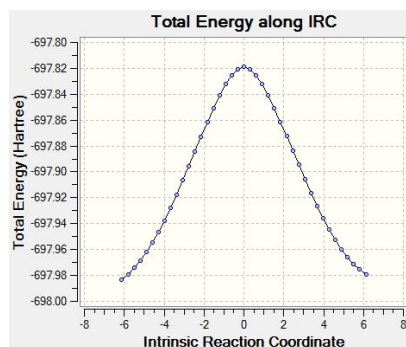
Cartesian coordinates for **S36** (R/R' = Ph)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.47435700 | 0.01420300 | -0.62638200 |
| C | -0.47455700 | 0.01425000 | 0.62675300 |
| C | -0.29266400 | 1.31788000 | 1.43616900 |
| C | -0.46555800 | 2.60388700 | 0.60932300 |
| C | 0.46581300 | 2.60374400 | -0.60895100 |
| C | 0.29239800 | 1.31781600 | -1.43580000 |
| H | -0.96598000 | 1.31847100 | 2.30147800 |
| H | -0.14128500 | -0.80015800 | 1.28096800 |
| H | 0.14099200 | -0.80023300 | -1.28053700 |
| H | -1.50182100 | 2.70333800 | 0.26499900 |
| H | -0.26187400 | 3.47662000 | 1.24220500 |
| H | 0.26243500 | 3.47658900 | -1.24177700 |
| H | 1.50213400 | 2.70276400 | -0.26467100 |
| H | -0.72562300 | 1.30698200 | -1.84691300 |
| H | 0.96537300 | 1.31829500 | -2.30136800 |
| H | 0.72521200 | 1.30688400 | 1.84763500 |
| C | 1.92423200 | -0.34153800 | -0.26530900 |
| C | 3.03122500 | 0.42389500 | -0.66226300 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.18731800 | -1.53737400 | 0.42891300 |
| C | 4.33920300 | 0.02848400 | -0.36000300 |
| H | 2.88845000 | 1.34055800 | -1.22220900 |
| C | 3.48858600 | -1.93869300 | 0.73309800 |
| H | 1.36234300 | -2.17808000 | 0.72947800 |
| C | 4.57638800 | -1.15158400 | 0.34433000 |
| H | 5.17162800 | 0.64868700 | -0.68125400 |
| H | 3.65200300 | -2.86978800 | 1.26887200 |
| H | 5.59105300 | -1.45884000 | 0.58031000 |
| C | -1.92435000 | -0.34153000 | 0.26552400 |
| C | -3.03143200 | 0.42431800 | 0.66132800 |
| C | -2.18716000 | -1.53787600 | -0.42796100 |
| C | -4.33930200 | 0.02879900 | 0.35865900 |
| H | -2.88885100 | 1.34136300 | 1.22069500 |
| C | -3.48828300 | -1.93928300 | -0.73255900 |
| H | -1.36201100 | -2.17882600 | -0.72755300 |
| C | -4.57621400 | -1.15174800 | -0.34493600 |
| H | -5.17184100 | 0.64931100 | 0.67901500 |
| H | -3.65154700 | -2.87075500 | -1.26772100 |
| H | -5.59078100 | -1.45908100 | -0.58124400 |

Cartesian coordinates for **TS36** (R/R' = Ph)

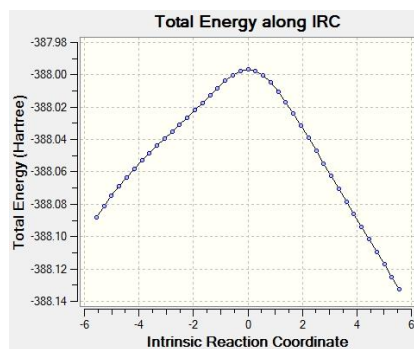
| | | | |
|---|-------------|-------------|-------------|
| C | 0.00213200 | 0.08653300 | -0.68935400 |
| C | -0.00211900 | 0.08638500 | 0.68914100 |
| C | 0.00461300 | 1.34817700 | 1.50724500 |
| C | 0.34389800 | 2.60508600 | 0.68732800 |
| C | -0.34367900 | 2.60526200 | -0.68694100 |
| C | -0.00450000 | 1.34852000 | -1.50717000 |
| H | 0.00806300 | -0.86217600 | -1.21198300 |
| H | -0.00820000 | -0.86243600 | 1.21156500 |
| H | 0.71521400 | 1.22067600 | 2.33110800 |
| H | 1.42929600 | 2.66032000 | 0.55352500 |
| H | -0.05347000 | 3.49787900 | -1.25231800 |
| H | -0.71515300 | 1.22125900 | -2.33102600 |
| H | 0.98613400 | 1.43989800 | -1.97009500 |
| H | -1.42906600 | 2.66045800 | -0.55305900 |
| H | 0.05369400 | 3.49757100 | 1.25291900 |
| H | -0.98604000 | 1.43951600 | 1.97013800 |
| C | -2.19386000 | -0.27701400 | -0.00311100 |
| C | -3.26979300 | 0.59237200 | 0.20019100 |
| C | -2.45295500 | -1.63451900 | -0.19979100 |
| C | -4.58721900 | 0.11187400 | 0.19247000 |
| H | -3.10906900 | 1.65528000 | 0.37627400 |
| C | -3.76542700 | -2.12690500 | -0.20949300 |
| H | -1.63133000 | -2.33943200 | -0.34875500 |
| C | -4.83576400 | -1.24900500 | -0.01500100 |
| H | -5.41684300 | 0.79757700 | 0.35210100 |
| H | -3.95104500 | -3.18732300 | -0.36646000 |
| H | -5.85616300 | -1.62221600 | -0.01975400 |
| C | 2.19378800 | -0.27712800 | 0.00292800 |
| C | 3.26968200 | 0.59229600 | -0.20039100 |
| C | 2.45291600 | -1.63460600 | 0.19973600 |
| C | 4.58712600 | 0.11184400 | -0.19254500 |
| H | 3.10896700 | 1.65518000 | -0.37664200 |
| C | 3.76540700 | -2.12693300 | 0.20957800 |
| H | 1.63130600 | -2.33953600 | 0.34869200 |
| C | 4.83571700 | -1.24900200 | 0.01508000 |
| H | 5.41673000 | 0.79756400 | -0.35220700 |
| H | 3.95106000 | -3.18732700 | 0.36665600 |
| H | 5.85613300 | -1.62216700 | 0.01993700 |

IRC for **TS36** (R/R' = Ph)Cartesian coordinates for **S37** (R/R' = CCH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.53172100 | -0.75492300 | 0.57745200 |
| C | 0.53171900 | -0.75492100 | -0.57746500 |
| C | 0.42022000 | 0.53936000 | -1.42454200 |
| C | 0.52018800 | 1.80882100 | -0.56616600 |
| C | -0.52017800 | 1.80881800 | 0.56617600 |
| C | -0.42021400 | 0.53934900 | 1.42454200 |
| H | 1.19702600 | 0.53141100 | -2.19649400 |
| H | 0.31584200 | -1.61285900 | -1.22650200 |
| H | -0.31584900 | -1.61286700 | 1.22648200 |
| H | 1.52893500 | 1.87904700 | -0.13788500 |
| H | 0.38650300 | 2.69226200 | -1.20191200 |
| H | -0.38648900 | 2.69225300 | 1.20193000 |
| H | -1.52892400 | 1.87905200 | 0.13789600 |
| H | 0.54857400 | 0.51628900 | 1.93854300 |
| H | -1.19701900 | 0.53139800 | 2.19649500 |
| H | -0.54856700 | 0.51630800 | -1.93854600 |
| C | 1.88306900 | -0.94282600 | -0.03652400 |
| C | -1.88307100 | -0.94281600 | 0.03650800 |
| C | 3.00160500 | -1.10869900 | 0.39683000 |
| C | -3.00161600 | -1.10868900 | -0.39682100 |
| H | 3.98686000 | -1.25658500 | 0.77645200 |
| H | -3.98689200 | -1.25655600 | -0.77639700 |

Cartesian coordinates for **T S37** (R/R' = CCH)

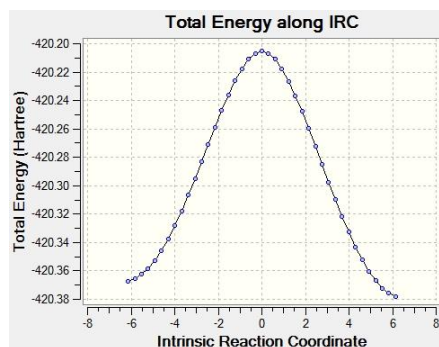
| | | | |
|---|-------------|-------------|-------------|
| C | 0.10287400 | -0.57183600 | -0.83055100 |
| C | -0.03904500 | -0.72768800 | 0.58482300 |
| C | 0.11540800 | 0.43137900 | 1.52756200 |
| C | 0.79325100 | 1.65306300 | 0.89087900 |
| C | 0.18901100 | 1.95127700 | -0.49026000 |
| C | 0.37680100 | 0.78455900 | -1.47265800 |
| H | -0.32918100 | -1.35380000 | -1.44808800 |
| H | -0.51873200 | -1.63566400 | 0.93820600 |
| H | 0.61063300 | 0.11149100 | 2.45042200 |
| H | 1.87499100 | 1.48052900 | 0.80599600 |
| H | 0.63523200 | 2.85751000 | -0.91366800 |
| H | -0.34169500 | 0.86567600 | -2.29160500 |
| H | 1.38230700 | 0.78736300 | -1.90873500 |
| H | -0.88667600 | 2.12564300 | -0.38058600 |
| H | 0.66580100 | 2.51342800 | 1.55616600 |
| H | -0.92611600 | 0.67115200 | 1.78335200 |
| C | -2.52520200 | -0.34708700 | -0.59548000 |
| C | -3.23380900 | -0.90563500 | 0.26299400 |
| C | 1.43550500 | -1.23478800 | -0.13408600 |
| C | 2.49944000 | -1.82399000 | -0.01892500 |
| H | 3.43877200 | -2.32468800 | 0.08289400 |
| H | -3.89074500 | -1.35416300 | 0.97984500 |

IRC for **TS37** (R/R' = CCH)Cartesian coordinates for **S38** (R/R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.53902100 | -0.77061700 | 0.56816000 |
| C | 0.53918000 | -0.77039000 | -0.56852100 |
| C | 0.45900700 | 0.52424300 | -1.41718200 |
| C | 0.53481700 | 1.79094700 | -0.55220800 |
| C | -0.53497100 | 1.79072500 | 0.55256900 |
| C | -0.45897400 | 0.52379700 | 1.41719700 |
| H | 1.25816700 | 0.51304400 | -2.16497700 |
| H | 0.36874600 | -1.63931600 | -1.21490500 |
| H | -0.36845700 | -1.63969600 | 1.21430900 |
| H | 1.53259500 | 1.86529100 | -0.09967500 |
| H | 0.41554400 | 2.67240600 | -1.19180900 |
| H | -0.41581600 | 2.67202100 | 1.19241700 |
| H | -1.53276100 | 1.86505100 | 0.10006200 |
| H | 0.49232500 | 0.49743400 | 1.96213300 |
| H | -1.25811200 | 0.51229800 | 2.16501000 |
| H | -0.49227600 | 0.49787200 | -1.96213900 |
| C | 1.87455000 | -0.94116400 | 0.02496100 |
| C | -1.87435100 | -0.94131700 | -0.02544100 |
| N | -2.92996100 | -1.07521000 | -0.49155700 |
| N | 2.92976400 | -1.07532800 | 0.49189400 |

Cartesian coordinates for **TS38** (R/R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.01610600 | -0.73079600 | 0.70408700 |
| C | -0.01688700 | -0.72989500 | -0.70574000 |
| C | -0.08731700 | 0.53336000 | -1.51164600 |
| C | -0.39084700 | 1.77907200 | -0.66038400 |
| C | 0.39264200 | 1.77777000 | 0.66221200 |
| C | 0.08781800 | 0.53122200 | 1.51173700 |
| H | 0.02277300 | -1.69054300 | 1.20896100 |
| H | -0.02464900 | -1.68894200 | -1.21184200 |
| H | -0.84301200 | 0.38588200 | -2.29083100 |
| H | -1.46599700 | 1.81474400 | -0.45371800 |
| H | 0.14952000 | 2.67264000 | 1.24331200 |
| H | 0.84329000 | 0.38190300 | 2.29079200 |
| H | -0.87168300 | 0.62524100 | 2.03474300 |
| H | 1.46782600 | 1.81265100 | 0.45559800 |
| H | -0.14682700 | 2.67449100 | -1.24026200 |
| H | 0.87224800 | 0.62716800 | -2.03456200 |
| C | 2.05629800 | -0.90781300 | -0.07738000 |
| N | 3.20686100 | -1.12165100 | -0.11131900 |
| C | -2.05744200 | -0.90583400 | 0.07526900 |
| N | -3.20767900 | -1.12088400 | 0.11258700 |

IRC for **TS38** (R/R' = CN)Cartesian coordinates for **S39** (R = CH₃ & R' = NH₂)

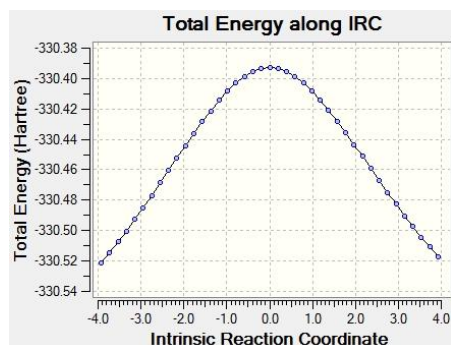
| | | | |
|---|-------------|-------------|-------------|
| C | 0.26977400 | 1.13081400 | 0.27754900 |
| C | -1.02218900 | 0.50163700 | -0.32435100 |
| C | -0.70057300 | -0.79831500 | -1.09666500 |
| C | 0.09573600 | -1.81382000 | -0.25887900 |
| C | 1.37605300 | -1.18351200 | 0.31241300 |
| C | 1.06631600 | 0.09991800 | 1.10218200 |
| H | -1.63274100 | -1.25051300 | -1.45912100 |
| H | -1.42085500 | 1.22929000 | -1.04728700 |
| H | -0.03712500 | 1.93979100 | 0.95412600 |
| H | -0.52537100 | -2.18421300 | 0.56799600 |
| H | 0.34236900 | -2.68931300 | -0.87235900 |
| H | 1.89749400 | -1.89973000 | 0.95921400 |
| H | 2.07235600 | -0.96007800 | -0.50913400 |
| H | 0.48664200 | -0.16549300 | 1.99587600 |
| H | 1.99126800 | 0.57237400 | 1.44996600 |
| H | -0.11840100 | -0.54936300 | -1.99559700 |
| C | -2.11304000 | 0.28961600 | 0.74069700 |
| H | -1.82158900 | -0.44411600 | 1.49910800 |
| H | -2.33971300 | 1.22777000 | 1.26071300 |
| H | -3.04117200 | -0.06695600 | 0.27939200 |
| N | 1.16235600 | 1.75937800 | -0.71119500 |
| H | 1.50617400 | 1.08523400 | -1.38950100 |
| H | 0.67170800 | 2.48164700 | -1.23270700 |

Cartesian coordinates for **TS39** (R = CH₃ & R' = NH₂)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.86850200 | 0.09677200 | -0.69726600 |
| C | 0.81915900 | 0.32947800 | 0.68135300 |
| C | -0.44233700 | 0.13657800 | 1.49282100 |
| C | -1.69455600 | 0.01087000 | 0.61032700 |
| C | -1.45129500 | -0.94106200 | -0.56998600 |
| C | -0.31241100 | -0.43719300 | -1.47318100 |
| H | 1.77488100 | 0.33761700 | -1.23650600 |
| H | 1.69339300 | 0.73936000 | 1.17061700 |
| H | -0.53161400 | 0.98996600 | 2.16932900 |
| H | -1.95852600 | 1.00370700 | 0.23058800 |
| H | -2.36300400 | -1.05292000 | -1.16751700 |
| H | 0.02300100 | -1.23036700 | -2.15392900 |
| H | -0.66202300 | 0.38610600 | -2.10162900 |
| H | -1.20885400 | -1.94116500 | -0.18497100 |
| H | -2.53648900 | -0.34208800 | 1.21694300 |
| H | -0.33919900 | -0.75704500 | 2.12471200 |
| C | 1.67855900 | -1.53207000 | 0.33608300 |
| H | 2.74579900 | -1.38014600 | 0.17833800 |
| H | 1.47280000 | -1.83498000 | 1.36282100 |
| H | 1.26451000 | -2.26540900 | -0.35635200 |
| N | 0.42138300 | 2.23938400 | -0.36963600 |
| H | 1.25712900 | 2.82890200 | -0.40918500 |

H -0.37521000 2.86254100 -0.53671500

IRC for **TS39** (R = CH₃ & R' = NH₂)



Cartesian coordinates for **S40** (R = CH₃ & R' = OH)

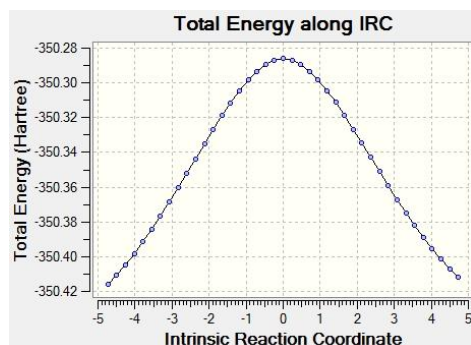
| | | | |
|---|-------------|-------------|-------------|
| C | -0.07318300 | -1.17137800 | 0.23078300 |
| C | 1.09238200 | -0.32628600 | -0.33688500 |
| C | 0.55714700 | 0.93014600 | -1.06368300 |
| C | -0.40117300 | 1.76589300 | -0.19723200 |
| C | -1.56242900 | 0.90940500 | 0.33246600 |
| C | -1.04751700 | -0.33448400 | 1.07809200 |
| H | 1.40102500 | 1.54439000 | -1.40242900 |
| H | 1.59432800 | -0.96112600 | -1.07862400 |
| H | 0.34129600 | -1.97478900 | 0.84985400 |
| H | 0.14524900 | 2.19891100 | 0.65122400 |
| H | -0.78644000 | 2.61236400 | -0.77873600 |
| H | -2.20613400 | 1.50039300 | 0.99476900 |
| H | -2.20323700 | 0.60336900 | -0.50845100 |
| H | -0.53441400 | -0.01723400 | 1.99589600 |
| H | -1.88075800 | -0.97567700 | 1.38724900 |
| H | 0.02969200 | 0.62239200 | -1.97919200 |
| C | 2.12869700 | 0.02210300 | 0.74567600 |
| H | 1.71798600 | 0.66225100 | 1.53322300 |
| H | 2.51287900 | -0.88534600 | 1.22569000 |
| H | 2.98164500 | 0.55055600 | 0.30536900 |
| O | -0.76262400 | -1.87690300 | -0.81515100 |
| H | -1.17566900 | -1.23762400 | -1.40993700 |

Cartesian coordinates for **TS40** (R = CH₃ & R' = OH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.73969400 | -0.46552000 | -0.73555700 |
| C | -0.63146700 | -0.71599400 | 0.62579800 |
| C | 0.36051500 | 0.00815300 | 1.50570900 |
| C | 1.47339500 | 0.68071800 | 0.68532900 |
| C | 0.89918800 | 1.47345400 | -0.49820300 |
| C | 0.08966600 | 0.56943400 | -1.44612300 |
| H | -1.37225100 | -1.11119400 | -1.33173200 |
| H | -1.18873100 | -1.54691800 | 1.04054600 |
| H | 0.78741900 | -0.73275300 | 2.18690300 |
| H | 2.12888200 | -0.10971400 | 0.30892100 |
| H | 1.70756000 | 1.94750000 | -1.06571800 |
| H | -0.54711200 | 1.16386200 | -2.11419300 |
| H | 0.76574600 | -0.01303900 | -2.07964300 |
| H | 0.26804000 | 2.29183900 | -0.12481500 |
| H | 2.05899400 | 1.34114100 | 1.33512900 |
| H | -0.16772000 | 0.74401600 | 2.12906300 |
| C | -2.19597300 | 0.56488500 | 0.30407200 |
| H | -2.97513200 | 0.31186400 | -0.41413100 |
| H | -2.54409900 | 0.35342600 | 1.31523600 |
| H | -1.85452800 | 1.59293700 | 0.21318200 |
| O | 0.85313300 | -2.00012800 | -0.43829400 |

H 0.57408800 -2.92271900 -0.53854700

IRC for **TS40** (R = CH₃ & R' = OH)

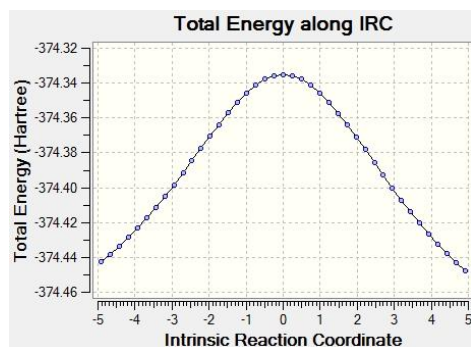


Cartesian coordinates for **S41** (R = CH₃ & R' = F)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.02503000 | -1.16298300 | 0.21260300 |
| C | 1.11497300 | -0.23253900 | -0.33577600 |
| C | 0.48574000 | 0.99294100 | -1.03584300 |
| C | -0.54894300 | 1.72029100 | -0.15953800 |
| C | -1.64363700 | 0.75359000 | 0.31974800 |
| C | -1.04117100 | -0.45934200 | 1.04770600 |
| H | 1.28146300 | 1.68327700 | -1.34307700 |
| H | 1.66065500 | -0.81496700 | -1.08975100 |
| H | 0.47477700 | -1.99220800 | 0.77187800 |
| H | -0.05535400 | 2.17626000 | 0.70998900 |
| H | -0.99638300 | 2.54608600 | -0.72572600 |
| H | -2.34920100 | 1.26893700 | 0.98223100 |
| H | -2.22060500 | 0.40105100 | -0.54431000 |
| H | -0.57888800 | -0.13976500 | 1.99172500 |
| H | -1.81861500 | -1.18616900 | 1.30897400 |
| H | -0.00762100 | 0.65278000 | -1.95467300 |
| F | -0.62661300 | -1.77207700 | -0.89950800 |
| C | 2.12146100 | 0.15361200 | 0.76240600 |
| H | 1.66681900 | 0.75178800 | 1.55859600 |
| H | 2.56295700 | -0.73575200 | 1.22706800 |
| H | 2.93879400 | 0.74396500 | 0.33481200 |

Cartesian coordinates for **TS41** (R = CH₃ & R' = F)

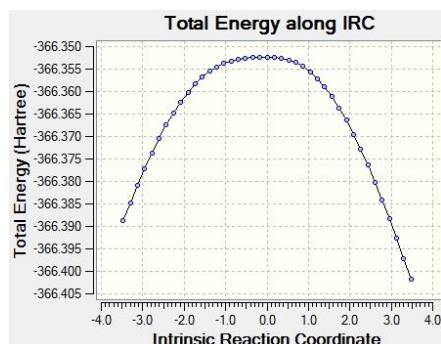
| | | | |
|---|-------------|-------------|-------------|
| C | -0.82705800 | -0.25300200 | -0.74469600 |
| C | -0.75903700 | -0.60743600 | 0.59287700 |
| C | 0.36820800 | -0.15809500 | 1.49261600 |
| C | 1.58244700 | 0.33943500 | 0.69050500 |
| C | 1.16415800 | 1.30345500 | -0.42899200 |
| C | 0.18862200 | 0.63069600 | -1.41042600 |
| H | -1.54238200 | -0.77239700 | -1.37072900 |
| H | -1.42612000 | -1.38710600 | 0.93987200 |
| H | 0.64613000 | -1.02335300 | 2.10062200 |
| H | 2.06522600 | -0.53713500 | 0.24949200 |
| H | 2.04383200 | 1.64678600 | -0.98405500 |
| H | -0.30942800 | 1.36598300 | -2.05506300 |
| H | 0.72922100 | -0.05933200 | -2.06790000 |
| H | 0.70730000 | 2.20457800 | 0.00406500 |
| H | 2.29294000 | 0.82807600 | 1.36665400 |
| H | 0.00912600 | 0.61362600 | 2.18803000 |
| C | -2.01489700 | 0.88660300 | 0.36928600 |
| F | 0.36759000 | -2.11982100 | -0.56804600 |
| H | -2.83006500 | 0.84263200 | -0.35169800 |
| H | -2.41092100 | 0.66401300 | 1.36029300 |
| H | -1.49782200 | 1.84208800 | 0.36581300 |

IRC for **TS41** (R = CH₃ & R' = F)Cartesian coordinates for **S42** (R = NH₂ & R' = OH)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.06131700 | -1.16996400 | 0.24068700 |
| C | 1.14431300 | -0.19834300 | -0.30233900 |
| C | 0.49941700 | 0.98484500 | -1.04980600 |
| C | -0.56365800 | 1.71450800 | -0.21000900 |
| C | -1.64106000 | 0.73981100 | 0.29354600 |
| C | -1.01743100 | -0.44039800 | 1.05938000 |
| H | 1.29194100 | 1.67293000 | -1.36174300 |
| H | 1.75003100 | -0.77016200 | -1.01509700 |
| H | 0.55365400 | -1.91729000 | 0.87369800 |
| H | -0.08827800 | 2.21038800 | 0.64842800 |
| H | -1.02091300 | 2.51521100 | -0.80352100 |
| H | -2.36316400 | 1.25939800 | 0.93432700 |
| H | -2.22077800 | 0.36547100 | -0.56405000 |
| H | -0.56493800 | -0.06651800 | 1.98852700 |
| H | -1.78425600 | -1.16489700 | 1.35567000 |
| H | 0.02966000 | 0.61001100 | -1.97045900 |
| N | 2.07043700 | 0.30191300 | 0.72378800 |
| H | 1.59034100 | 0.81229500 | 1.45918700 |
| H | 2.57689700 | -0.46161700 | 1.16426600 |
| O | -0.51359700 | -1.94872100 | -0.82095800 |
| H | -1.03186700 | -1.37159500 | -1.39683800 |

Cartesian coordinates for **TS42** (R = NH₂ & R' = OH)

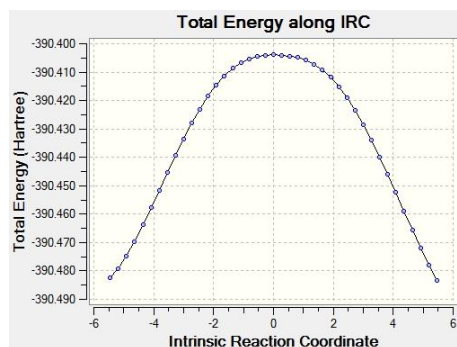
| | | | |
|---|-------------|-------------|-------------|
| C | -0.96642100 | -0.09730600 | -0.68916400 |
| C | -0.92449400 | -0.18238700 | 0.75714400 |
| C | 0.34597800 | 0.11039400 | 1.53830000 |
| C | 1.58835700 | 0.20743200 | 0.63637500 |
| C | 1.31311300 | 1.02057100 | -0.63663100 |
| C | 0.23457800 | 0.33149600 | -1.49082200 |
| H | -1.73608400 | -0.66338600 | -1.19727300 |
| H | -1.65172400 | -0.83713900 | 1.22144600 |
| H | 0.47632500 | -0.70997200 | 2.24717700 |
| H | 1.84232700 | -0.81683300 | 0.34375000 |
| H | 2.22685400 | 1.11364600 | -1.23358500 |
| H | -0.07663600 | 0.95217100 | -2.34092100 |
| H | 0.62302100 | -0.62402900 | -1.85977400 |
| H | 1.02079300 | 2.05478400 | -0.38346500 |
| H | 2.41829600 | 0.64497800 | 1.20335000 |
| H | 0.20206000 | 1.03013900 | 2.12620100 |
| N | -1.64620000 | 1.08751000 | 0.16959600 |
| O | 0.06564500 | -2.25218500 | -0.26687100 |
| H | -0.06572000 | -3.20716200 | -0.32245700 |
| H | -2.65743400 | 1.14384000 | 0.21818600 |
| H | -1.17051400 | 1.98266800 | 0.23395900 |

IRC for **TS42** (R = NH₂ & R' = OH)Cartesian coordinates for **S43** (R = NH₂ & R' = F)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.13823400 | 1.15582800 | 0.22411100 |
| C | -1.15736200 | 0.12312900 | -0.30074600 |
| C | -0.43875200 | -1.02659000 | -1.02848400 |
| C | 0.67646500 | -1.66320700 | -0.18045100 |
| C | 1.69346700 | -0.60735500 | 0.28343400 |
| C | 1.00325000 | 0.54479700 | 1.03134100 |
| H | -1.18505400 | -1.77388100 | -1.31755400 |
| H | -1.79945200 | 0.64496600 | -1.02006000 |
| H | -0.65456600 | 1.93518500 | 0.79838000 |
| H | 0.24590300 | -2.17251900 | 0.69450800 |
| H | 1.18155200 | -2.44338300 | -0.76208300 |
| H | 2.45506400 | -1.06166900 | 0.92816200 |
| H | 2.21954900 | -0.20198000 | -0.58979000 |
| H | 0.58960000 | 0.18100300 | 1.98245700 |
| H | 1.71791700 | 1.33559000 | 1.28567100 |
| H | 0.00230000 | -0.62731700 | -1.94969200 |
| F | 0.42231500 | 1.82107400 | -0.90290800 |
| N | -2.04155300 | -0.40161700 | 0.74792300 |
| H | -1.53062900 | -0.88961100 | 1.47729300 |
| H | -2.58514500 | 0.33565900 | 1.18817400 |

Cartesian coordinates for **TS43** (R = NH₂ & R' = F)

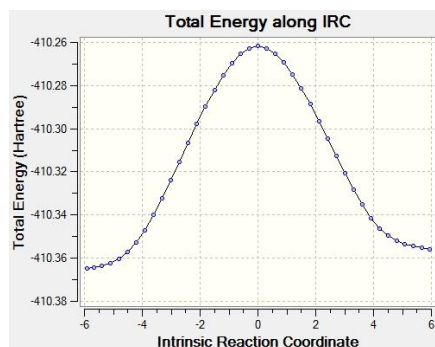
| | | | |
|---|-------------|-------------|-------------|
| C | 0.96247800 | -0.13841600 | -0.67556500 |
| C | 0.92370700 | 0.22054800 | 0.72184100 |
| C | -0.37553100 | 0.24018500 | 1.50825000 |
| C | -1.61716400 | 0.14695900 | 0.60470700 |
| C | -1.44834600 | -0.91352300 | -0.49224600 |
| C | -0.27971000 | -0.54874700 | -1.42364000 |
| H | 1.79700200 | 0.23198800 | -1.25779000 |
| H | 1.73075100 | 0.84796500 | 1.08031900 |
| H | -0.39521500 | 1.18299300 | 2.05947400 |
| H | -1.74202800 | 1.12429000 | 0.12920500 |
| H | -2.36306000 | -0.99441300 | -1.08930700 |
| H | -0.04961400 | -1.35813900 | -2.12799100 |
| H | -0.53503600 | 0.35086500 | -1.99185900 |
| H | -1.30033600 | -1.91166500 | -0.04488200 |
| H | -2.49921200 | -0.07058300 | 1.21786700 |
| H | -0.36136200 | -0.56917600 | 2.25342200 |
| F | 0.32361900 | 2.12368400 | -0.60790100 |
| N | 1.48891100 | -1.22368600 | 0.38837800 |
| H | 2.48550400 | -1.39481700 | 0.47024200 |
| H | 0.90505400 | -2.02870000 | 0.59368700 |

IRC for **TS43** (R = NH₂ & R' = F)Cartesian coordinates for **S44** (R = OH & R' = F)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.04555600 | -1.17012500 | 0.24305600 |
| C | 1.15678800 | -0.22822100 | -0.25212500 |
| C | 0.57889000 | 0.97498700 | -1.00902000 |
| C | -0.51050000 | 1.70866800 | -0.20628200 |
| C | -1.62864800 | 0.74507000 | 0.22304800 |
| C | -1.06632600 | -0.45558300 | 1.00336900 |
| H | 1.39885400 | 1.65134600 | -1.27647900 |
| H | 1.81612400 | -0.80140300 | -0.91102100 |
| H | 0.48650900 | -1.97472500 | 0.83953100 |
| H | -0.07520500 | 2.18823800 | 0.68483300 |
| H | -0.92116200 | 2.52765700 | -0.80774400 |
| H | -2.37308100 | 1.26882300 | 0.83377600 |
| H | -2.15170000 | 0.37919700 | -0.66910600 |
| H | -0.65533100 | -0.12224500 | 1.96694400 |
| H | -1.85570100 | -1.17843900 | 1.23733800 |
| H | 0.14443600 | 0.60653000 | -1.94637000 |
| F | -0.52171500 | -1.78810200 | -0.90474600 |
| O | 1.98385000 | 0.15368000 | 0.85456600 |
| H | 1.55632400 | 0.86971900 | 1.34220700 |

Cartesian coordinates for **TS44** (R = OH & R' = F)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.90270000 | -0.37427800 | 0.60770600 |
| C | -0.90365900 | 0.36054000 | -0.60889200 |
| C | 0.36326600 | 0.77058100 | -1.30115900 |
| C | 1.61430700 | 0.58007300 | -0.42565200 |
| C | 1.58153300 | -0.75763500 | 0.32793900 |
| C | 0.36088600 | -0.83879100 | 1.25992900 |
| H | -1.84009300 | -0.50101800 | 1.13482300 |
| H | -1.84439900 | 0.76035200 | -0.96560600 |
| H | 0.25115600 | 1.81963200 | -1.59216500 |
| H | 1.65823500 | 1.40176200 | 0.29589100 |
| H | 2.49331100 | -0.88046600 | 0.92241600 |
| H | 0.21094800 | -1.85535900 | 1.64021500 |
| H | 0.49128900 | -0.17984300 | 2.12647200 |
| H | 1.54840000 | -1.58898100 | -0.38614000 |
| H | 2.50814800 | 0.63982700 | -1.05619600 |
| H | 0.43309600 | 0.18344000 | -2.22537000 |
| F | -0.87292100 | 1.64218600 | 1.00197000 |
| O | -1.08752700 | -1.42661800 | -0.88501300 |
| H | -2.03538500 | -1.60902500 | -0.99119000 |

IRC for **TS44** (R = OH & R' = F)Cartesian coordinates for **S45** (R = CH₃ & R' = C(O)CH₃)

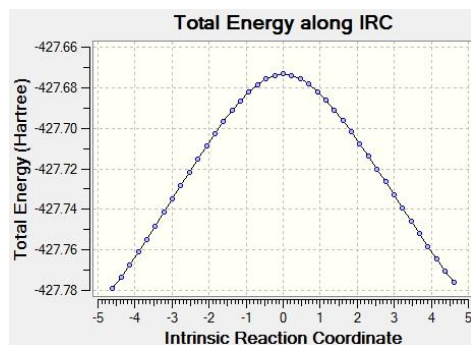
| | | | |
|---|-------------|-------------|-------------|
| C | 0.46287200 | 0.25608500 | 0.66042500 |
| C | -0.38517700 | 1.15576700 | -0.30306500 |
| C | -1.22353300 | 0.29265300 | -1.27187600 |
| C | -2.10310900 | -0.74023200 | -0.54985900 |
| C | -1.25100300 | -1.65917800 | 0.33713900 |
| C | -0.38478200 | -0.85532500 | 1.32149100 |
| H | -1.83943300 | 0.95399000 | -1.89492300 |
| H | 0.30995700 | 1.75192500 | -0.91076300 |
| H | 0.84761600 | 0.91550700 | 1.45226200 |
| H | -2.86076900 | -0.22809400 | 0.05964400 |
| H | -2.65443000 | -1.33420000 | -1.28896100 |
| H | -1.89569200 | -2.34555700 | 0.90046200 |
| H | -0.59978500 | -2.27233100 | -0.29379200 |
| H | -1.03580200 | -0.38229100 | 2.06893900 |
| H | 0.27765100 | -1.53261900 | 1.87282100 |
| H | -0.54722100 | -0.23891700 | -1.95396600 |
| C | -1.24463300 | 2.15661000 | 0.48981800 |
| H | -1.95033300 | 1.65766500 | 1.16088300 |
| H | -0.61578000 | 2.81416000 | 1.10079600 |
| H | -1.82600000 | 2.78855800 | -0.19099000 |
| C | 1.69735000 | -0.27549000 | -0.06959300 |
| O | 1.75696700 | -1.39922300 | -0.54295200 |
| C | 2.89021900 | 0.66466300 | -0.15875300 |
| H | 3.56943400 | 0.33464800 | -0.94685400 |
| H | 2.58981700 | 1.70378200 | -0.32553900 |
| H | 3.42581000 | 0.63423300 | 0.79924000 |

Cartesian coordinates for **TS45** (R = CH₃ & R' = C(O)CH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.41809700 | 0.61766100 | -0.86021200 |
| C | 0.35864200 | 0.97569300 | 0.45811600 |
| C | 0.71377000 | 0.03988200 | 1.58202200 |
| C | 0.84701200 | -1.42538200 | 1.12790100 |
| C | 1.56983600 | -1.54113700 | -0.22252600 |
| C | 0.83625300 | -0.74570400 | -1.31463600 |
| H | 0.09380100 | 1.33199800 | -1.60876500 |
| H | 0.00248600 | 1.96776000 | 0.71327500 |
| H | -0.04864500 | 0.13153700 | 2.36522100 |
| H | -0.15234600 | -1.86283200 | 1.03304800 |
| H | 1.64081300 | -2.59246600 | -0.52214900 |
| H | 1.44474000 | -0.66079100 | -2.22271300 |
| H | -0.08823400 | -1.26986300 | -1.60270200 |
| H | 2.59704800 | -1.16883900 | -0.12454500 |
| H | 1.37862300 | -1.99926700 | 1.89526100 |
| H | 1.65078900 | 0.39275900 | 2.03480100 |
| C | 2.45289000 | 1.84628600 | -0.36978600 |
| H | 2.24044500 | 2.65255700 | -1.06906400 |
| H | 2.68768900 | 2.18843200 | 0.63677200 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.13228700 | 1.08477200 | -0.74666600 |
| C | -2.04674500 | 0.02403900 | -0.17981400 |
| O | -2.30591100 | -1.05840500 | -0.65116000 |
| C | -3.14221200 | 0.97596200 | 0.30287900 |
| H | -4.14368100 | 0.55550300 | 0.13852100 |
| H | -2.99131700 | 1.18037900 | 1.36911700 |
| H | -3.04246900 | 1.93180000 | -0.22379600 |

IRC for **TS45** (R = CH₃ & R' = C(O)CH₃)



Cartesian coordinates for **S46** (R = NH₂ & R' = C(O)CH₃)

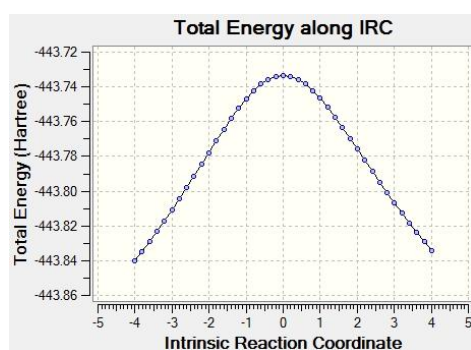
| | | | |
|---|-------------|-------------|-------------|
| C | 0.46722400 | 0.25505700 | 0.66829700 |
| C | -0.37708200 | 1.18375600 | -0.28539200 |
| C | -1.20443400 | 0.34339700 | -1.27448400 |
| C | -2.10725900 | -0.68203400 | -0.56968700 |
| C | -1.28400100 | -1.61952300 | 0.32564700 |
| C | -0.40939900 | -0.83738200 | 1.32073100 |
| H | -1.79765300 | 1.02742900 | -1.89064500 |
| H | 0.31727900 | 1.80597000 | -0.86346300 |
| H | 0.86149200 | 0.91013200 | 1.45904600 |
| H | -2.87143000 | -0.16235600 | 0.02696600 |
| H | -2.65756800 | -1.26253600 | -1.31969300 |
| H | -1.94853700 | -2.29334100 | 0.88085400 |
| H | -0.63882200 | -2.24471500 | -0.29937400 |
| H | -1.05642100 | -0.34953600 | 2.06372700 |
| H | 0.23029400 | -1.52927700 | 1.88029100 |
| H | -0.51865700 | -0.19131400 | -1.94350500 |
| N | -1.25105600 | 2.12341100 | 0.42607500 |
| H | -1.92826200 | 1.64340300 | 1.01164000 |
| H | -0.71665200 | 2.74536700 | 1.02682400 |
| C | 1.69031700 | -0.29552700 | -0.06415500 |
| C | 2.89807700 | 0.62483000 | -0.15421100 |
| O | 1.72813500 | -1.41782800 | -0.54388400 |
| H | 3.58310400 | 0.26804600 | -0.92530600 |
| H | 2.61390400 | 1.66368300 | -0.35111000 |
| H | 3.41958200 | 0.61234100 | 0.81182500 |

Cartesian coordinates for **TS46** (R = NH₂ & R' = C(O)CH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.09025800 | 0.65222700 | -0.66089500 |
| C | -0.11030400 | 0.56892500 | 0.74023400 |
| C | 0.71209100 | -0.43542200 | 1.50916000 |
| C | 1.45271600 | -1.45610700 | 0.62253800 |
| C | 1.95979100 | -0.81733600 | -0.67798500 |
| C | 0.78823300 | -0.24976600 | -1.49394000 |
| H | -0.59026200 | 1.49109900 | -1.13596300 |
| H | -0.63502700 | 1.33712300 | 1.30087500 |
| H | 0.07886600 | -0.95017100 | 2.24330400 |
| H | 0.77771700 | -2.28373100 | 0.37721500 |
| H | 2.49817200 | -1.56009000 | -1.27781500 |
| H | 1.14821500 | 0.32833000 | -2.34886600 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.18544100 | -1.07763800 | -1.89299400 |
| H | 2.65343500 | -0.00092700 | -0.45040000 |
| H | 2.28642700 | -1.88207100 | 1.19207800 |
| H | 1.42986000 | 0.16086200 | 2.08112200 |
| N | 1.37704000 | 2.36122500 | 0.14327800 |
| H | 0.77636800 | 3.19692000 | 0.13436300 |
| H | 2.32413100 | 2.76170800 | 0.19863300 |
| C | -1.68295900 | -0.28800600 | -0.06856900 |
| C | -2.90191500 | 0.60147700 | 0.00334500 |
| O | -1.70950900 | -1.48881700 | -0.16631900 |
| H | -3.48852500 | 0.32515800 | 0.88672400 |
| H | -2.64854800 | 1.66150200 | 0.05565800 |
| H | -3.52384300 | 0.41793400 | -0.87966300 |

IRC for **TS46** (R = NH₂ & R' = C(O)CH₃)



Cartesian coordinates for **S47** (R = OH & R' = C(O)CH₃)

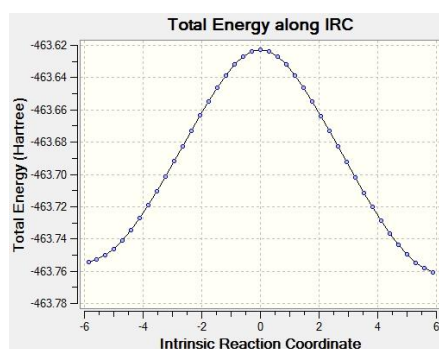
| | | | |
|---|-------------|-------------|-------------|
| C | 0.46609900 | 0.23082600 | 0.68126200 |
| C | -0.35806100 | 1.19489500 | -0.23067800 |
| C | -1.21136400 | 0.42988800 | -1.25279900 |
| C | -2.12185900 | -0.61822600 | -0.59183800 |
| C | -1.30378300 | -1.60639900 | 0.25218800 |
| C | -0.42121100 | -0.88131600 | 1.28334300 |
| H | -1.79792100 | 1.15636600 | -1.82664000 |
| H | 0.32576900 | 1.86467200 | -0.76163000 |
| H | 0.85083300 | 0.86443900 | 1.49162900 |
| H | -2.87722600 | -0.12121800 | 0.03722400 |
| H | -2.68884200 | -1.15210600 | -1.36320000 |
| H | -1.97239500 | -2.30282900 | 0.77296500 |
| H | -0.66444200 | -2.20352600 | -0.40553800 |
| H | -1.06146100 | -0.42386600 | 2.05145100 |
| H | 0.21271500 | -1.60499400 | 1.80723200 |
| H | -0.54090800 | -0.07608400 | -1.95964500 |
| O | -1.14613200 | 2.08573200 | 0.56811100 |
| H | -1.87907600 | 1.59434900 | 0.96178000 |
| C | 1.69213400 | -0.29958600 | -0.06502200 |
| C | 2.88276000 | 0.63928300 | -0.17208600 |
| O | 1.74360300 | -1.42664700 | -0.53123300 |
| H | 3.54926100 | 0.30708600 | -0.97003300 |
| H | 2.58258800 | 1.67907800 | -0.33422900 |
| H | 3.43304300 | 0.60976300 | 0.77739900 |

Cartesian coordinates for **TS47** (R = OH & R' = C(O)CH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.06601000 | 0.71845200 | -0.74678400 |
| C | 0.00168100 | 0.78908500 | 0.63922300 |
| C | 0.70178500 | -0.18893700 | 1.54382600 |
| C | 1.31481700 | -1.38956000 | 0.79819200 |
| C | 1.92506800 | -0.97029200 | -0.54750400 |
| C | 0.85828000 | -0.34061800 | -1.45756500 |
| H | -0.44243600 | 1.47964700 | -1.33034600 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.55190100 | 1.60418600 | 1.09362300 |
| H | 0.01119000 | -0.52800000 | 2.32722900 |
| H | 0.54018900 | -2.14541600 | 0.62454500 |
| H | 2.36360700 | -1.84065100 | -1.04873400 |
| H | 1.31492700 | 0.11489500 | -2.34143200 |
| H | 0.16451600 | -1.11459900 | -1.81720900 |
| H | 2.71597200 | -0.23159300 | -0.38620900 |
| H | 2.07613800 | -1.85299900 | 1.43531300 |
| H | 1.48311300 | 0.39271500 | 2.04430900 |
| O | 1.69079000 | 1.98578400 | -0.01339600 |
| H | 1.43445200 | 2.91629100 | -0.11224000 |
| C | -1.81924500 | -0.25403600 | -0.10300000 |
| C | -3.00732300 | 0.66246000 | 0.08661300 |
| O | -1.87437400 | -1.43813800 | -0.26552300 |
| H | -3.13211800 | 0.84394800 | 1.16117700 |
| H | -2.83934500 | 1.62957300 | -0.39483600 |
| H | -3.91606200 | 0.19150200 | -0.30185100 |

IRC for **TS47** (R = OH & R' = C(O)CH₃)



Cartesian coordinates for **S48** (R = F & R' = C(O)CH₃)

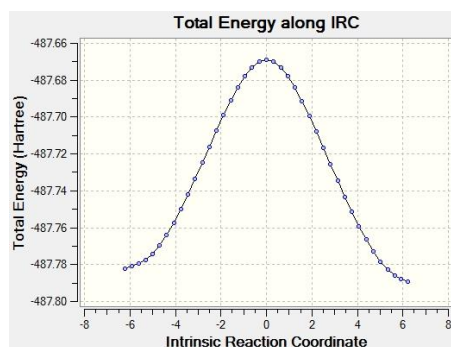
| | | | |
|---|-------------|-------------|-------------|
| C | 0.46912800 | 0.22226600 | 0.67074300 |
| C | -0.33780700 | 1.17689500 | -0.23823900 |
| C | -1.24569600 | 0.46567500 | -1.23352700 |
| C | -2.15987600 | -0.56397000 | -0.55279000 |
| C | -1.33797100 | -1.57956200 | 0.25338700 |
| C | -0.42575700 | -0.88186100 | 1.27682300 |
| H | -1.82925700 | 1.22142500 | -1.77131500 |
| H | 0.32523100 | 1.88261900 | -0.75138400 |
| H | 0.86177700 | 0.85408300 | 1.47912300 |
| H | -2.86131100 | -0.03991200 | 0.10846000 |
| H | -2.76233400 | -1.07676800 | -1.31147300 |
| H | -2.00733900 | -2.26936000 | 0.78161400 |
| H | -0.72516600 | -2.18157900 | -0.42555900 |
| H | -1.04616300 | -0.41260400 | 2.05031000 |
| H | 0.20840800 | -1.61958500 | 1.78060900 |
| H | -0.60671800 | -0.03523100 | -1.97338400 |
| F | -1.14482600 | 1.98018700 | 0.61235500 |
| C | 1.69315000 | -0.31195400 | -0.08570400 |
| C | 2.90608700 | 0.60058700 | -0.14823600 |
| H | 3.59133500 | 0.25857000 | -0.92566000 |
| H | 2.63002000 | 1.64640600 | -0.31780000 |
| H | 3.42307500 | 0.56060300 | 0.81933700 |
| O | 1.71679100 | -1.42235100 | -0.58860100 |

Cartesian coordinates for **TS48** (R = F & R' = C(O)CH₃)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.00686800 | 0.69638100 | -0.72545500 |
| C | -0.06534700 | 0.72367500 | 0.65817200 |
| C | 0.71503600 | -0.21564400 | 1.53031200 |
| C | 1.41340500 | -1.34757000 | 0.75513200 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.97881300 | -0.84549200 | -0.58123300 |
| C | 0.86151000 | -0.27466900 | -1.46991200 |
| H | -0.52314700 | 1.47791200 | -1.27430900 |
| H | -0.62149500 | 1.52694900 | 1.13072900 |
| H | 0.07271900 | -0.61465000 | 2.32608400 |
| H | 0.69993700 | -2.15930200 | 0.57034400 |
| H | 2.48454900 | -1.66182200 | -1.10873800 |
| H | 1.27723100 | 0.25360100 | -2.33355200 |
| H | 0.23409700 | -1.08626500 | -1.86575500 |
| H | 2.70533000 | -0.04822400 | -0.39850700 |
| H | 2.21388200 | -1.76319800 | 1.37672300 |
| H | 1.45317100 | 0.43101100 | 2.01984600 |
| F | 1.46073400 | 2.12451800 | 0.02794200 |
| C | -1.77348700 | -0.30656200 | -0.09723600 |
| C | -2.97969500 | 0.58138700 | 0.06593400 |
| O | -1.77137000 | -1.49098900 | -0.23704400 |
| H | -2.79969300 | 1.58106900 | -0.33533500 |
| H | -3.84678500 | 0.12002100 | -0.41571500 |
| H | -3.18565200 | 0.68111600 | 1.13878100 |

IRC for **TS48** (R = F & R' = C(O)CH₃)



Cartesian coordinates for **S49** (R = CH₃ & R' = CN)

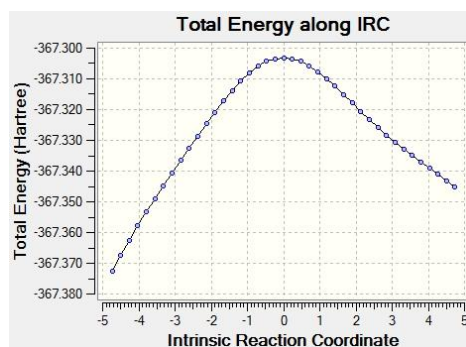
| | | | |
|---|-------------|-------------|-------------|
| C | -0.64133600 | -0.57225100 | 0.63509400 |
| C | 0.49538800 | -1.08803800 | -0.30442500 |
| C | 0.92601800 | 0.02347600 | -1.28644400 |
| C | 1.29690300 | 1.34179600 | -0.58616400 |
| C | 0.15414100 | 1.84052900 | 0.31240100 |
| C | -0.27343900 | 0.76831700 | 1.32534600 |
| H | 1.76792300 | -0.33704100 | -1.89018700 |
| H | 0.07897400 | -1.91497800 | -0.89301800 |
| H | -0.82591400 | -1.32980300 | 1.40833300 |
| H | 2.20456200 | 1.20645300 | 0.01748000 |
| H | 1.54019500 | 2.10062100 | -1.33913200 |
| H | 0.45572400 | 2.74907000 | 0.84680100 |
| H | -0.70774000 | 2.11551500 | -0.31041100 |
| H | 0.54716600 | 0.56967000 | 2.02512300 |
| H | -1.12219400 | 1.11478400 | 1.92455300 |
| H | 0.10152100 | 0.21420300 | -1.98610400 |
| C | 1.66910300 | -1.65823600 | 0.50906100 |
| H | 2.15770400 | -0.90564700 | 1.13557300 |
| H | 1.33587300 | -2.47100900 | 1.16441700 |
| H | 2.42979100 | -2.06707000 | -0.16449500 |
| C | -1.90373300 | -0.43814900 | -0.11091000 |
| N | -2.90026600 | -0.33563400 | -0.70038400 |

Cartesian coordinates for **TS49** (R = CH₃ & R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.07788500 | -0.84862000 | -0.72636900 |
| C | -0.14923200 | -0.94737600 | 0.66192900 |
| C | -0.45388800 | 0.24881500 | 1.54065900 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.33370200 | 1.58409900 | 0.78171300 |
| C | -0.97919500 | 1.52588700 | -0.61109600 |
| C | -0.33792800 | 0.42242300 | -1.46654400 |
| H | 0.40165000 | -1.65855400 | -1.26620800 |
| H | 0.31156600 | -1.81348900 | 1.12352900 |
| H | 0.27809400 | 0.21182600 | 2.35254600 |
| H | 0.73144300 | 1.80839700 | 0.66717700 |
| H | -0.85148700 | 2.48448100 | -1.12408600 |
| H | -0.88969600 | 0.22995400 | -2.39397100 |
| H | 0.68857700 | 0.70858400 | -1.75008900 |
| H | -2.06418100 | 1.37015900 | -0.52560300 |
| H | -0.78508900 | 2.38297900 | 1.37911000 |
| H | -1.44449000 | 0.13388500 | 2.00033100 |
| C | -1.71304500 | -1.59944700 | -0.08992200 |
| H | -1.89936600 | -2.16630100 | 0.82288300 |
| H | -2.43836200 | -0.80161400 | -0.21140400 |
| H | -1.71998900 | -2.30812600 | -0.91775400 |
| C | 2.58605400 | -0.52766400 | 0.50442000 |
| N | 2.63346500 | 0.03844500 | -0.53217100 |

IRC for **TS49** (R = CH₃ & R' = CN)



Cartesian coordinates for **S50** (R = NH₂ & R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.67469400 | -0.52538200 | 0.65297500 |
| C | 0.43654200 | -1.13624600 | -0.27927900 |
| C | 0.92307100 | -0.07976900 | -1.28779700 |
| C | 1.38885500 | 1.22183700 | -0.61258100 |
| C | 0.29203400 | 1.81541200 | 0.28668100 |
| C | -0.20382700 | 0.79261000 | 1.31934100 |
| H | 1.72988000 | -0.51912000 | -1.88292000 |
| H | -0.01768300 | -1.96445700 | -0.83441100 |
| H | -0.90272900 | -1.26194700 | 1.43476900 |
| H | 2.29453100 | 1.03601500 | -0.01707300 |
| H | 1.67926100 | 1.94802500 | -1.38047400 |
| H | 0.66266100 | 2.70792600 | 0.80421600 |
| H | -0.55267700 | 2.14195400 | -0.33454600 |
| H | 0.60874400 | 0.54130300 | 2.01344300 |
| H | -1.01458200 | 1.20911700 | 1.92604800 |
| H | 0.09902200 | 0.15081700 | -1.97457600 |
| N | 1.56629000 | -1.70276000 | 0.45472000 |
| H | 2.06042600 | -1.01570400 | 1.01510900 |
| H | 1.28390600 | -2.46492600 | 1.06408700 |
| C | -1.92267500 | -0.32108700 | -0.09710900 |
| N | -2.90437400 | -0.17056100 | -0.70144200 |

Cartesian coordinates for **TS50** (R = NH₂ & R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.00905300 | 0.90167300 | 0.72360400 |
| C | 0.10562500 | 0.88230600 | -0.73618700 |
| C | -0.24454300 | -0.38483100 | -1.51122900 |
| C | -0.66231100 | -1.55843900 | -0.60430700 |

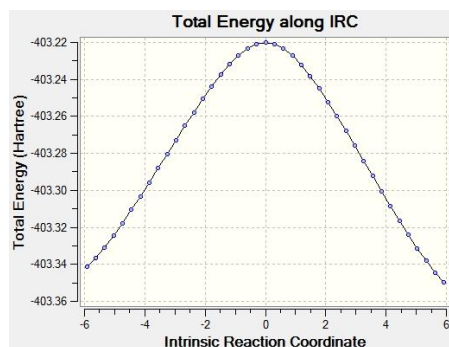
| | | | |
|---|-------------|-------------|-------------|
| C | -1.53890500 | -1.10856000 | 0.57364500 |
| C | -0.76767500 | -0.13996100 | 1.48885300 |
| H | 0.57125600 | 1.64932100 | 1.26494500 |
| H | 0.92243500 | 1.46193200 | -1.15596300 |
| H | 0.64558000 | -0.66491200 | -2.07917900 |
| H | 0.24598400 | -2.02368400 | -0.20816400 |
| H | -1.85759900 | -1.97323900 | 1.16467800 |
| H | -1.42749800 | 0.35093900 | 2.21378700 |
| H | -0.00861500 | -0.68579400 | 2.05490300 |
| H | -2.46819300 | -0.64440100 | 0.20513500 |
| H | -1.18288900 | -2.31219600 | -1.20436800 |
| H | -1.03293200 | -0.14375600 | -2.23794700 |
| C | 2.30835200 | -0.11574300 | 0.80458400 |
| N | 2.94605200 | -0.34927500 | -0.15881300 |
| N | -1.05128700 | 1.76730000 | -0.34210700 |
| H | -0.93509100 | 2.76965400 | -0.43339500 |
| H | -1.99336800 | 1.43128500 | -0.51177400 |

Cartesian coordinates for **S51** (R = OH & R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.69898100 | -0.48977800 | 0.66881300 |
| C | 0.38474000 | -1.16580900 | -0.23064100 |
| C | 0.94303800 | -0.18203700 | -1.26847100 |
| C | 1.45236300 | 1.12516700 | -0.63405600 |
| C | 0.37089500 | 1.79340100 | 0.23111400 |
| C | -0.17628200 | 0.82893700 | 1.29384900 |
| H | 1.73931200 | -0.68212800 | -1.83114700 |
| H | -0.06966900 | -2.02181400 | -0.73796500 |
| H | -0.94488800 | -1.20123200 | 1.46594300 |
| H | 2.34469600 | 0.93045700 | -0.01864000 |
| H | 1.78574200 | 1.80825000 | -1.42318900 |
| H | 0.77342000 | 2.68833900 | 0.71932200 |
| H | -0.45270500 | 2.13086000 | -0.41198000 |
| H | 0.61612900 | 0.56506900 | 2.00606800 |
| H | -0.97371900 | 1.30115700 | 1.87650200 |
| H | 0.14491000 | 0.05246800 | -1.98382900 |
| C | -1.93056100 | -0.26024000 | -0.10011400 |
| N | -2.89770100 | -0.07898800 | -0.71879200 |
| O | 1.40127400 | -1.73321500 | 0.59580600 |
| H | 2.03921900 | -1.05063300 | 0.84105400 |

Cartesian coordinates for **TS51** (R = OH & R' = CN)

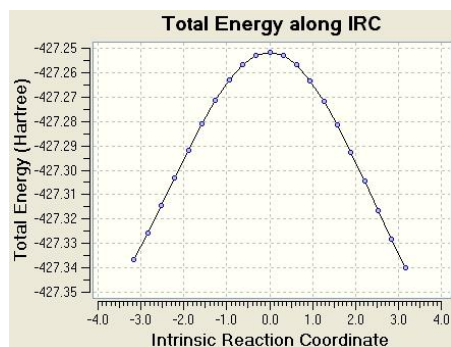
| | | | |
|---|-------------|-------------|-------------|
| C | -0.10388100 | -0.96752400 | -0.65804900 |
| C | -0.03871200 | -0.88841100 | 0.76478600 |
| C | -0.35242900 | 0.38163000 | 1.51566700 |
| C | -0.49823100 | 1.60958300 | 0.59777200 |
| C | -1.26755000 | 1.28905400 | -0.69263300 |
| C | -0.56725100 | 0.18343200 | -1.50474300 |
| H | 0.33276300 | -1.83346700 | -1.13882700 |
| H | 0.44669000 | -1.70099900 | 1.28932800 |
| H | 0.45411500 | 0.53918500 | 2.23709300 |
| H | 0.50448300 | 1.96149600 | 0.33533400 |
| H | -1.35274300 | 2.18538800 | -1.31492900 |
| H | -1.20488600 | -0.20046700 | -2.30913000 |
| H | 0.33544700 | 0.57873100 | -1.98219200 |
| H | -2.30257800 | 0.99653200 | -0.45603500 |
| H | -0.99624400 | 2.41521400 | 1.14690000 |
| H | -1.26096700 | 0.20951900 | 2.10875500 |
| C | 2.18331100 | -0.23688200 | -0.09582000 |
| N | 3.28509900 | 0.16043000 | -0.17934300 |
| O | -1.48323500 | -1.68199800 | 0.19818900 |
| H | -2.21742700 | -1.04345800 | 0.19171500 |

IRC for **TS51** (R = OH & R' = CN)Cartesian coordinates for **S52** (R = F & R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.72009500 | -0.45120200 | 0.66496000 |
| C | 0.32601400 | -1.16857600 | -0.22248700 |
| C | 0.97187300 | -0.25076100 | -1.25256700 |
| C | 1.53090900 | 1.03649900 | -0.62422000 |
| C | 0.46339400 | 1.77004000 | 0.20323900 |
| C | -0.14082400 | 0.85170600 | 1.27548600 |
| H | 1.75786400 | -0.81000200 | -1.77153300 |
| H | -0.11488300 | -2.05292100 | -0.69319200 |
| H | -0.99797800 | -1.14261300 | 1.46991800 |
| H | 2.38318400 | 0.78380800 | 0.01864700 |
| H | 1.91464100 | 1.69063400 | -1.41500500 |
| H | 0.89870100 | 2.65292800 | 0.68496900 |
| H | -0.33385400 | 2.13538300 | -0.45838500 |
| H | 0.63339700 | 0.55488300 | 1.99163800 |
| H | -0.92521900 | 1.36669500 | 1.83931600 |
| H | 0.20769700 | -0.00369800 | -2.00137700 |
| C | -1.93869500 | -0.19123800 | -0.11564600 |
| N | -2.89925800 | 0.01451700 | -0.73598000 |
| F | 1.32397700 | -1.65061400 | 0.65714200 |

Cartesian coordinates for **TS52** (R = F & R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.15211200 | 0.90935700 | 0.60390100 |
| C | 0.22450100 | 0.73235000 | -0.79832500 |
| C | -0.32859800 | -0.48042800 | -1.48349300 |
| C | -0.68112000 | -1.61614900 | -0.50949500 |
| C | -1.40527900 | -1.08602500 | 0.73798100 |
| C | -0.54653800 | -0.06714100 | 1.50779800 |
| H | 0.57512700 | 1.81620100 | 1.02045300 |
| H | 0.68885100 | 1.51808500 | -1.38310600 |
| H | 0.37747800 | -0.81088000 | -2.25205900 |
| H | 0.23883700 | -2.13522100 | -0.21383100 |
| H | -1.66216400 | -1.91462900 | 1.40584900 |
| H | -1.16039200 | 0.52799500 | 2.19184900 |
| H | 0.21055500 | -0.56406200 | 2.12498500 |
| H | -2.34028400 | -0.60115700 | 0.44004100 |
| H | -1.30695800 | -2.34959100 | -1.02783300 |
| H | -1.22255300 | -0.12114900 | -2.00761500 |
| C | 1.97540200 | 0.08167500 | 0.10948500 |
| N | 3.07645600 | -0.29760500 | 0.21030100 |
| F | -1.36406500 | 1.76397800 | -0.30866100 |

IRC for **TS52** (R = F & R' = CN)Cartesian coordinates for **S53** (R = C(O)CH₃ & R' = CN)

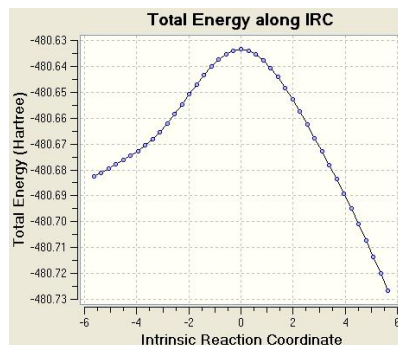
| | | | |
|---|-------------|-------------|-------------|
| C | 0.51437700 | -0.81486200 | -0.53431100 |
| C | -0.46890000 | -0.36373600 | 0.60370700 |
| C | 0.09464700 | 0.83985300 | 1.39053900 |
| C | 0.60631200 | 1.99360300 | 0.51051900 |
| C | 1.59460200 | 1.50214300 | -0.55668000 |
| C | 0.98060800 | 0.37985800 | -1.40448300 |
| H | -0.67598700 | 1.20577900 | 2.07799000 |
| H | -0.57626500 | -1.21394000 | 1.28927400 |
| H | 0.01052900 | -1.54767500 | -1.17806500 |
| H | -0.24383100 | 2.48257500 | 0.02500900 |
| H | 1.08913200 | 2.74194500 | 1.15005800 |
| H | 1.88916900 | 2.33081600 | -1.21073500 |
| H | 2.51440000 | 1.13686900 | -0.07980700 |
| H | 0.10380000 | 0.76003600 | -1.94164400 |
| H | 1.69120100 | 0.01899400 | -2.15568800 |
| H | 0.91940600 | 0.46750500 | 2.01233900 |
| C | -1.86001500 | -0.12341700 | -0.00101700 |
| C | 1.66358500 | -1.52169800 | 0.05466200 |
| N | 2.56638100 | -2.08648000 | 0.51992700 |
| O | -2.25037000 | 0.98541300 | -0.32288800 |
| C | -2.75027400 | -1.34423000 | -0.15336700 |
| H | -3.57777900 | -1.12275700 | -0.82926100 |
| H | -2.19586500 | -2.22050300 | -0.50538000 |
| H | -3.15927600 | -1.60266300 | 0.83210300 |

Cartesian coordinates for **TS53** (R = C(O)CH₃ & R' = CN)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.18079461 | -0.92093917 | -0.61429799 |
| C | -0.11562561 | -0.84182617 | 0.80853701 |
| C | -0.42934261 | 0.42821483 | 1.55941801 |
| C | -0.57514461 | 1.65616783 | 0.64152301 |
| C | -1.34446361 | 1.33563883 | -0.64888199 |
| C | -0.64416461 | 0.23001683 | -1.46099199 |
| H | 0.25584939 | -1.78688217 | -1.09507599 |
| H | 0.36977639 | -1.65441417 | 1.33307901 |
| H | 0.37720139 | 0.58576983 | 2.28084401 |
| H | 0.42756939 | 2.00808083 | 0.37908501 |
| H | -1.42965661 | 2.23197283 | -1.27117799 |
| H | -1.28179961 | -0.15388217 | -2.26537899 |
| H | 0.25853339 | 0.62531583 | -1.93844099 |
| H | -2.37949161 | 1.04311683 | -0.41228399 |
| H | -1.07315761 | 2.46179883 | 1.19065101 |
| H | -1.33788061 | 0.25610383 | 2.15250601 |
| C | 2.10639739 | -0.19029717 | -0.05206899 |
| N | 3.20818539 | 0.20701483 | -0.13559199 |
| C | -2.40447567 | -2.04282412 | 0.29057473 |
| C | -3.24341193 | -2.51574677 | -0.91114492 |
| H | -2.70507615 | -3.26892883 | -1.44762547 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.17034588 | -2.92035374 | -0.56187907 |
| H | -3.43771102 | -1.68654685 | -1.55889129 |
| O | -3.35051302 | -1.46983067 | 0.82871211 |

IRC for **TS53** (R = C(O)CH₃ & R' = CN)

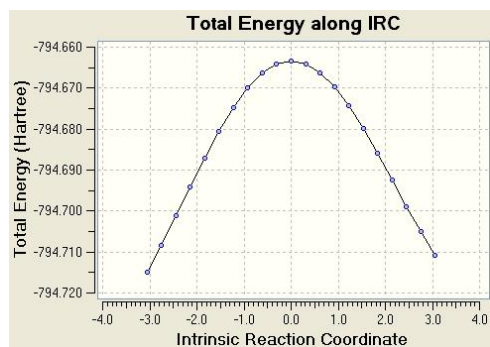


Cartesian coordinates for **S54** (R = F & R' = Cl)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.68242600 | -0.36300500 | 0.64332900 |
| C | 0.32627500 | -1.17061600 | -0.18500200 |
| C | 1.11062400 | -0.33762000 | -1.19082900 |
| C | 1.72797000 | 0.91967600 | -0.55622600 |
| C | 0.66676600 | 1.75715300 | 0.17584500 |
| C | -0.07896800 | 0.91668600 | 1.22313300 |
| H | 1.88171200 | -0.97400100 | -1.63860700 |
| H | -0.16588400 | -2.02322100 | -0.66141900 |
| H | -1.08694400 | -1.00002600 | 1.43152500 |
| H | 2.51228300 | 0.62126900 | 0.15074500 |
| H | 2.21553600 | 1.51893500 | -1.33349500 |
| H | 1.13550900 | 2.61674000 | 0.66842500 |
| H | -0.05188400 | 2.16204100 | -0.54804800 |
| H | 0.62408200 | 0.59817600 | 2.00485700 |
| H | -0.86372400 | 1.49860600 | 1.71673200 |
| H | 0.42120700 | -0.05274000 | -1.99509400 |
| F | 1.23568800 | -1.71981500 | 0.75963600 |
| Cl | -2.12732500 | 0.01052400 | -0.42905000 |

Cartesian coordinates for **TS54** (R = F & R' = Cl)

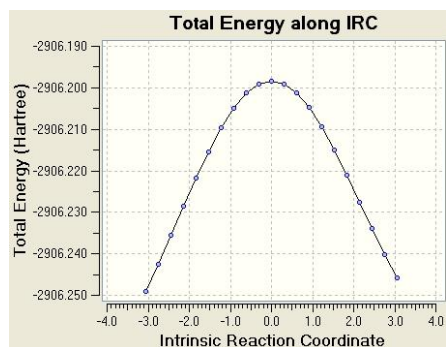
| | | | |
|----|-------------|-------------|-------------|
| C | 0.16051300 | 0.90170600 | 0.58461300 |
| C | 0.22568100 | 0.66868100 | -0.82637500 |
| C | -0.45808600 | -0.49368800 | -1.47438000 |
| C | -0.94980200 | -1.54821000 | -0.46858900 |
| C | -1.62062600 | -0.89688400 | 0.75000400 |
| C | -0.65987500 | 0.04523200 | 1.49883500 |
| H | 0.68832000 | 1.75742600 | 0.98335700 |
| H | 0.79360900 | 1.36234600 | -1.43135700 |
| H | 0.22202700 | -0.92880100 | -2.21323600 |
| H | -0.09687700 | -2.15380800 | -0.14352100 |
| H | -1.97481100 | -1.66726400 | 1.44276900 |
| H | -1.20635300 | 0.71879800 | 2.16859000 |
| H | 0.03875500 | -0.51764600 | 2.12809700 |
| H | -2.49579500 | -0.32445800 | 0.42501100 |
| H | -1.65255600 | -2.22086700 | -0.97108800 |
| H | -1.29856000 | -0.06275100 | -2.03447000 |
| F | -1.16679000 | 1.85245700 | -0.39061300 |
| Cl | 2.19391300 | -0.27624200 | 0.16333700 |

IRC for **TS54** (R = F & R' = Cl)Cartesian coordinates for **S55** (R = F & R' = Br)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.10883200 | -0.37316800 | 0.77794100 |
| C | 0.79789000 | -1.16950600 | -0.16378800 |
| C | 1.45952800 | -0.32794100 | -1.24849700 |
| C | 2.13254800 | 0.93285200 | -0.68100700 |
| C | 1.14895900 | 1.76102700 | 0.16140900 |
| C | 0.53169500 | 0.91518400 | 1.28566800 |
| H | 2.18277100 | -0.95729700 | -1.77840800 |
| H | 0.26315000 | -2.02589500 | -0.58312300 |
| H | -0.42132100 | -1.01253500 | 1.60369000 |
| H | 2.99018400 | 0.63916400 | -0.06296200 |
| H | 2.52802700 | 1.53690600 | -1.50543900 |
| H | 1.65831200 | 2.62778100 | 0.59775600 |
| H | 0.35168100 | 2.15415500 | -0.48225800 |
| H | 1.32148000 | 0.60993300 | 1.98673900 |
| H | -0.20082300 | 1.48958400 | 1.86083100 |
| H | 0.68575200 | -0.04709400 | -1.97314200 |
| F | 1.81533000 | -1.71372500 | 0.67015900 |
| Br | -1.81336900 | -0.00062500 | -0.18529900 |

Cartesian coordinates for **TS55** (R = F & R' = Br)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.35327200 | 0.91862800 | 0.57879500 |
| C | -0.33100000 | 0.71323500 | -0.83630900 |
| C | -0.96576600 | -0.47931900 | -1.48192600 |
| C | -1.34040800 | -1.58313900 | -0.47894300 |
| C | -1.99829200 | -1.00258000 | 0.78271600 |
| C | -1.07896800 | -0.00393500 | 1.51197200 |
| H | 0.10105900 | 1.82006600 | 0.96666800 |
| H | 0.13704100 | 1.46929600 | -1.45180400 |
| H | -0.29936500 | -0.85552800 | -2.26431200 |
| H | -0.43836100 | -2.14159200 | -0.20469800 |
| H | -2.26454800 | -1.80922800 | 1.47365200 |
| H | -1.65291100 | 0.62685700 | 2.19989300 |
| H | -0.33070500 | -0.52393000 | 2.11953100 |
| H | -2.92547900 | -0.48934900 | 0.50733100 |
| H | -2.02077700 | -2.29023500 | -0.96492500 |
| H | -1.85950800 | -0.09083500 | -1.98703300 |
| F | -1.82287700 | 1.78935000 | -0.32509400 |
| Br | 1.83901900 | -0.09134300 | 0.05924900 |

IRC for **TS55** (R = F & R' = Br)Cartesian coordinates for **S56** (R = Cl & R' = Br)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.15984400 | -0.39180100 | 0.64852700 |
| C | 0.81113500 | -0.70519600 | -0.49262000 |
| C | 1.11612200 | 0.49910800 | -1.38535300 |
| C | 1.47988500 | 1.76282500 | -0.59161200 |
| C | 0.40473900 | 2.09359500 | 0.45657900 |
| C | 0.15423200 | 0.90258700 | 1.39347800 |
| H | 1.90850900 | 0.23166800 | -2.09098000 |
| H | 0.45033500 | -1.54965100 | -1.07889000 |
| H | -0.22789400 | -1.23776100 | 1.33031300 |
| H | 2.44830900 | 1.61840100 | -0.09644700 |
| H | 1.60203900 | 2.60186400 | -1.28590100 |
| H | 0.70866600 | 2.96252100 | 1.05121100 |
| H | -0.53061300 | 2.36781000 | -0.04754400 |
| H | 1.05975200 | 0.70722800 | 1.98432800 |
| H | -0.64966500 | 1.11767300 | 2.10362100 |
| H | 0.21021100 | 0.68624500 | -1.97681200 |
| Br | -1.99999600 | -0.33036800 | -0.13942800 |
| Cl | 2.36368200 | -1.34763700 | 0.28312400 |

Cartesian coordinates for **TS56** (R = Cl & R' = Br)

| | | | |
|----|-------------|-------------|-------------|
| C | 0.31192700 | -0.54614200 | 0.69474000 |
| C | 0.31759800 | -0.52053600 | -0.73649500 |
| C | 0.57199900 | 0.73887300 | -1.51359000 |
| C | 0.52506600 | 2.00944900 | -0.64724700 |
| C | 1.25452500 | 1.81677700 | 0.69218800 |
| C | 0.66032800 | 0.66169200 | 1.51995600 |
| H | 0.13892200 | -1.49213800 | 1.18792600 |
| H | 0.13146600 | -1.44401500 | -1.26651700 |
| H | -0.15240400 | 0.78722700 | -2.33315700 |
| H | -0.52001400 | 2.28311100 | -0.46497900 |
| H | 1.20500700 | 2.73792100 | 1.28185500 |
| H | 1.36002100 | 0.33516500 | 2.29624800 |
| H | -0.24976400 | 0.97900500 | 2.04068900 |
| H | 2.31315700 | 1.60767300 | 0.50533000 |
| H | 0.97861300 | 2.83539800 | -1.20476500 |
| H | 1.55741800 | 0.62017600 | -1.97885700 |
| Br | -2.03163400 | -0.33482500 | 0.03313000 |
| Cl | 2.49977200 | -1.32301900 | -0.07533200 |

IRC for **TS56** (R = Cl & R' = Br)