

Supporting Information

On the Mechanism of Conversion of Substituted Glycals to Chiral Acenes via Diels- Alder Reaction: A Computational Study

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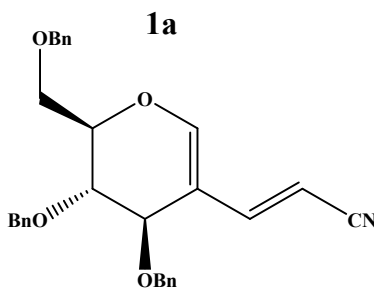
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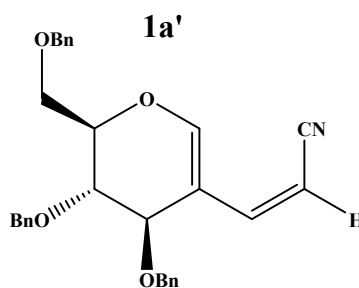
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Scheme S1: *E* and *Z* configuration of **1a**



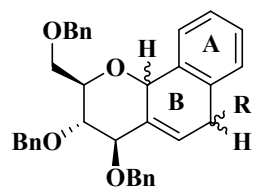
(*E*)-3-((2*R*,3*S*,4*R*)-3,4-bis(benzyloxy)-2-((benzyloxy)methyl)-3,4-dihydro-2*H*-pyran-5-yl)acrylonitrile



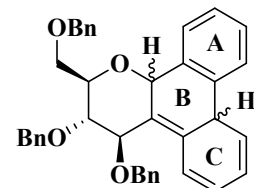
(*Z*)-3-((2*R*,3*S*,4*R*)-3,4-bis(benzyloxy)-2-((benzyloxy)methyl)-3,4-dihydro-2*H*-pyran-5-yl)acrylonitrile

Table S1: Aromaticity (NICS (0)) for A, B, and C rings calculated at SMD_{ACN}-M062X/6-31G(d) level of theory.

| | 3 | | 4 | | TS2 | | 5 | | 6 | | TS3 | | 7 | | 3a | | | | | | | | | | |
|---|-----------|-------|----------|-----------|------------|------|------------|------|-----------|-----------|------------|-------|-----------|-------|-----------|-------------|------------|-------|-----------|-------|--------|-----------|-------|--------|--|
| | A | B | A | B | A | B | A | B | A | B | A | B | A | B | A | B | | | | | | | | | |
| R | -8.81 | 1.52 | -8.63 | 1.81 | -8.79 | 1.54 | -7.50 | 1.40 | -7.24 | 0.44 | -8.52 | -7.77 | -9.18 | -6.88 | -9.31 | -8.73 | | | | | | | | | |
| S | -8.81 | 0.91 | -8.61 | 1.99 | -8.55 | 2.07 | -7.53 | 0.72 | -7.20 | 0.49 | -8.65 | -7.36 | -9.03 | -8.89 | -9.19 | -9.39 | | | | | | | | | |
| | 8 | | 9 | | TS6 | | 10 | | 11 | | TS7 | | 12 | | 3a | | TS5 | | | | | | | | |
| | A | B | A | B | A | B | A | B | A | B | A | B | A | B | A | B | A | B | | | | | | | |
| R | -8.65 | 1.80 | -8.44 | 1.85 | -8.53 | 1.39 | -7.59 | 1.00 | -7.13 | 0.49 | -8.40 | -7.63 | -9.12 | -7.71 | -9.31 | -8.73 | -8.79 | -0.92 | | | | | | | |
| S | -8.77 | 0.79 | -8.59 | 0.77 | -8.42 | 1.61 | -7.77 | 0.47 | -7.29 | -0.46 | -8.42 | -7.70 | -8.69 | -9.52 | -9.19 | -9.39 | -8.92 | -2.12 | | | | | | | |
| | 13 | | | 14 | | | TS9 | | | 15 | | | 16 | | | TS10 | | | 17 | | | 3b | | | |
| | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C | |
| R | -8.73 | 0.04 | 4.95 | -8.56 | 0.37 | 4.60 | -8.36 | 2.07 | 3.24 | -7.79 | 0.43 | 2.76 | -7.75 | 2.41 | -1.85 | -8.90 | -3.78 | -7.29 | -8.99 | -4.49 | -8.95 | -9.07 | -4.90 | -9.25 | |
| S | -8.91 | -0.32 | 4.38 | -8.79 | -0.78 | 3.69 | -8.42 | 0.53 | -0.89 | -9.12 | 1.05 | 3.31 | -7.97 | 1.75 | -1.94 | -8.71 | -3.95 | -7.39 | -9.04 | -6.07 | -10.27 | -9.18 | -6.33 | -10.08 | |



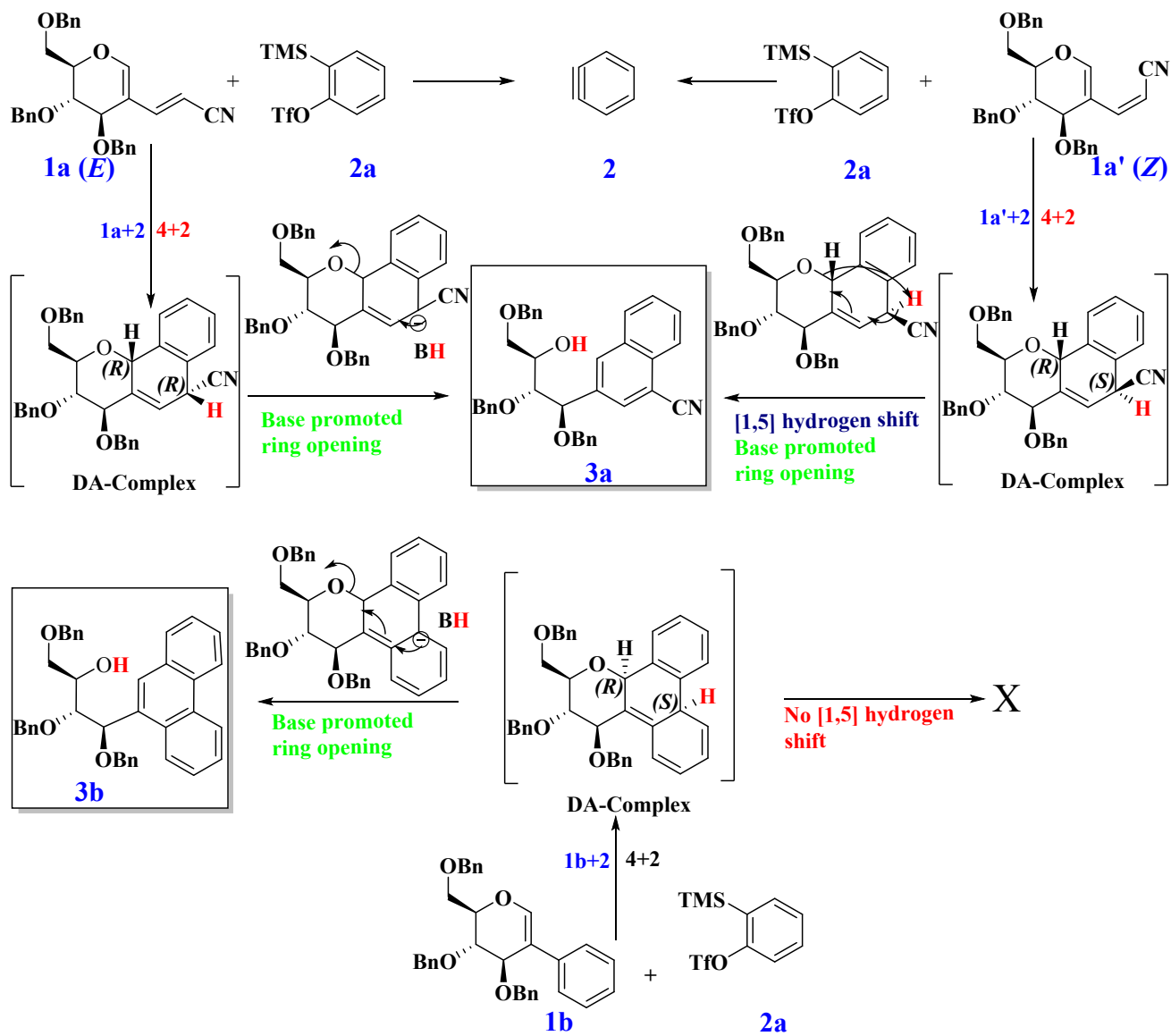
DA-adduct from vinyl diene



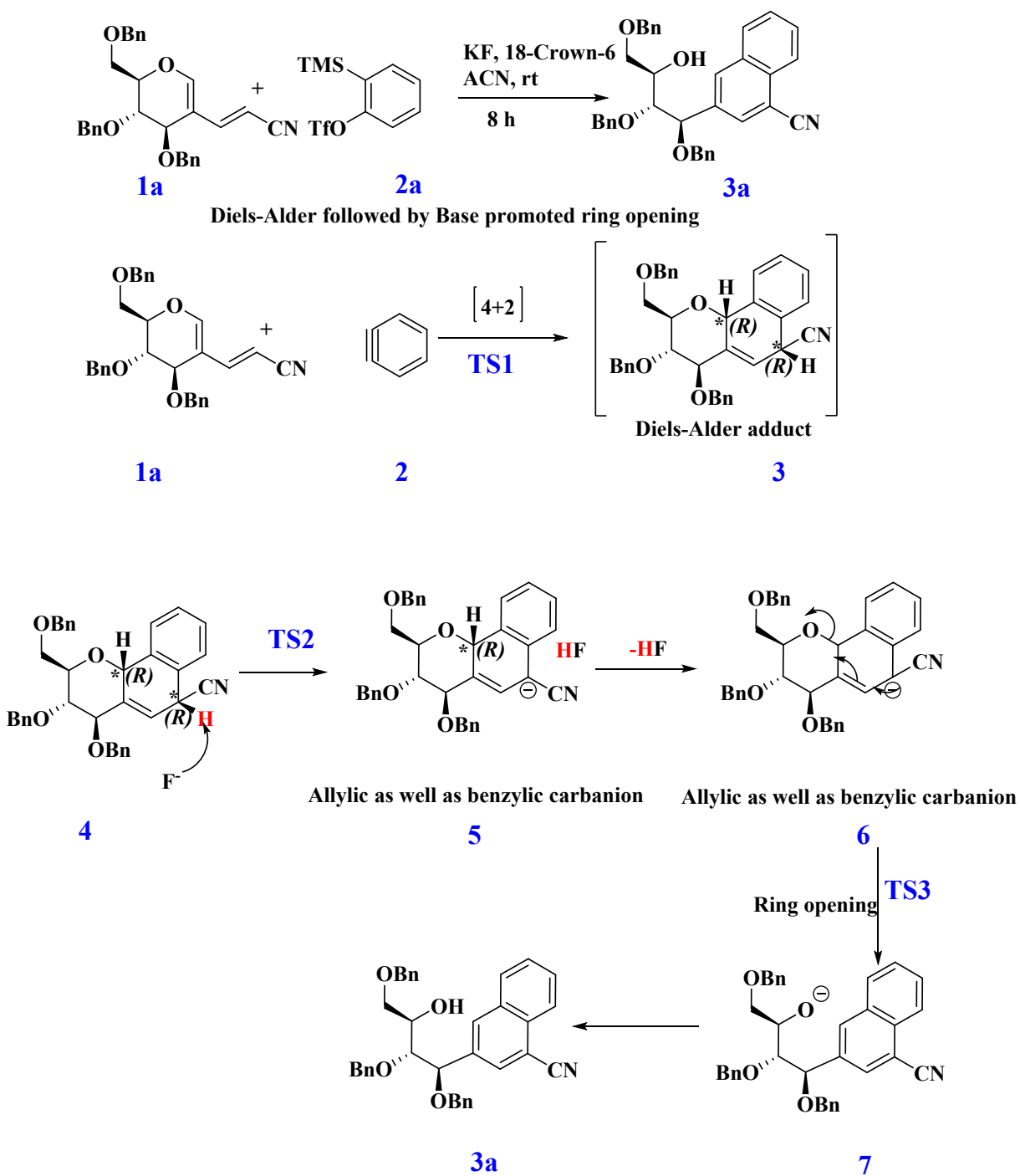
DA-adduct from aryl diene

A, B, and C denote rings, which are considered for aromaticity (NICS (0)) calculations.

Scheme S2: Schematic mechanism of annulative π -extension reactions



Scheme S3: Base promoted tandem Diels-Alder and ring opening reaction of **1a**.



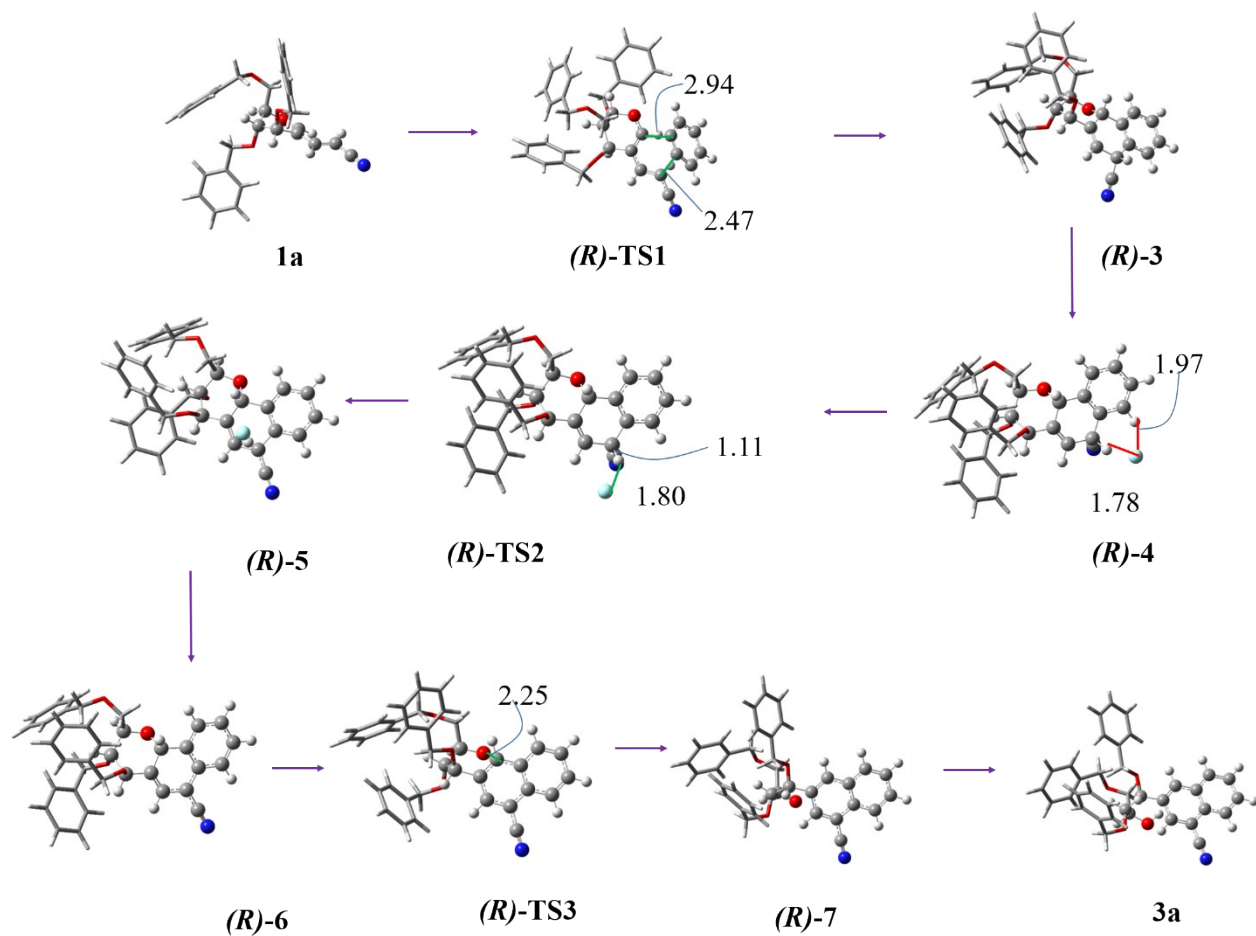


Figure S1: *R*-stereoisomeric pathway: The $\text{SMD}_{\text{ACN}}\text{-M062X/6-31G(d)}$ computed Diels-Alder and base catalyzed ring opening reaction of **1a**. Distances are given in Å.

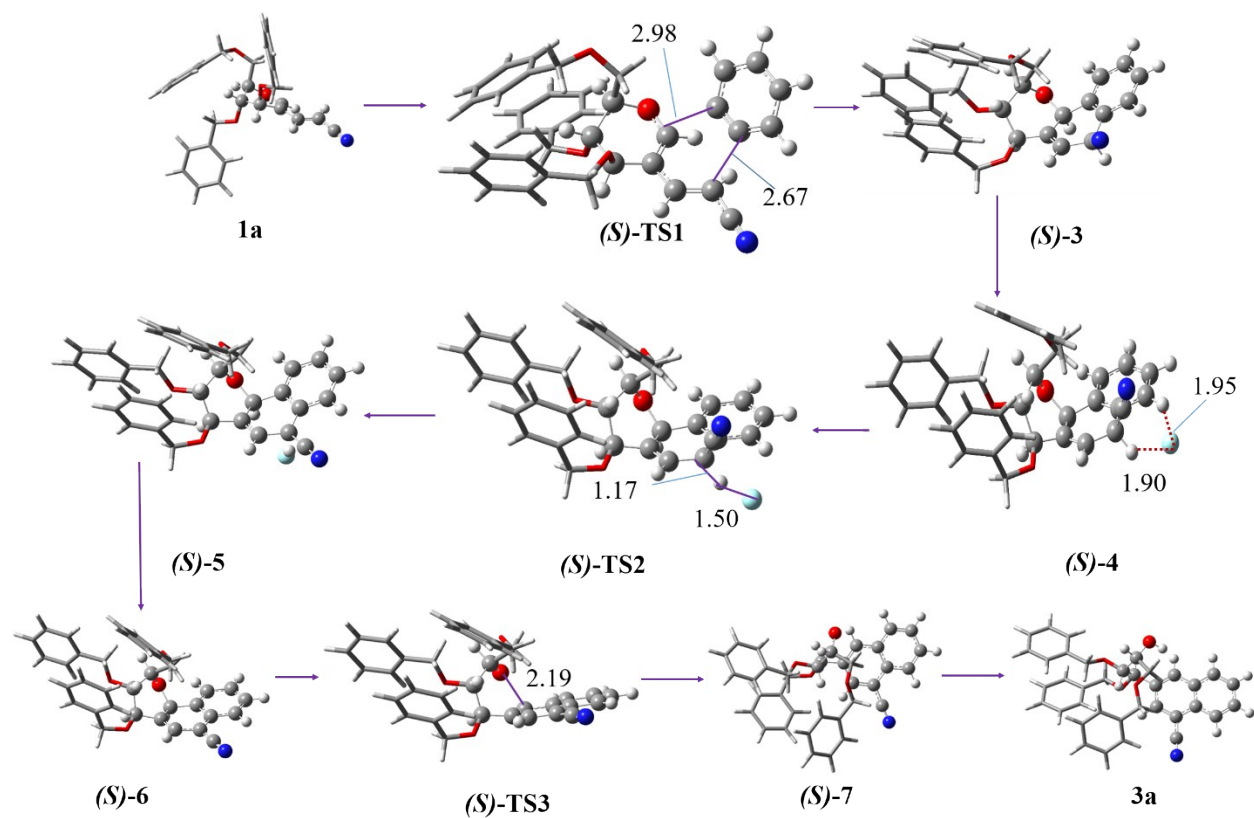


Figure S2: *S*-stereoisomeric pathway: The SMD_{ACN}-M062X/6-31G(d) computed Diels-Alder and base catalyzed ring opening reaction of **1a**. Distances are given in Å.

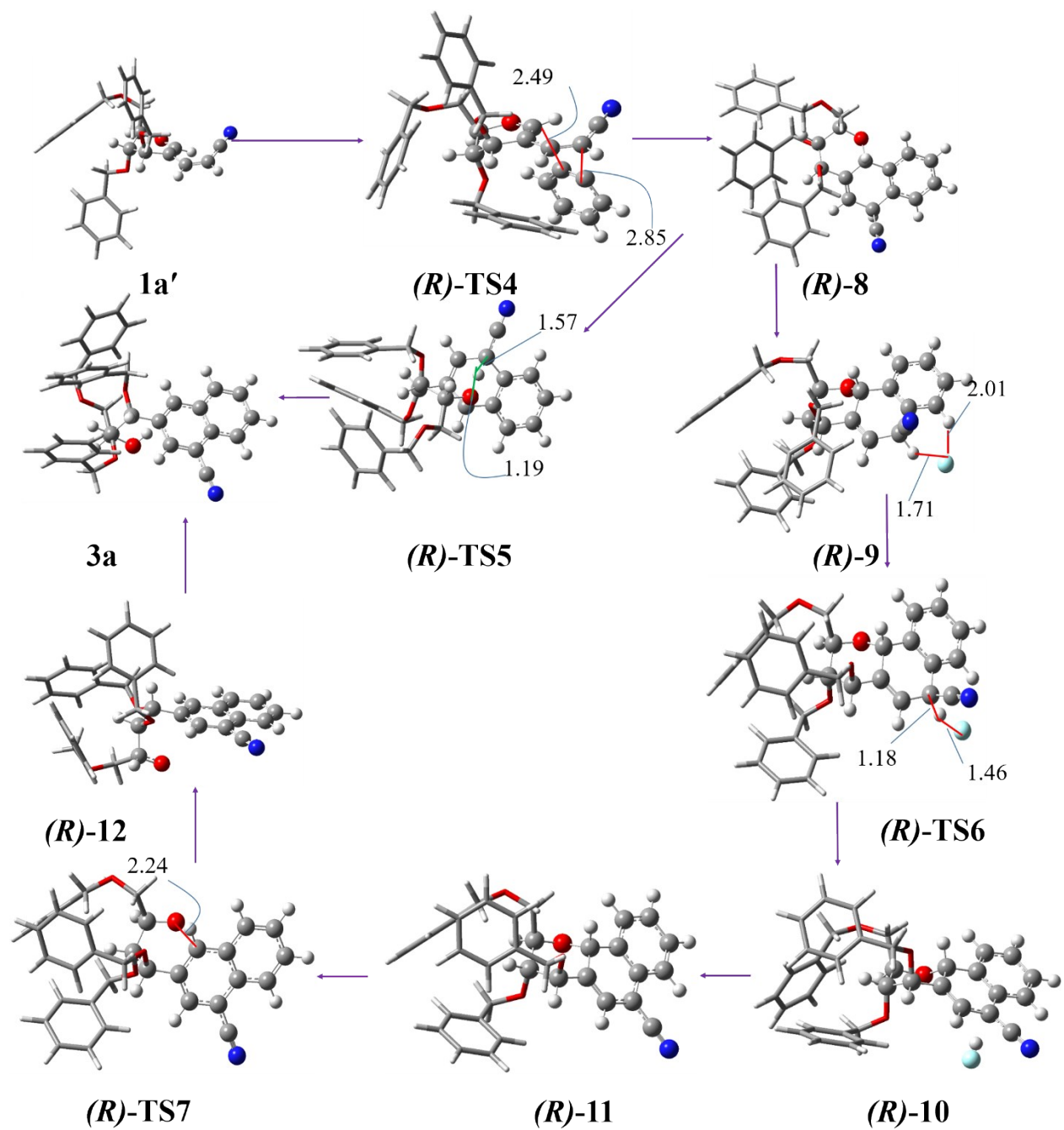


Figure S3: *R*-stereoisomeric pathway:The SMD_{ACN}-M062X/6-31G(d) computed Diels-Alder and base catalyzed ring opening reaction of **1a'**. Distances are given in Å.

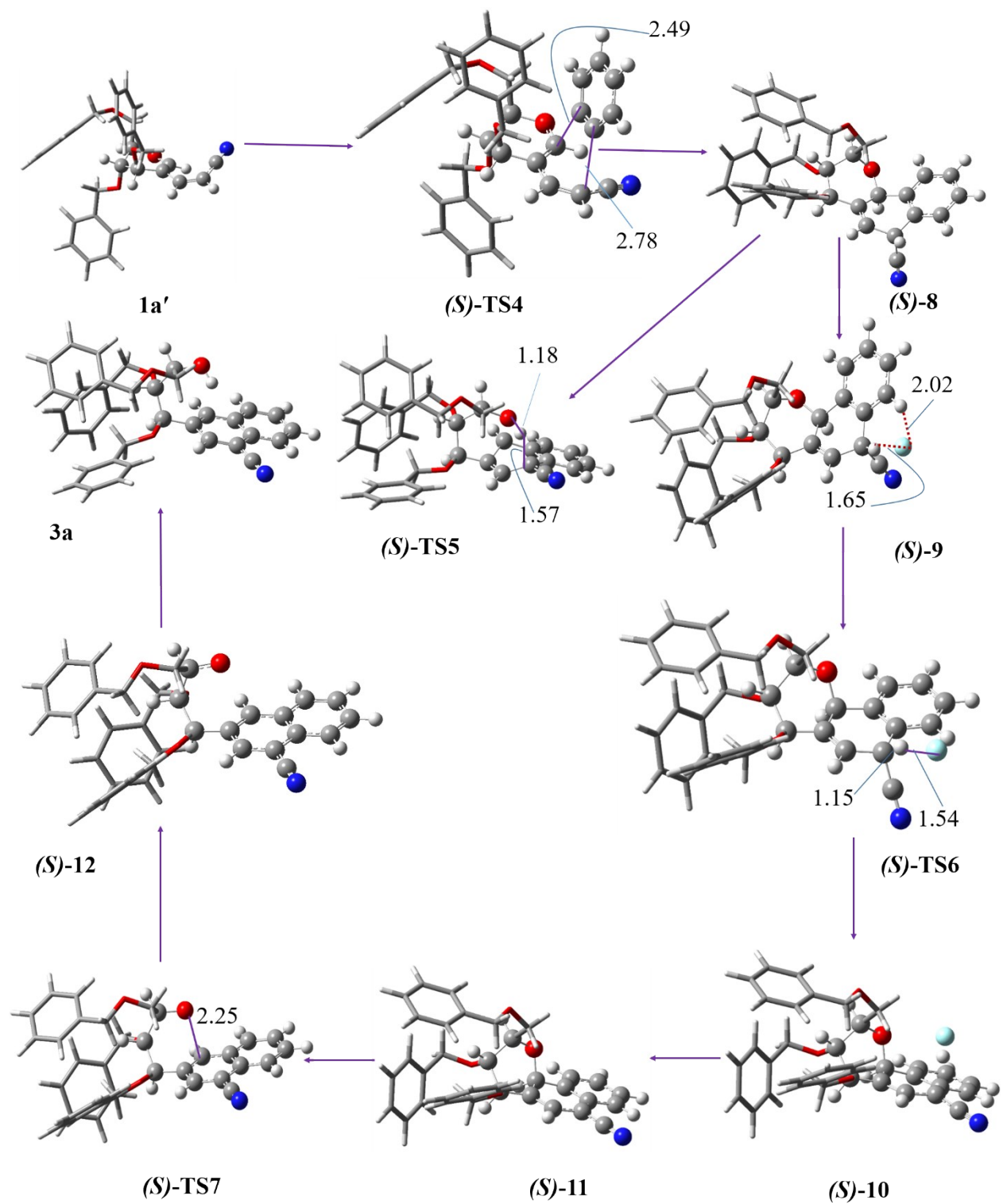
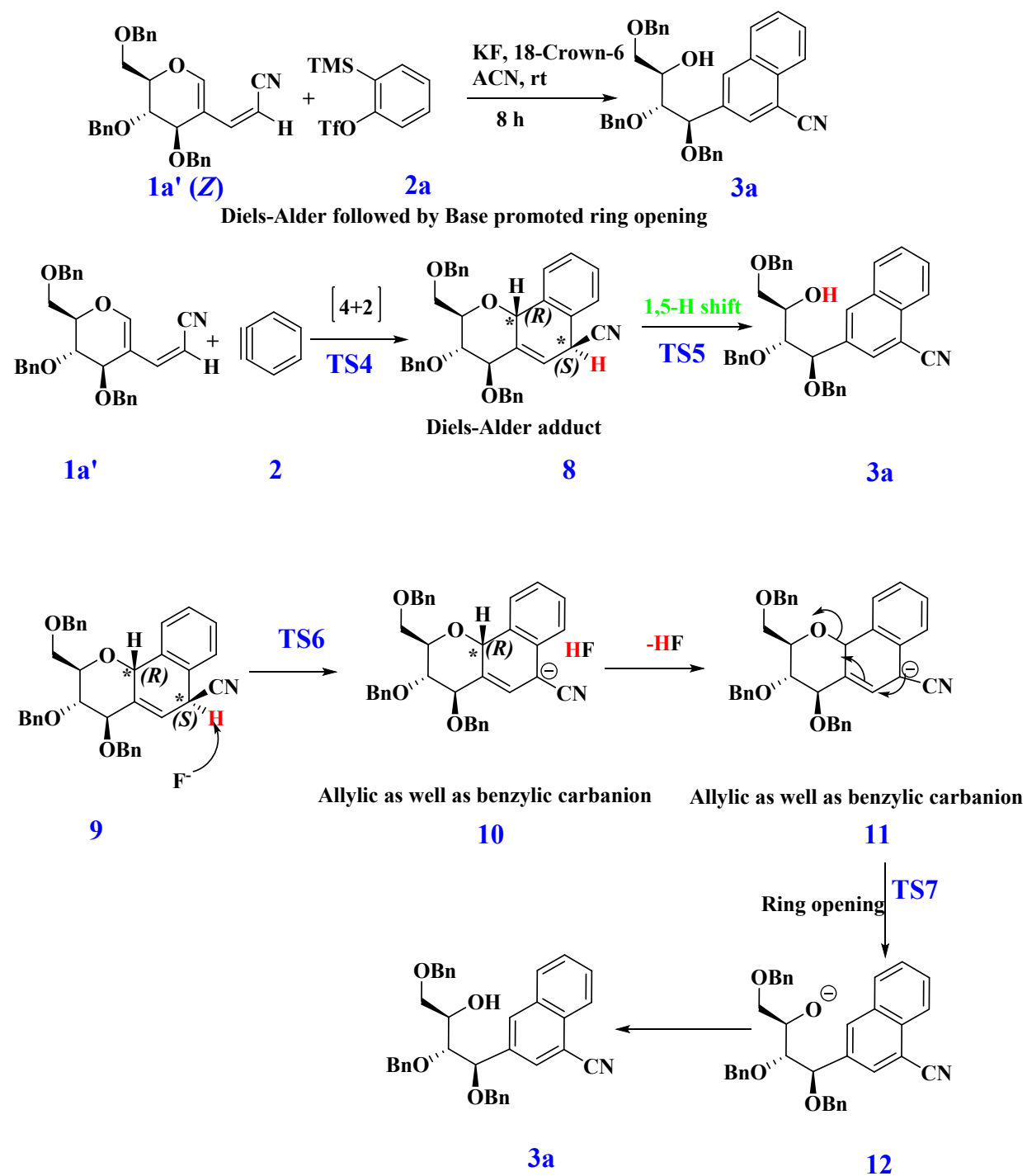
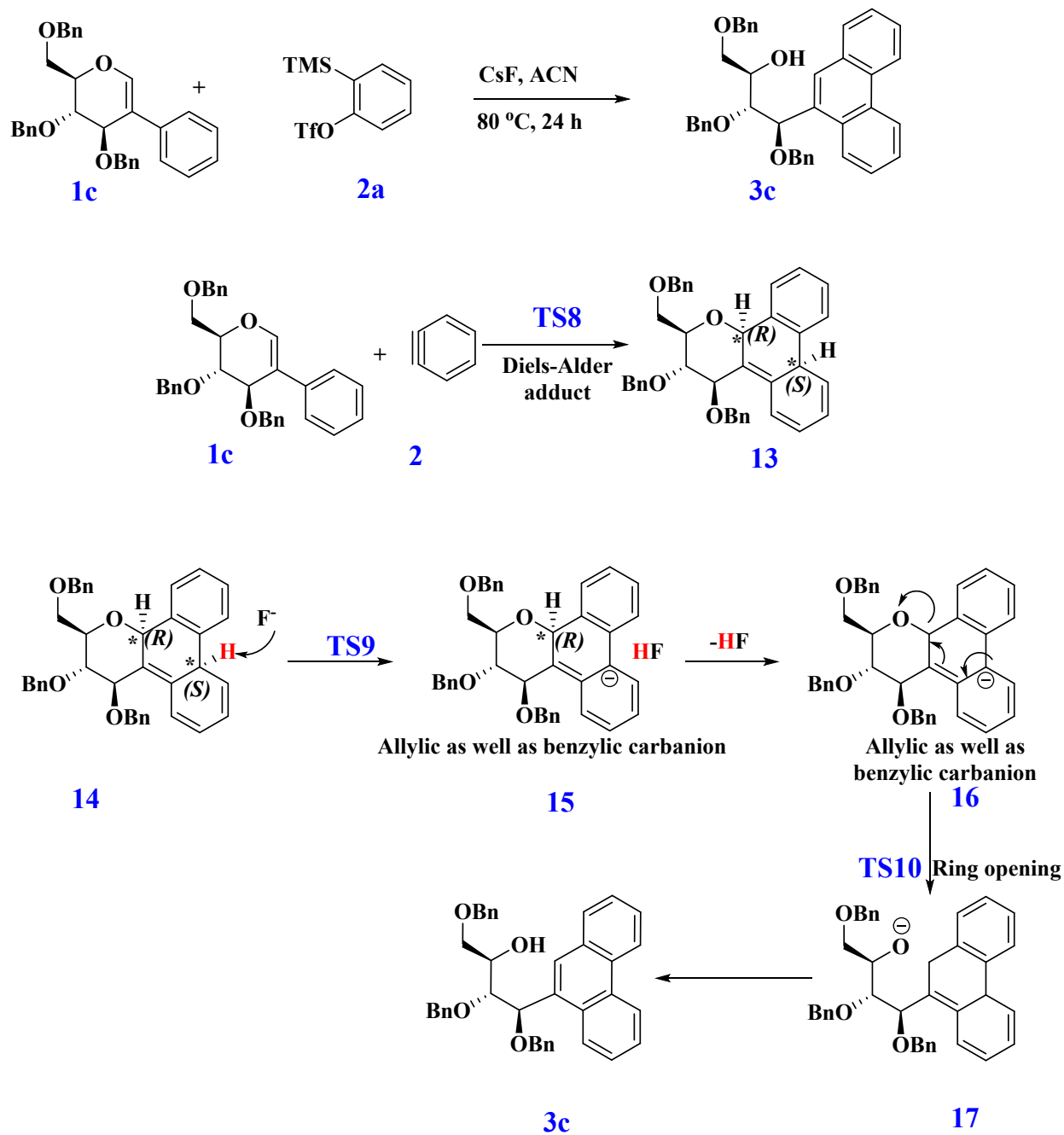


Figure S4: *S*-stereoisomeric pathway: The SMD_{ACN}-M062X/6-31G(d) computed Diels-Alder and base catalyzed ring opening reaction of **1a'**. Distances are given in Å.

Scheme S4: Base promoted tandem Diels-Alder and ring opening reaction **1a'**.



Scheme S5: Synthesis of phenanthrene derivatives using 2-aryl -D-Glucal (**1b**)



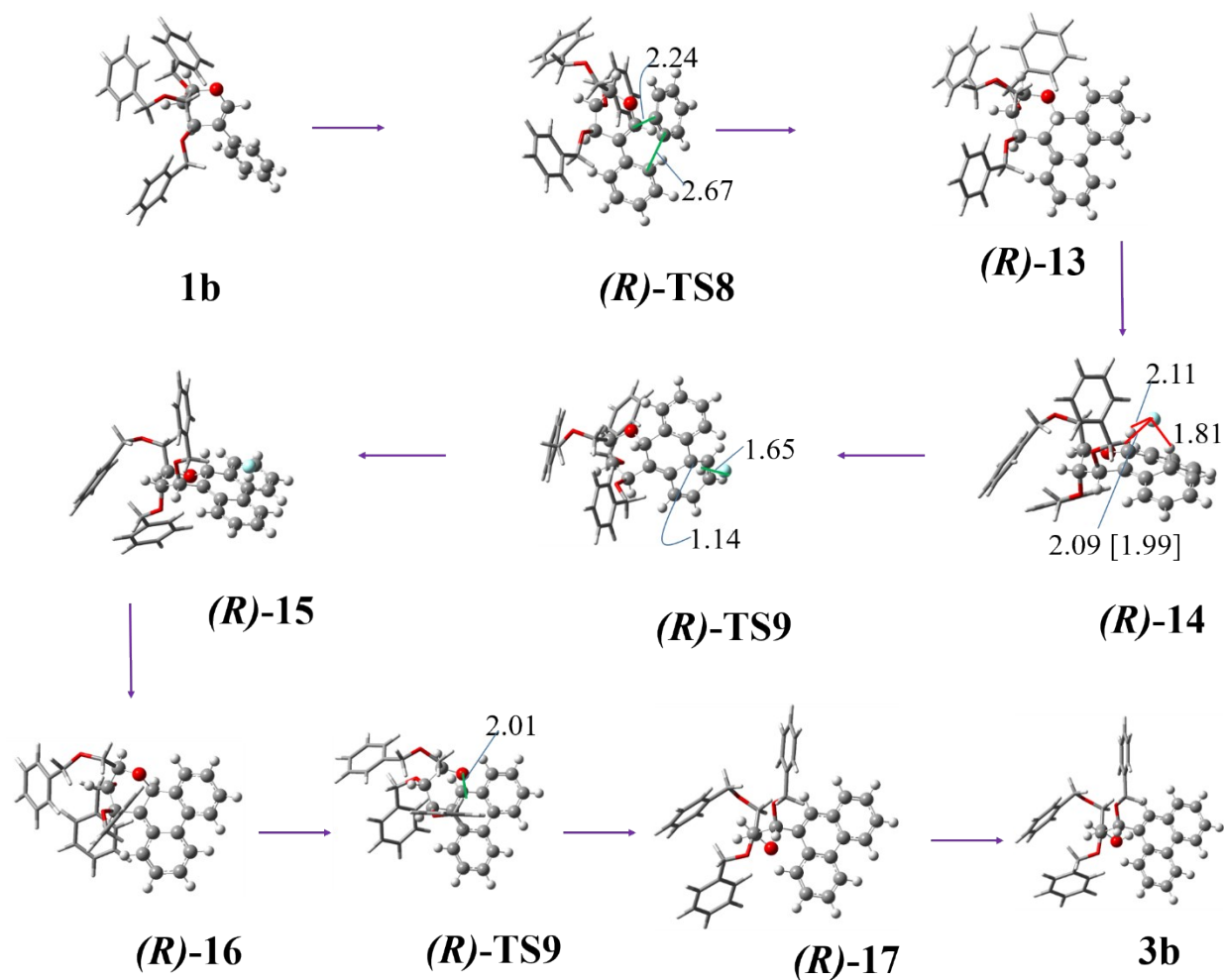


Figure S5: *R*-stereoisomeric pathway: The SMD_{ACN}-M062X/6-31G(d) computed Diels-Alder and base catalyzed ring opening reaction of **1b**. Distances are given in Å.

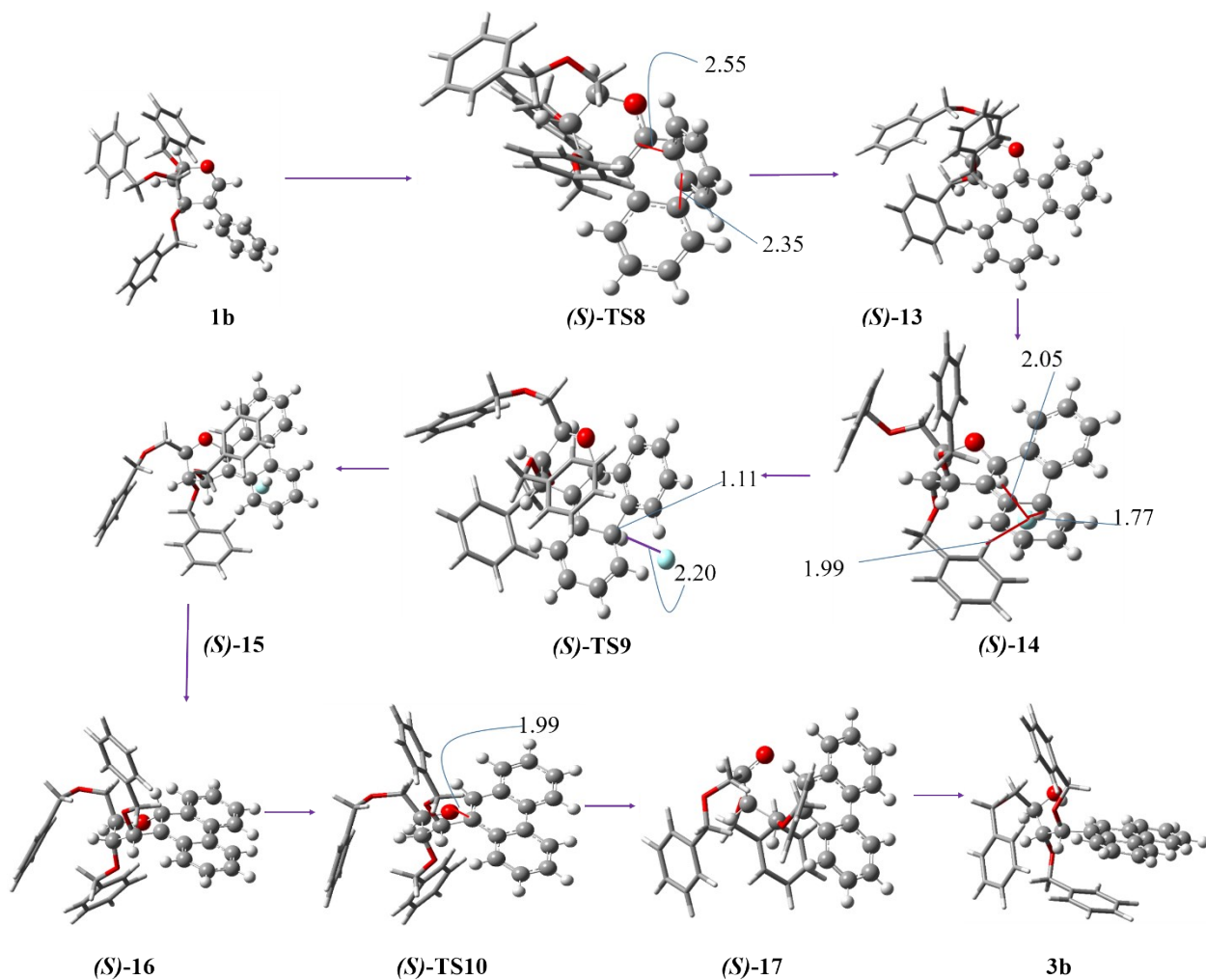


Figure S6: *S*-stereoisomeric pathway: The $\text{SMD}_{\text{ACN}}\text{-M062X/6-31G(d)}$ computed Diels-Alder and base catalyzed ring opening reaction of **1b**. Distances are given in Å.

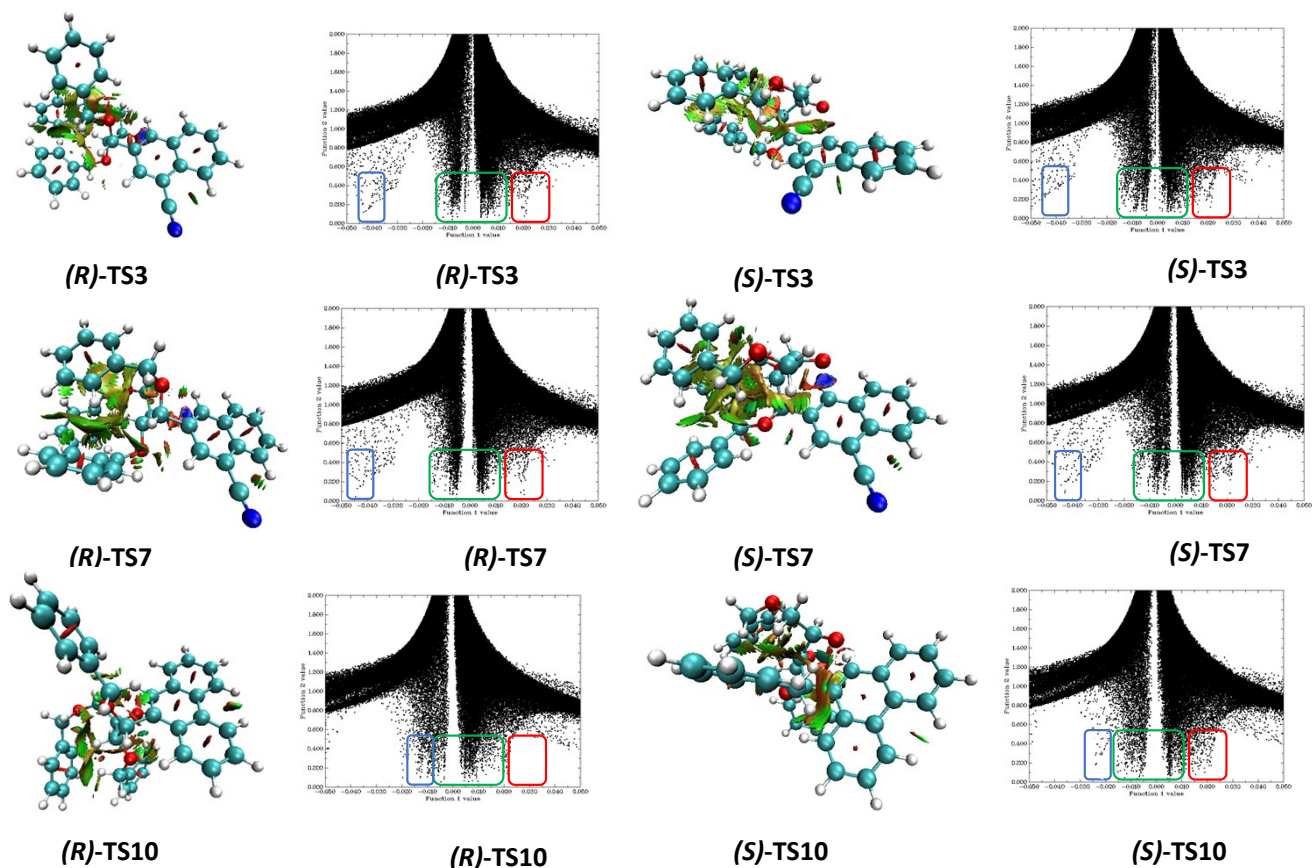


Figure S7: Noncovalent interactions reduced density gradient isosurface plots for all the transition state structures were calculated. Red color indicates steric repulsion, whereas green, and light-green represent the noncovalent interactions and the blue color corresponds to hydrogen bonding interaction. All the scatter plots are given for the NCI plot.

Table S2: π stacking interactions between the benzene ring centers.

| TS | Distance between the benzene ring centers (Å) |
|-------|---|
| S-TS2 | 4.7 (off center parallel stacking) 2.5(Edge to face π stacking) 2.5(CH- π stacking) |
| R-TS2 | 5.6(Not proper orientation), 2.5(CH- π stacking), 2.46(CH- π stacking) |
| S-TS3 | 4.7 (off center parallel stacking) 2.8(CH- π stacking) |
| R-TS3 | 5.6(Not proper orientation), 2.5(Edge to face stacking) |

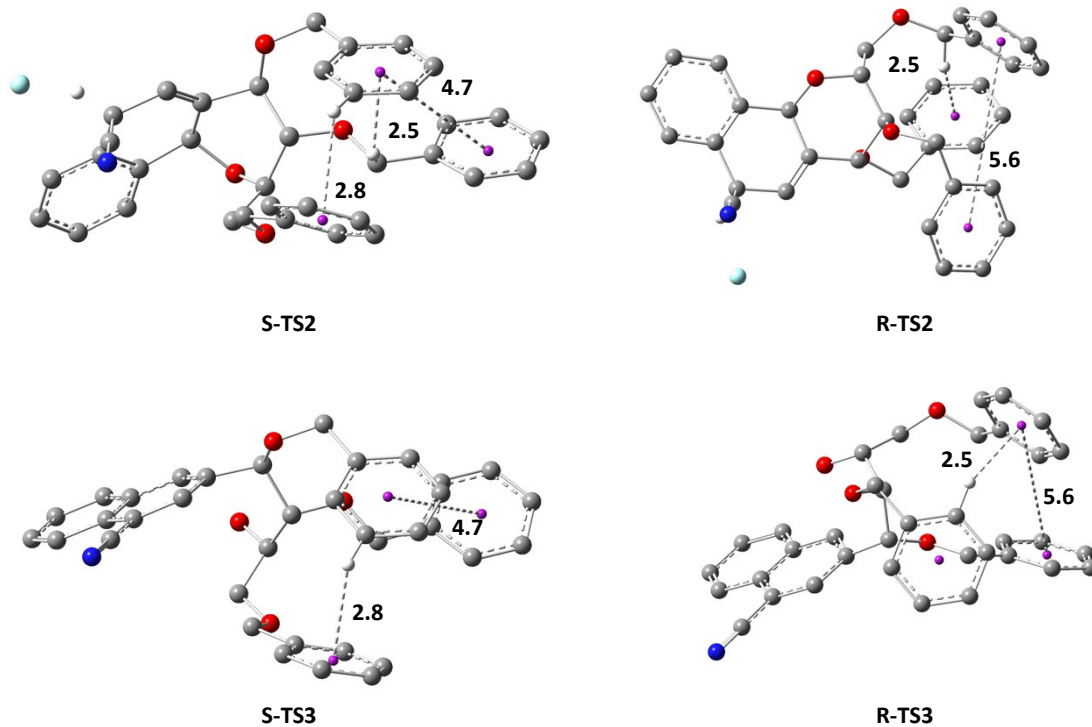


Figure S8: Distance between the benzene ring centers in benzyl groups (Å) for structures refer in Table S2.

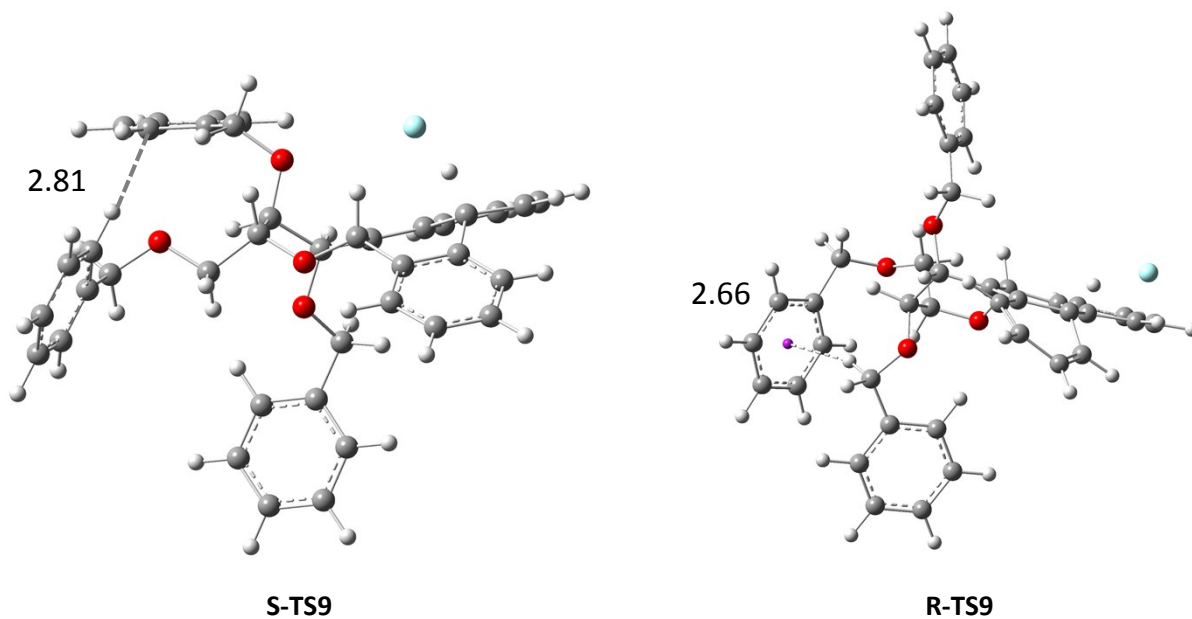


Figure S9: The transition state geometries for the proton abstraction step in **1b**. The CH- π interaction distances are shown in (Å).

Table S3: NICS values and barrier height for the transition states.

| TS | Barrier height | | A ring | | B ring | | C ring | |
|------|----------------|------|--------|-------|--------|-------|--------|-------|
| | R | S | R | S | R | S | R | S |
| TS3 | 12.1 | 18.3 | -8.52 | -8.65 | -7.77 | -7.36 | | |
| TS7 | 22.6 | 19.4 | -8.40 | -8.42 | -7.63 | -7.70 | | |
| TS10 | 10.9 | 11.6 | -8.90 | -8.71 | -3.78 | -3.95 | -7.29 | -7.39 |

Table S4: The calculated rate constant of the DA reactions at 298 K temperature.

| TS | ΔG^\ddagger | k (s ⁻¹) |
|-------|---------------------|------------------------|
| S-TS1 | 7.9 | 1.04x10 ⁻⁰² |
| R-TS4 | 8.5 | 3.56x10 ⁻⁰³ |
| R-TS8 | 13.8 | 4.94x10 ⁻⁰⁷ |

$$k = \frac{k_B T}{h} \exp\left(-\frac{\Delta G^\ddagger}{RT}\right) \dots\dots 1$$

Table S5: Cartesian Coordinate of the systems examined using SMD_{ACN}-M062X/6-31G(d) level of theory, the absolute Gibbs free energy values (G) of the ground state and transition state geometries in Hartree and the number of imaginary frequencies.

| 1a G(M062X/6-31G(d)): -1515.15737 Number of Imaginary frequency: 0 | | | | 1a' G(M062X/6-31G(d)): -1515.15648 Number of Imaginary frequency: 0 | | | |
|---|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -0.48035600 | 0.16642500 | 0.36173500 | C | -0.48442600 | 0.30503700 | 0.23905400 |
| C | 0.70831800 | 0.97005400 | -0.16337200 | C | 0.59520700 | 1.06924000 | -0.52622600 |
| C | 0.95064500 | 2.17498200 | 0.71364500 | C | 0.78007700 | 2.44933300 | 0.06007200 |
| C | 0.36161200 | 2.24425900 | 1.92757500 | C | 0.24112500 | 2.73663500 | 1.26546400 |
| C | -0.43315500 | -0.00077600 | 1.88350500 | C | -0.34822600 | 0.48166900 | 1.75399600 |
| H | 0.46119800 | 1.31161900 | -1.18042300 | H | 0.26136500 | 1.16886100 | -1.57084900 |
| H | -0.46776600 | -0.81516500 | -0.12435400 | H | -0.39791500 | -0.75435400 | -0.02493500 |
| H | -1.37808900 | -0.42928800 | 2.22987700 | H | -1.22855500 | 0.06140400 | 2.25009200 |
| H | 0.39032000 | 3.14288500 | 2.53883400 | H | 0.21131000 | 3.74495700 | 1.66947800 |
| O | -0.37143300 | 1.29272900 | 2.51158800 | O | -0.38302800 | 1.88233800 | 2.08120500 |
| C | 0.70401700 | -0.85571500 | 2.46795000 | C | 0.89460100 | -0.12280800 | 2.42778400 |
| H | 1.66052700 | -0.62209800 | 1.98737100 | H | 1.80213500 | 0.10145800 | 1.85614000 |
| H | 0.77398300 | -0.59552900 | 3.52788100 | H | 0.97683100 | 0.35087900 | 3.41021200 |
| O | 1.80136100 | 0.06355600 | -0.23493400 | O | 1.75630800 | 0.25133900 | -0.48753900 |
| O | -1.64685300 | 0.87639700 | -0.00535300 | O | -1.73238900 | 0.81290600 | -0.19029200 |
| O | 0.44386700 | -2.24307800 | 2.43537800 | O | 0.77981600 | -1.50701800 | 2.68033100 |
| C | -2.78901200 | 0.05126600 | -0.12230900 | C | -2.78394700 | -0.12331500 | -0.06676700 |

| | | | | | | | |
|---|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | -2.57909700 | -0.78237600 | -0.81185200 | H | -2.51136600 | -1.06051400 | -0.57884300 |
| H | -3.05030400 | -0.39576100 | 0.84865100 | H | -2.96169100 | -0.37669900 | 0.98908200 |
| C | 2.93857000 | 0.57785100 | -0.90154300 | C | 2.79922800 | 0.66331200 | -1.35568600 |
| H | 2.65219300 | 0.97782000 | -1.88575000 | H | 2.40697500 | 0.81848000 | -2.37114000 |
| H | 3.37459500 | 1.40706700 | -0.32446700 | H | 3.22385900 | 1.61684300 | -1.00967000 |
| C | 0.54562700 | -2.87513400 | 1.17203300 | C | 0.96479200 | -2.36851600 | 1.57119200 |
| H | 1.14845300 | -2.27220100 | 0.47891600 | H | 1.48779200 | -1.85008800 | 0.75621200 |
| H | 1.08388800 | -3.81803600 | 1.33283300 | H | 1.61619100 | -3.18531600 | 1.90820500 |
| C | 3.96157900 | -0.51808900 | -1.06209000 | C | 3.86034600 | -0.40652800 | -1.35821400 |
| C | 4.80112400 | -0.52183700 | -2.17769200 | C | 4.38831600 | -0.88770400 | -2.55615700 |
| C | 4.11692600 | -1.50982000 | -0.08954500 | C | 4.33429400 | -0.92274900 | -0.14737200 |
| C | 5.78517400 | -1.49766800 | -2.32129300 | C | 5.38265900 | -1.86582500 | -2.54854900 |
| H | 4.67975900 | 0.24329600 | -2.94075200 | H | 4.01733500 | -0.49691100 | -3.50040600 |
| C | 5.09487100 | -2.49177200 | -0.23714300 | C | 5.32061200 | -1.90451500 | -0.13800900 |
| H | 3.46906700 | -1.51491500 | 0.78306000 | H | 3.92394900 | -0.55253300 | 0.78922100 |
| C | 5.93324200 | -2.48739500 | -1.35121900 | C | 5.84911600 | -2.37739900 | -1.34011800 |
| H | 6.42962200 | -1.48947100 | -3.19545000 | H | 5.78517500 | -2.23337700 | -3.48795200 |
| H | 5.20453100 | -3.26060400 | 0.52233700 | H | 5.68106400 | -2.29969100 | 0.80733900 |
| H | 6.69530800 | -3.25274400 | -1.46407100 | H | 6.61993500 | -3.14278900 | -1.33248700 |
| C | -3.95654600 | 0.85735700 | -0.63371000 | C | -4.04975300 | 0.43558800 | -0.66704200 |
| C | -3.86684900 | 2.23026500 | -0.85847100 | C | -4.10562100 | 1.70986600 | -1.22909400 |
| C | -5.16508500 | 0.20045600 | -0.88600800 | C | -5.20072100 | -0.35940700 | -0.65704400 |
| C | -4.97346800 | 2.93763000 | -1.33067900 | C | -5.30036700 | 2.18481200 | -1.77282200 |
| H | -2.93004900 | 2.74199400 | -0.66449200 | H | -3.21399200 | 2.32770100 | -1.23788900 |
| C | -6.26789000 | 0.90557700 | -1.35600200 | C | -6.39080500 | 0.11373400 | -1.19936200 |
| H | -5.23587000 | -0.87204700 | -0.71334900 | H | -5.15686900 | -1.35618100 | -0.22172800 |
| C | -6.17475900 | 2.28015000 | -1.58053400 | C | -6.44402300 | 1.39092000 | -1.76003400 |
| H | -4.89283700 | 4.00712200 | -1.50377400 | H | -5.33454700 | 3.17998300 | -2.20725600 |
| H | -7.20065300 | 0.38357700 | -1.54939200 | H | -7.27786200 | -0.51286900 | -1.18628700 |
| H | -7.03471900 | 2.83239600 | -1.94811500 | H | -7.37264000 | 1.76302800 | -2.18266900 |
| C | -0.80993600 | -3.17461400 | 0.56246200 | C | -0.34205700 | -2.94948400 | 1.06809700 |
| C | -0.90633900 | -3.46783800 | -0.80198400 | C | -0.40372800 | -3.51708900 | -0.20871500 |
| C | -1.96757300 | -3.18031600 | 1.34174400 | C | -1.48910600 | -2.93705100 | 1.86266500 |
| C | -2.13979600 | -3.75874000 | -1.37842500 | C | -1.59429600 | -4.06060500 | -0.68436500 |
| H | -0.00761400 | -3.45785300 | -1.41540900 | H | 0.48574900 | -3.52066300 | -0.83557100 |
| C | -3.20511800 | -3.46888200 | 0.76497200 | C | -2.68322900 | -3.48073400 | 1.38722500 |
| H | -1.89526200 | -2.95158800 | 2.40075200 | H | -1.44214500 | -2.49291300 | 2.85239200 |
| C | -3.29601300 | -3.75664600 | -0.59520100 | C | -2.74035600 | -4.04194600 | 0.11331300 |
| H | -2.20119200 | -3.98035000 | -2.44007600 | H | -1.63151400 | -4.49269200 | -1.68032900 |
| H | -4.10006200 | -3.46652000 | 1.38107400 | H | -3.57081300 | -3.46312300 | 2.01370000 |
| H | -4.25989700 | -3.97793700 | -1.04454200 | H | -3.67069100 | -4.46113400 | -0.25879000 |
| C | 1.68607900 | 3.31068300 | 0.18099700 | C | 1.38821900 | 3.48290900 | -0.76366400 |
| C | 2.32940000 | 4.25092300 | 0.90441300 | C | 2.07496500 | 4.58078600 | -0.38284800 |
| C | 2.97254700 | 5.35126000 | 0.26273900 | C | 2.39464400 | 4.88378200 | 0.97602400 |
| N | 3.50464000 | 6.24643100 | -0.24843100 | N | 2.67525100 | 5.14455500 | 2.07110500 |
| H | 1.71543900 | 3.38579500 | -0.90665900 | H | 1.28697900 | 3.33411800 | -1.83910600 |
| H | 2.39950300 | 4.21570300 | 1.98760600 | H | 2.44630300 | 5.28403800 | -1.12033800 |
| 1b G(M062X/6-31G(d)): -1576.48624 Number of Imaginary frequency: 0 | | | | 2a G(M062X/6-31G(d)): -230.76494 Number of Imaginary frequency: 0 | | | |
| C | -0.61104500 | 0.04005400 | 0.47234900 | C | -1.46520200 | -0.13226100 | -0.00035400 |
| C | 0.64559500 | 0.74796200 | -0.03506000 | C | -0.70340200 | 1.05190900 | -0.00007400 |
| C | 0.99335200 | 1.91076200 | 0.86292800 | C | 0.70332900 | 1.05195000 | -0.00007900 |
| C | 0.43200600 | 1.98733900 | 2.08172200 | C | 1.46519800 | -0.13217200 | -0.00036400 |
| C | -0.59051600 | -0.16323800 | 1.98967000 | C | 0.62280700 | -1.23180800 | 0.00042500 |
| H | 0.42753100 | 1.10528400 | -1.05145200 | C | -0.62270700 | -1.23180100 | 0.00042900 |
| H | -0.67780200 | -0.92803700 | -0.03504900 | H | -2.54937500 | -0.13212000 | -0.00010400 |
| H | -1.57547100 | -0.51135400 | 2.31805900 | H | -1.22698300 | 2.00454800 | 0.00017000 |
| H | 0.57802200 | 2.84398600 | 2.73504400 | H | 1.22684900 | 2.00462300 | 0.00016100 |
| O | -0.40463400 | 1.09545800 | 2.65055300 | H | 2.54937200 | -0.13194900 | -0.00012100 |
| C | 0.45301700 | -1.14222300 | 2.55308800 | | | | |
| H | 1.43819800 | -0.96719900 | 2.10659700 | | | | |
| H | 0.51617800 | -0.94024200 | 3.62604700 | | | | |
| O | 1.65103200 | -0.25670700 | -0.11132600 | | | | |
| O | -1.71346100 | 0.85014800 | 0.11099200 | | | | |
| O | 0.07658600 | -2.49947800 | 2.44399300 | | | | |
| C | -2.90897200 | 0.11702200 | -0.05616500 | | | | |
| H | -2.75146900 | -0.69636100 | -0.78336200 | | | | |
| H | -3.21405500 | -0.35677400 | 0.88912300 | | | | |

| | | | |
|--|-------------|-------------|-------------|
| C | 2.84977600 | 0.14021900 | -0.75404500 |
| H | 2.62589500 | 0.62934500 | -1.71357600 |
| H | 3.39167800 | 0.86608500 | -0.13115600 |
| C | 0.22224900 | -3.09541700 | 1.16762500 |
| H | 0.89440300 | -2.50269800 | 0.53294100 |
| H | 0.69950800 | -4.07169000 | 1.32338000 |
| C | 3.69764800 | -1.08684500 | -0.97472300 |
| C | 4.36812400 | -1.28010900 | -2.18278900 |
| C | 3.83942200 | -2.03651800 | 0.04258200 |
| C | 5.17313600 | -2.40278400 | -2.37441600 |
| H | 4.25607800 | -0.54899800 | -2.97970500 |
| C | 4.63523700 | -3.16254800 | -0.15025700 |
| H | 3.31899500 | -1.89172300 | 0.98616100 |
| C | 5.30612200 | -3.34778800 | -1.35965500 |
| H | 5.68865900 | -2.54204200 | -3.32015500 |
| H | 4.73440300 | -3.89615600 | 0.64464600 |
| H | 5.92690000 | -4.22606200 | -1.50983300 |
| C | -4.01063100 | 1.02852800 | -0.53652300 |
| C | -3.81947500 | 2.40057700 | -0.69364500 |
| C | -5.26158800 | 0.47443900 | -0.82670600 |
| C | -4.86802400 | 3.20908000 | -1.13571300 |
| H | -2.84971000 | 2.83213400 | -0.46960200 |
| C | -6.30638100 | 1.28024300 | -1.26702500 |
| H | -5.41143200 | -0.59693800 | -0.70681000 |
| C | -6.11190800 | 2.65385500 | -1.42311900 |
| H | -4.70852500 | 4.27695100 | -1.25489400 |
| H | -7.27274500 | 0.83756600 | -1.49024000 |
| H | -6.92616400 | 3.28446300 | -1.76748600 |
| C | -1.10813100 | -3.29725100 | 0.46908900 |
| C | -1.13863100 | -3.51689200 | -0.91214600 |
| C | -2.30829000 | -3.27855500 | 1.18057900 |
| C | -2.34932700 | -3.71303600 | -1.57139400 |
| H | -0.20632700 | -3.52206300 | -1.47326400 |
| C | -3.52284100 | -3.47313300 | 0.52095900 |
| H | -2.28642400 | -3.10276700 | 2.25174600 |
| C | -3.54774500 | -3.68916000 | -0.85547600 |
| H | -2.35948000 | -3.87723900 | -2.64503800 |
| H | -4.45130800 | -3.45301300 | 1.08492500 |
| H | -4.49320800 | -3.83734700 | -1.36901000 |
| C | 1.87862200 | 3.00678500 | 0.40059900 |
| C | 1.82583500 | 3.47846400 | -0.92022700 |
| C | 2.79400300 | 3.60652800 | 1.27982000 |
| C | 2.65019600 | 4.51886600 | -1.34067400 |
| H | 1.12333300 | 3.04240100 | -1.62470400 |
| C | 3.60942800 | 4.65459700 | 0.86168500 |
| H | 2.87845600 | 3.23086700 | 2.29594100 |
| C | 3.54397300 | 5.11492400 | -0.45221300 |
| H | 2.58803400 | 4.86909100 | -2.36698600 |
| H | 4.30941100 | 5.10139200 | 1.56191000 |
| H | 4.18683300 | 5.92528400 | -0.78222000 |
| R-TS1 | | | |
| G(M062X/6-31G(d)): -1745.90661 | | | |
| Number of Imaginary frequency: -118.22 | | | |
| 0 1 | | | |
| C | -0.47124000 | -0.24922000 | 0.20020200 |
| C | 0.37604400 | -1.52629500 | 0.18049300 |
| C | 1.70079200 | -1.30718400 | 0.86830800 |
| C | 1.94317300 | -0.14871500 | 1.54654800 |
| C | -0.33736700 | 0.50045800 | 1.52914500 |
| H | 0.57623000 | -1.75180700 | -0.87503900 |
| H | -1.52159000 | -0.52710600 | 0.04855700 |
| H | -0.82151500 | 1.47985100 | 1.46354900 |
| H | 2.90398400 | 0.08773600 | 1.99213800 |
| O | 1.04666100 | 0.80304600 | 1.79140900 |
| C | -0.89266500 | -0.23373200 | 2.76778000 |
| H | -0.75987100 | -1.31875900 | 2.67725800 |
| H | -0.31387100 | 0.11663900 | 3.62699300 |
| O | -0.30990000 | -2.62049800 | 0.77380900 |
| O | -0.01133000 | 0.52972200 | -0.88788900 |
| S-TS1 | | | |
| G(M062X/6-31G(d)): -1745.90976 | | | |
| Number of Imaginary frequency: -35.16 | | | |
| 0 1 | | | |
| C | 0.48485300 | -0.29563800 | -0.47808600 |
| C | -0.86595100 | 0.20032000 | -1.01213100 |
| C | -1.93614200 | -0.85424700 | -0.88378400 |
| C | -1.68363800 | -2.01353700 | -0.22457500 |
| C | 0.31152700 | -1.20102300 | 0.74420500 |
| H | -0.72544100 | 0.40905800 | -2.08072800 |
| H | 1.08060700 | 0.58082400 | -0.19905400 |
| H | 1.26732900 | -1.66440700 | 1.00848400 |
| H | -2.37250800 | -2.85335000 | -0.21537400 |
| O | -0.54640800 | -2.30885400 | 0.41063600 |
| C | -0.26885000 | -0.52288300 | 2.00298300 |
| H | -1.00311100 | 0.24875800 | 1.73828300 |
| H | -0.77839300 | -1.30662000 | 2.57167100 |
| O | -1.27685600 | 1.38946400 | -0.34935100 |
| O | 1.10896500 | -0.99001900 | -1.54227600 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| O | -2.23596000 | 0.07659100 | 3.06442700 | O | 0.71033700 | 0.00290200 | 2.87227100 |
| C | -0.81987900 | 1.64939400 | -1.21043300 | C | 2.52037000 | -1.09529700 | -1.44750300 |
| H | -0.90997600 | 1.66591300 | -2.30379500 | H | 2.93453300 | -0.76573900 | -2.40914000 |
| H | -1.83415600 | 1.52474100 | -0.80484300 | H | 2.90577100 | -0.40841800 | -0.68090300 |
| C | -0.76758400 | -3.61415700 | -0.13941200 | C | -1.16686600 | 2.58197500 | -1.12111400 |
| H | 0.02671700 | -3.82924700 | -0.86656900 | H | -1.56972000 | 2.39833000 | -2.12674700 |
| H | -0.92581200 | -4.51007700 | 0.46722800 | H | -1.81776900 | 3.30588700 | -0.62343800 |
| C | -3.20157000 | -0.49511100 | 2.20207000 | C | 1.33616400 | 1.19723300 | 2.44530800 |
| H | -2.81968900 | -1.42083000 | 1.74551600 | H | 0.68394800 | 1.75829300 | 1.75898400 |
| H | -4.05456900 | -0.77321800 | 2.83323500 | H | 1.47032500 | 1.81573700 | 3.34141000 |
| C | -2.05017600 | -3.27288300 | -0.87021700 | C | 0.22952800 | 3.16146200 | -1.23134000 |
| C | -2.04732600 | -2.46206600 | -2.01242400 | C | 1.19161100 | 2.60106500 | -2.08244800 |
| C | -3.26295800 | -3.81469300 | -0.43407800 | C | 0.55649800 | 4.31986200 | -0.52134400 |
| C | -3.22899700 | -2.20952800 | -2.70633100 | C | 2.44582900 | 3.19000800 | -2.22167300 |
| H | -1.11159500 | -2.04127400 | -2.37541000 | H | 0.95614300 | 1.70660300 | -2.65578300 |
| C | -4.44575900 | -3.57460600 | -1.13278700 | C | 1.80658000 | 4.92200700 | -0.67016400 |
| H | -3.27405800 | -4.44974900 | 0.44886100 | H | -0.18449000 | 4.76564200 | 0.13835100 |
| C | -4.42959200 | -2.77413900 | -2.27394700 | C | 2.75249600 | 4.35951000 | -1.52429800 |
| H | -3.21086000 | -1.58387400 | -3.59411400 | H | 3.17960500 | 2.74505200 | -2.88795300 |
| H | -5.37689800 | -4.01472800 | -0.78779000 | H | 2.03807100 | 5.83041000 | -0.12159600 |
| H | -5.34816300 | -2.58817500 | -2.82323500 | H | 3.72486000 | 4.82791800 | -1.64725400 |
| C | -0.22679400 | 2.95859500 | -0.73517800 | C | 2.99708500 | -2.50197200 | -1.15563900 |
| C | 1.10059300 | 3.03967600 | -0.31418700 | C | 2.10929800 | -3.56667800 | -1.01150600 |
| C | -1.00889200 | 4.11743200 | -0.75477900 | C | 4.37150800 | -2.74075900 | -1.04696300 |
| C | 1.63601700 | 4.26143000 | 0.09398500 | C | 2.58720300 | -4.85147700 | -0.74676100 |
| H | 1.70593300 | 2.13791100 | -0.29979500 | H | 1.04368600 | -3.38219500 | -1.10062100 |
| C | -0.47382400 | 5.33796400 | -0.35144900 | C | 4.84836700 | -4.02106800 | -0.78422300 |
| H | -2.04244600 | 4.05991200 | -1.08981600 | H | 5.06962100 | -1.91494700 | -1.16912300 |
| C | 0.85154900 | 5.41304600 | 0.07764400 | C | 3.95487100 | -5.08273600 | -0.63062000 |
| H | 2.66965000 | 4.31048500 | 0.42650300 | H | 1.88442200 | -5.67213000 | -0.63297200 |
| H | -1.09233900 | 6.23078400 | -0.36736400 | H | 5.91774300 | -4.19265000 | -0.69946100 |
| H | 1.26785300 | 6.36339900 | 0.39880500 | H | 4.32570300 | -6.08255300 | -0.42455400 |
| C | -3.66893900 | 0.46599600 | 1.13010300 | C | 2.68731800 | 0.95334500 | 1.80511800 |
| C | -4.14600600 | -0.02840800 | -0.08529200 | C | 3.21933500 | 1.90070700 | 0.92790400 |
| C | -3.66300700 | 1.84460500 | 1.35100300 | C | 3.42713100 | -0.19315500 | 2.10270800 |
| C | -4.61485500 | 0.83934500 | -1.06929000 | C | 4.47607000 | 1.70975200 | 0.35720300 |
| H | -4.13808800 | -1.10176800 | -0.26262800 | H | 2.63784400 | 2.78728300 | 0.68256400 |
| C | -4.13337900 | 2.71516900 | 0.36841500 | C | 4.68425300 | -0.38683900 | 1.53106400 |
| H | -3.28426400 | 2.23143600 | 2.29268100 | H | 3.01103300 | -0.93397400 | 2.77920500 |
| C | -4.60956200 | 2.21602500 | -0.84435300 | C | 5.21246300 | 0.56362600 | 0.65755100 |
| H | -4.97618400 | 0.43979300 | -2.01338500 | H | 4.87413800 | 2.45103800 | -0.33077900 |
| H | -4.12654300 | 3.78636700 | 0.55003400 | H | 5.25053000 | -1.28395400 | 1.76560800 |
| H | -4.97210100 | 2.89682700 | -1.60912800 | H | 6.19046600 | 0.41025900 | 0.21013400 |
| C | 2.72672300 | -2.27887900 | 0.66612600 | C | -3.21982400 | -0.56707600 | -1.46362200 |
| C | 3.99749200 | -2.22501500 | 1.16380000 | C | -4.32149500 | -1.35999300 | -1.43118400 |
| C | 4.94637400 | -3.23677600 | 0.82468600 | C | -5.55796200 | -0.90811500 | -1.98263200 |
| N | 5.73934600 | -4.03453200 | 0.54052100 | N | -6.57612100 | -0.54886400 | -2.40754500 |
| H | 2.48503100 | -3.09346300 | -0.01593800 | H | -3.31953600 | 0.41859700 | -1.91692100 |
| H | 4.29931700 | -1.54704700 | 1.95552500 | H | -4.31613000 | -2.37879500 | -1.05856000 |
| C | 6.00249300 | -0.67731200 | -0.86006000 | C | -6.00349700 | -0.78167600 | 1.58093700 |
| C | 6.43452500 | 0.40666300 | -1.64417800 | C | -6.06344900 | -0.69799600 | 2.98481100 |
| C | 5.67581600 | 1.58236900 | -1.76922000 | C | -4.94955900 | -0.96180500 | 3.80165800 |
| C | 4.44259900 | 1.74817900 | -1.11942100 | C | -3.69848400 | -1.32668000 | 3.27578600 |
| C | 4.04925700 | 0.64231000 | -0.36041600 | C | -3.70347600 | -1.38481700 | 1.88311900 |
| C | 4.78384600 | -0.38320600 | -0.28573400 | C | -4.72807600 | -1.14198900 | 1.20048700 |
| H | 6.57690600 | -1.59140600 | -0.74971600 | H | -6.85462300 | -0.58334600 | 0.93826600 |
| H | 7.38455100 | 0.32785400 | -2.16624200 | H | -7.00544600 | -0.41907600 | 3.45014300 |
| H | 6.05604400 | 2.38775700 | -2.39261700 | H | -5.06138400 | -0.87792900 | 4.87970700 |
| H | 3.86963800 | 2.66556100 | -1.22985300 | H | -2.84656300 | -1.53138400 | 3.91757600 |
| R-3 G(M062X/6-31G(d)): -1746.05991 Number of Imaginary frequency: 0 | | | | S-3 G(M062X/6-31G(d)): -1746.06678 Number of Imaginary frequency: 0 | | | |
| C | -0.08065100 | 0.13897500 | 0.43529800 | C | 0.10539400 | -0.96169400 | 0.04936300 |
| C | 0.63589700 | 0.66726900 | -0.82700800 | C | 0.83303000 | -1.50858500 | 1.28742400 |
| C | 2.12282600 | 0.47035100 | -0.69540100 | C | 2.30411400 | -1.25027500 | 1.11131700 |
| C | 2.51220100 | -0.91840400 | -0.27634000 | C | 2.89210200 | -1.97088700 | -0.07396600 |
| C | 0.45095300 | -1.22717100 | 0.89837100 | C | 0.95592000 | -1.12916800 | -1.22901500 |
| H | 0.41732300 | 1.73674000 | -0.92473400 | H | 0.65983000 | -2.59836600 | 1.30748800 |
| H | -1.15829900 | 0.06010200 | 0.21902300 | H | -0.09090700 | 0.10626800 | 0.21859700 |

| | | | | | | | |
|--------------------|-------------|-------------|-------------|--------------------|-------------|-------------|-------------|
| H | 0.13129400 | -1.35618700 | 1.93654000 | H | 0.29380600 | -1.47454900 | -2.02889500 |
| H | 2.15916700 | -1.63256700 | -1.03829800 | O | 1.91604000 | -2.17057500 | -1.09267400 |
| O | 1.87455600 | -1.21676500 | 0.96809500 | C | 1.57567700 | 0.19646500 | -1.68125600 |
| C | -0.05830000 | -2.44805400 | 0.10674000 | H | 2.26427500 | 0.58801600 | -0.92234800 |
| H | -0.30231900 | -2.18900000 | -0.93012900 | H | 2.14271400 | 0.04880500 | -2.60877400 |
| H | 0.74785700 | -3.19005400 | 0.10303300 | O | 0.40557800 | -0.92900600 | 2.49695700 |
| O | 0.20861900 | -0.02411700 | -1.99420600 | O | -1.12327700 | -1.65730400 | -0.05618000 |
| O | 0.15539900 | 1.06562300 | 1.48568300 | O | 0.50786800 | 1.10110900 | -1.89943900 |
| O | -1.16146800 | -3.09339800 | 0.71964900 | C | -2.09015400 | -0.94808600 | -0.80074400 |
| C | -0.99959500 | 1.78468800 | 1.89508000 | H | -2.29836700 | 0.02077400 | -0.31906800 |
| H | -1.80674700 | 1.08833400 | 2.16428500 | H | -1.71262800 | -0.72807300 | -1.81192400 |
| H | -0.69733500 | 2.32256300 | 2.79931400 | C | -0.91404900 | -1.24630900 | 2.90862400 |
| C | -0.97194800 | 0.50843000 | -2.59189300 | H | -1.19375600 | -2.25072300 | 2.56661500 |
| H | -1.31969400 | 1.39193900 | -2.04108700 | H | -0.88364100 | -1.26352600 | 4.00473300 |
| H | -0.70467700 | 0.83449200 | -3.60551600 | C | 0.65692800 | 2.33576500 | -1.23138400 |
| C | -2.42078900 | -2.48454400 | 0.51776300 | H | 1.00559800 | 2.16677100 | -0.20022100 |
| H | -2.41774700 | -1.88030300 | -0.39871300 | H | 1.42114100 | 2.95172600 | -1.72978700 |
| H | -3.14271600 | -3.29778400 | 0.36610500 | C | -1.94551700 | -0.23845700 | 2.44842700 |
| C | -2.07594300 | -0.51876400 | -2.65566100 | C | -3.27619900 | -0.62652900 | 2.28584700 |
| C | -3.38033400 | -0.18588800 | -2.28917000 | C | -1.59083300 | 1.09030500 | 2.20378000 |
| C | -1.80232700 | -1.81888400 | -3.09402700 | C | -4.23768200 | 0.29323700 | 1.87119500 |
| C | -4.39982300 | -1.13793400 | -2.35541500 | H | -3.55759100 | -1.66245500 | 2.46438500 |
| H | -3.59932000 | 0.82387100 | -1.94733600 | C | -2.54886900 | 2.01091300 | 1.78135700 |
| C | -2.81385900 | -2.77332600 | -3.14839000 | H | -0.55509400 | 1.39605800 | 2.32780000 |
| H | -0.78721400 | -2.08250900 | -3.38107500 | C | -3.87506500 | 1.61445700 | 1.61052900 |
| C | -4.11687800 | -2.43427700 | -2.77830700 | H | -5.26655800 | -0.02803400 | 1.73263400 |
| H | -5.41171200 | -0.86635500 | -2.06781800 | H | -2.25908900 | 3.03889600 | 1.57775000 |
| H | -2.58833000 | -3.78232100 | -3.48159300 | H | -4.61884400 | 2.33061000 | 1.27208200 |
| H | -4.90659900 | -3.17868900 | -2.82301500 | C | -3.35952400 | -1.75430600 | -0.90020300 |
| C | -1.48378800 | 2.75480300 | 0.84007200 | C | -3.42935800 | -3.08108600 | -0.47613100 |
| C | -0.62589800 | 3.75642300 | 0.36975700 | C | -4.50089500 | -1.14779200 | -1.43394900 |
| C | -2.76127000 | 2.64565800 | 0.29166800 | C | -4.62556700 | -3.79211500 | -0.58628400 |
| C | -1.03795700 | 4.62677400 | -0.63408600 | H | -2.54753900 | -3.55201600 | -0.05385700 |
| H | 0.37568100 | 3.83884800 | 0.78718000 | C | -5.69214300 | -1.85696700 | -1.54739400 |
| C | -3.18186100 | 3.52227100 | -0.71149100 | H | -4.45252000 | -0.10769500 | -1.75206400 |
| H | -3.43003200 | 1.86624000 | 0.65059000 | C | -5.75804800 | -3.18523300 | -1.12244000 |
| C | -2.31940200 | 4.51019400 | -1.17846400 | H | -4.66937700 | -4.82446200 | -0.25048700 |
| H | -0.36272000 | 5.39771100 | -0.99407200 | H | -6.57181800 | -1.37394400 | -1.96318400 |
| H | -4.17987300 | 3.42621600 | -1.13008600 | H | -6.68825500 | -3.73945000 | -1.20671200 |
| H | -2.64183200 | 5.18951400 | -1.96213200 | C | -0.65799700 | 3.07403300 | -1.18561600 |
| C | -2.87890100 | -1.63696100 | 1.68844000 | C | -0.70914200 | 4.30808200 | -0.52880900 |
| C | -3.92823400 | -0.72973200 | 1.51273000 | C | -1.82135600 | 2.55719200 | -1.75516000 |
| C | -2.31124100 | -1.77724900 | 2.95606300 | C | -1.90667400 | 5.00983500 | -0.43256900 |
| C | -4.39807500 | 0.02827700 | 2.58346900 | H | 0.19789800 | 4.71617600 | -0.08726800 |
| H | -4.37777900 | -0.61642200 | 0.52754500 | C | -3.02459600 | 3.25939900 | -1.65499700 |
| C | -2.77173400 | -1.01044600 | 4.02647400 | H | -1.78304600 | 1.60536700 | -2.27490900 |
| H | -1.50716600 | -2.49281000 | 3.09869000 | C | -3.07259600 | 4.48287900 | -0.99238300 |
| C | -3.81597900 | -0.10575300 | 3.84437500 | H | -1.93325700 | 5.96599700 | 0.08231500 |
| H | -5.21134500 | 0.73257600 | 2.43112900 | H | -3.92650200 | 2.84639200 | -2.09878200 |
| H | -2.31594500 | -1.12542000 | 5.00588600 | H | -4.00975500 | 5.02639700 | -0.91478500 |
| H | -4.17450700 | 0.49068600 | 4.67816800 | C | 3.02054700 | -0.45337300 | 1.89681900 |
| C | 2.98939900 | 1.45842300 | -0.88703800 | C | 4.49001900 | -0.19021100 | 1.64625200 |
| C | 4.48361500 | 1.28413600 | -0.76552200 | C | 4.80228700 | 1.20008700 | 2.02063800 |
| C | 5.01602900 | 2.32030200 | 0.13991700 | N | 5.04189800 | 2.29122100 | 2.31699400 |
| N | 5.42749100 | 3.13380100 | 0.85059200 | H | 2.56955900 | 0.01166800 | 2.76756500 |
| H | 2.64246200 | 2.45283200 | -1.16088600 | C | 6.09306600 | 0.09614000 | -0.30100100 |
| H | 4.94206200 | 1.48515200 | -1.74487000 | C | 6.49499900 | -0.16422200 | -1.60602900 |
| C | 6.28376000 | -0.34385200 | -0.09288800 | C | 5.72151300 | -0.99409100 | -2.41736200 |
| C | 6.72096400 | -1.59275000 | 0.32686100 | C | 4.55684100 | -1.56060100 | -1.91282800 |
| C | 5.79388000 | -2.61349100 | 0.54937900 | C | 4.14943300 | -1.30555300 | -0.60106700 |
| C | 4.44269700 | -2.37065000 | 0.34615200 | C | 4.92037000 | -0.46800300 | 0.20890400 |
| C | 3.99410200 | -1.11444000 | -0.07721900 | H | 6.69278000 | 0.74994600 | 0.32755800 |
| C | 4.92130400 | -0.09586300 | -0.29303600 | H | 7.40753000 | 0.28189800 | -1.98936400 |
| H | 7.00201300 | 0.45487400 | -0.26431700 | H | 6.02562600 | -1.19888500 | -3.43946600 |
| H | 7.78072800 | -1.77227700 | 0.48001400 | H | 3.94138600 | -2.20255800 | -2.53586500 |
| H | 6.12789000 | -3.59283600 | 0.87815400 | H | 3.15267000 | -2.98980600 | 0.24639100 |
| H | 3.71110200 | -3.15575100 | 0.51860300 | H | 5.08493000 | -0.82103500 | 2.32424800 |
| R-4 | | | | S-4 | | | |
| G(M062X/6-31G(d)): | -1845.96541 | | | G(M062X/6-31G(d)): | -1845.96960 | | |

| Number of Imaginary frequency: 0 | | | | Number of Imaginary frequency: 0 | | | |
|----------------------------------|-------------|--------------|-------------|----------------------------------|-------------|-------------|-------------|
| C | -0.06818900 | 0.14928600 | 0.41500900 | C | 0.10072700 | -1.02355600 | 0.02827100 |
| C | 0.65740900 | 0.65200300 | -0.85573100 | C | 0.83723600 | -1.59828000 | 1.25157500 |
| C | 2.13939800 | 0.45713200 | -0.69364300 | C | 2.28537500 | -1.24841100 | 1.04674500 |
| C | 2.51261500 | -0.93559900 | -0.26758000 | C | 2.89010400 | -1.99902600 | -0.10763700 |
| C | 0.45676100 | -1.20883900 | 0.91251900 | C | 0.94835800 | -1.15931900 | -1.26031100 |
| H | 0.43845800 | 1.71944700 | -0.97559600 | H | 0.70188100 | -2.69293000 | 1.24055700 |
| H | -1.14476600 | 0.06684600 | 0.19359000 | H | -0.08924200 | 0.03916700 | 0.23285200 |
| H | 0.12953700 | -1.31127900 | 1.95150200 | H | 0.27958800 | -1.50391700 | -2.05554500 |
| H | 2.13226300 | -1.65187300 | -1.01412400 | O | 1.92575000 | -2.18625000 | -1.15063000 |
| O | 1.87949200 | -1.21070600 | 0.98751900 | C | 1.56569300 | 0.16753700 | -1.71471400 |
| C | -0.05952100 | -2.44302400 | 0.14555200 | H | 2.31183300 | 0.52336000 | -0.99529500 |
| H | -0.30433100 | -2.20263100 | -0.89558200 | H | 2.06971800 | 0.02344900 | -2.67814900 |
| H | 0.74352500 | -3.18824300 | 0.15412600 | O | 0.39869400 | -1.06722600 | 2.47956100 |
| O | 0.23122500 | -0.06183600 | -2.01120300 | O | -1.13510600 | -1.70377700 | -0.10133600 |
| O | 0.15978400 | 1.09788200 | 1.44778700 | O | 0.52437900 | 1.11800700 | -1.85503200 |
| O | -1.16462000 | -3.07274000 | 0.77190800 | C | -2.09113900 | -0.95047500 | -0.81658600 |
| C | -1.00048500 | 1.81394200 | 1.84430600 | H | -2.28215100 | 0.00251500 | -0.29739700 |
| H | -1.80540700 | 1.11703000 | 2.11886200 | H | -1.71052300 | -0.69643800 | -1.81893400 |
| H | -0.70552000 | 2.36448900 | 2.74340300 | C | -0.92464900 | -1.39546300 | 2.86699500 |
| C | -0.94978700 | 0.45666400 | -2.61799800 | H | -1.21067900 | -2.37896300 | 2.47329500 |
| H | -1.29190000 | 1.35769900 | -2.09225200 | H | -0.90256200 | -1.46790300 | 3.96111900 |
| H | -0.68683900 | 0.75130000 | -3.64237700 | C | 0.71070600 | 2.27328000 | -1.06413400 |
| C | -2.42160800 | -2.46332100 | 0.56042400 | H | 1.01803300 | 1.98888500 | -0.04451500 |
| H | -2.41627100 | -1.87110900 | -0.36379300 | C | 1.52182000 | 2.89292500 | -1.47718500 |
| H | -3.14643100 | -3.27591500 | 0.41856400 | H | -1.94571300 | -0.35767700 | 2.45229500 |
| C | -2.06043800 | -0.56539400 | -2.64933100 | C | -3.28176600 | -0.72416400 | 2.28247400 |
| C | -3.36207700 | -0.21511800 | -2.28894200 | C | -1.57796700 | 0.97571400 | 2.25722700 |
| C | -1.79642800 | -1.87818000 | -3.05492000 | C | -4.23518600 | 0.22137000 | 1.90947600 |
| C | -4.38767000 | -1.16202000 | -2.32840100 | H | -3.57384800 | -1.76349500 | 2.41954000 |
| H | -3.57405400 | 0.80469400 | -1.97366300 | C | -2.52856500 | 1.92297500 | 1.87929800 |
| C | -2.81381800 | -2.82748200 | -3.08193000 | H | -0.53786800 | 1.26534300 | 2.38422400 |
| H | -0.78378700 | -2.15496900 | -3.33831300 | C | -3.85989900 | 1.54810900 | 1.70035700 |
| C | -4.11390900 | -2.47075600 | -2.71809700 | H | -5.26794100 | -0.08350600 | 1.76266200 |
| H | -5.39720300 | -0.87680200 | -2.04571600 | H | -2.22769900 | 2.95490400 | 1.71461500 |
| H | -2.59521900 | -3.84619100 | -3.38924600 | H | -4.59722300 | 2.28547900 | 1.39451700 |
| H | -4.90844800 | -3.211108500 | -2.74102400 | C | -3.37563800 | -1.72753200 | -0.94644700 |
| C | -1.48484500 | 2.76955200 | 0.77624900 | C | -3.47407600 | -3.06423100 | -0.56166200 |
| C | -0.62531500 | 3.76344200 | 0.29291700 | C | -4.50245800 | -1.08237300 | -1.46573800 |
| C | -2.76314000 | 2.65630700 | 0.23071500 | C | -4.68406600 | -3.74722500 | -0.69660700 |
| C | -1.03676900 | 4.62306300 | -0.72028400 | H | -2.60309200 | -3.56447400 | -0.15065500 |
| H | 0.37652600 | 3.84871600 | 0.70893600 | C | -5.70736500 | -1.76346300 | -1.60395000 |
| C | -3.18306600 | 3.52210100 | -0.78223900 | H | -4.43250500 | -0.03468400 | -1.75364800 |
| H | -3.43319200 | 1.88265700 | 0.59975700 | C | -5.80184100 | -3.10205200 | -1.21854700 |
| C | -2.31922400 | 4.50289000 | -1.26155900 | H | -4.74996300 | -4.78792800 | -0.39154500 |
| H | -0.36015300 | 5.38806500 | -1.09012900 | H | -6.57534100 | -1.25037300 | -2.00834900 |
| H | -4.18177000 | 3.42329300 | -1.19858000 | H | -6.74276500 | -3.63428400 | -1.32306100 |
| H | -2.64108400 | 5.17364500 | -2.05280700 | C | -0.56738000 | 3.06956300 | -0.98799100 |
| C | -2.87812800 | -1.59864100 | 1.71908100 | C | -0.56427500 | 4.27982800 | -0.28625400 |
| C | -3.92950900 | -0.69607400 | 1.53215000 | C | -1.75282500 | 2.62317900 | -1.57118300 |
| C | -2.30481600 | -1.71625500 | 2.98629600 | C | -1.73131200 | 5.02674900 | -0.15989900 |
| C | -4.39519300 | 0.08032300 | 2.59141800 | H | 0.36109900 | 4.63281300 | 0.16528300 |
| H | -4.38321200 | -0.60007800 | 0.54707300 | C | -2.92508200 | 3.37060100 | -1.44118500 |
| C | -2.76162200 | -0.93153500 | 4.04527700 | H | -1.75339700 | 1.69140800 | -2.12691400 |
| H | -1.49873100 | -2.42783800 | 3.13707400 | C | -2.91961600 | 4.57028600 | -0.73464600 |
| C | -3.80730000 | -0.03093000 | 3.85186000 | H | -1.71609100 | 5.96416500 | 0.38874400 |
| H | -5.20985100 | 0.78112100 | 2.43044000 | H | -3.84470100 | 3.01235600 | -1.89603900 |
| H | -2.30140500 | -1.02911700 | 5.02451300 | H | -3.83264600 | 5.15009700 | -0.63471100 |
| H | -4.16282900 | 0.57965200 | 4.67665600 | C | 2.91247900 | -0.28346000 | 1.71466700 |
| C | 3.01246400 | 1.45464100 | -0.80661300 | C | 4.26158100 | 0.25628800 | 1.31612500 |
| C | 4.48533500 | 1.29968400 | -0.54383700 | C | 4.06302700 | 1.69081400 | 1.02334600 |
| C | 4.83831800 | 2.15552600 | 0.60269400 | N | 3.81004400 | 2.79122600 | 0.76609300 |
| N | 5.07887600 | 2.83294800 | 1.50976800 | H | 2.41147100 | 0.20986700 | 2.54333300 |
| H | 2.66612900 | 2.45442900 | -1.06495100 | C | 6.12874000 | 0.02223900 | -0.34363300 |
| H | 5.16898400 | 1.70928600 | -1.31940800 | C | 6.68668100 | -0.51402500 | -1.49733900 |
| C | 6.29357700 | -0.39712000 | -0.18339100 | C | 5.99484400 | -1.48610400 | -2.22538300 |
| C | 6.73350800 | -1.68432700 | 0.09635900 | C | 4.75993000 | -1.93557600 | -1.77502100 |
| C | 5.80942200 | -2.71638700 | 0.28670400 | C | 4.18846400 | -1.40573200 | -0.61268200 |
| C | 4.45089000 | -2.45252600 | 0.17207800 | C | 4.86685200 | -0.40711000 | 0.08679700 |
| C | 3.99429100 | -1.15900700 | -0.10617100 | H | 6.62679200 | 0.75654000 | 0.29387900 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 4.92085100 | -0.12895600 | -0.26095200 | H | 7.66446900 | -0.17955500 | -1.83303200 |
| H | 6.95771900 | 0.44370400 | -0.39377700 | H | 6.42566600 | -1.90175400 | -3.13179400 |
| H | 7.79826100 | -1.89260600 | 0.15759800 | H | 4.22179400 | -2.70686400 | -2.31990300 |
| H | 6.15073600 | -3.72401300 | 0.50603800 | H | 3.10133300 | -3.02357800 | 0.23176800 |
| H | 3.72277600 | -3.25118400 | 0.29509800 | H | 5.02828900 | 0.29210000 | 2.10841000 |
| F | 6.88716700 | 2.19965900 | -1.29269800 | F | 6.53521300 | 1.44723500 | 2.12007400 |
| R-TS2 G(M062X/6-31G(d)): -1845.95869 Number of Imaginary frequency: -45.89 | | | | S-TS2 G(M062X/6-31G(d)): -1845.96956 Number of Imaginary frequency: -87.18 | | | |
| -1 I | | | | -1 I | | | |
| C | 0.05260400 | 0.11073900 | -0.42434700 | C | -0.09479900 | -1.05979300 | 0.05232800 |
| C | -0.67128200 | 0.71301400 | 0.80140800 | C | 0.64066700 | -1.55021700 | 1.31156300 |
| C | -2.15205400 | 0.48588000 | 0.67911800 | C | 2.08886200 | -1.22458400 | 1.07310500 |
| C | -2.51461600 | -0.93644100 | 0.36578200 | C | 2.68632800 | -2.06994200 | -0.01921900 |
| C | -0.46280500 | -1.28949200 | -0.80103400 | C | 0.74216900 | -1.31037500 | -1.22713600 |
| H | -0.46739300 | 1.78947900 | 0.82589700 | H | 0.49392800 | -2.64113700 | 1.38284500 |
| H | 1.13105400 | 0.05156300 | -0.20451700 | H | -0.26327500 | 0.01904100 | 0.17284500 |
| H | -0.14051900 | -1.47942100 | -1.82916300 | H | 0.06306200 | -1.71397400 | -1.98514100 |
| H | -2.12754500 | -1.58631100 | 1.16857000 | O | 1.71473600 | -2.33127900 | -1.04210200 |
| O | -1.88654100 | -1.31329700 | -0.86488200 | C | 1.37187700 | -0.03322300 | -1.79374700 |
| C | 0.06981400 | -2.44700900 | 0.06813500 | H | 2.14140600 | 0.35685100 | -1.11785500 |
| H | 0.32431400 | -2.11247700 | 1.08071400 | H | 1.85277100 | -0.26098800 | -2.75289600 |
| H | -0.72819800 | -3.19456900 | 0.13581100 | O | 0.21355500 | -0.92605200 | 2.50011500 |
| O | -0.22281700 | 0.10902000 | 2.01059600 | O | -1.34533800 | -1.72221800 | -0.01613500 |
| O | -0.18544100 | 0.96754200 | -1.53243200 | O | 0.35159000 | 0.93041300 | -1.99002900 |
| O | 1.17251600 | -3.12536800 | -0.51020400 | C | -2.29352700 | -1.00694700 | -0.77887800 |
| C | 0.96626100 | 1.66328200 | -1.98690500 | H | -2.45382400 | -0.01002000 | -0.33773000 |
| H | 1.77467500 | 0.95405800 | -2.21692700 | H | -1.92163900 | -0.84614000 | -1.80351100 |
| H | 0.66001100 | 2.14518900 | -2.92114800 | C | -1.11438900 | -1.19894200 | 2.91033100 |
| C | 0.95895900 | 0.69344700 | 2.55142100 | H | -1.42429300 | -2.19882300 | 2.58200200 |
| H | 1.30311200 | 1.52673800 | 1.92481600 | H | -1.09115200 | -1.20069800 | 4.00708600 |
| H | 0.70009300 | 1.10710200 | 3.53525000 | C | 0.56164000 | 2.12052400 | -1.25890100 |
| C | 2.43185900 | -2.50737200 | -0.34331400 | H | 0.83802900 | 1.88221000 | -0.21874900 |
| H | 2.43189900 | -1.85836600 | 0.54245600 | H | 1.40205800 | 2.68901800 | -1.68667700 |
| H | 3.15496300 | -3.31190200 | -0.15437400 | C | -2.11266800 | -0.16668300 | 2.43071700 |
| C | 2.06518400 | -0.32307300 | 2.69582200 | C | -3.46038000 | -0.50744000 | 2.30420000 |
| C | 3.37060900 | -0.01543900 | 2.31138900 | C | -1.71080100 | 1.13691700 | 2.13031300 |
| C | 1.79233000 | -1.58721200 | 3.22919800 | C | -4.39233700 | 0.43313300 | 1.86962100 |
| C | 4.39168800 | -0.95761900 | 2.45291300 | H | -3.77901500 | -1.52357100 | 2.52814100 |
| H | 3.58805000 | 0.96575000 | 1.89361400 | C | -2.63967200 | 2.07833200 | 1.68891400 |
| C | 2.80571500 | -2.53267500 | 3.35965300 | H | -0.66192400 | 1.40620600 | 2.22589100 |
| H | 0.77584700 | -1.83030700 | 3.52921800 | C | -3.98265100 | 1.72794800 | 1.55193700 |
| C | 4.10958600 | -2.21932900 | 2.97064400 | H | -5.43537000 | 0.14841100 | 1.75994000 |
| H | 5.40433600 | -0.70586300 | 2.15015600 | H | -2.31259000 | 3.08545300 | 1.44213600 |
| H | 2.58137500 | -3.51400600 | 3.76805200 | H | -4.70319200 | 2.45981900 | 1.19733000 |
| H | 4.90034700 | -2.95654500 | 3.07426400 | C | -3.59889100 | -1.75879600 | -0.82383000 |
| C | 1.45534800 | 2.69718100 | -0.99603900 | C | -3.71906700 | -3.06284600 | -0.34438300 |
| C | 0.59237600 | 3.70998800 | -0.56025800 | C | -4.72355500 | -1.12184900 | -1.35765600 |
| C | 2.74762100 | 2.63993200 | -0.47508400 | C | -4.94950400 | -3.72007800 | -0.39631400 |
| C | 1.01370700 | 4.64096600 | 0.38363000 | H | -2.84940700 | -3.55687800 | 0.07698700 |
| H | -0.42124200 | 3.75181000 | -0.95401100 | C | -5.94895600 | -1.77758200 | -1.41334200 |
| C | 3.17769200 | 3.57757200 | 0.46671000 | H | -4.63548900 | -0.09887700 | -1.71980900 |
| H | 3.42120300 | 1.85293200 | -0.80695800 | C | -6.06582900 | -3.08256900 | -0.93084400 |
| C | 2.30990000 | 4.57592500 | 0.90059200 | H | -5.03333400 | -4.73404700 | -0.01522800 |
| H | 0.33344100 | 5.41873200 | 0.71859100 | H | -6.81544100 | -1.27067800 | -1.82852100 |
| H | 4.18738300 | 3.52064800 | 0.86405600 | H | -7.02258800 | -3.59510900 | -0.96949800 |
| H | 2.63978700 | 5.30264500 | 1.63725800 | C | -0.68894900 | 2.96309000 | -1.25225500 |
| C | 2.88729800 | -1.72030600 | -1.55644100 | C | -0.64957200 | 4.21716800 | -0.63383400 |
| C | 3.93683600 | -0.80560300 | -1.42756300 | C | -1.88542800 | 2.51747500 | -1.81319200 |
| C | 2.32259100 | -1.92841400 | -2.81613500 | C | -1.79119900 | 5.01002400 | -0.56905500 |
| C | 4.41042100 | -0.10726600 | -2.53641600 | H | 0.28446900 | 4.56922300 | -0.19982300 |
| H | 4.38493900 | -0.64120000 | -0.44902000 | C | -3.03259000 | 3.31101500 | -1.74426200 |
| C | 2.78654700 | -1.22092200 | -3.92520700 | H | -1.91560600 | 1.54906900 | -2.30223900 |
| H | 1.51891200 | -2.65068900 | -2.92286800 | C | -2.99096000 | 4.55530800 | -1.12102400 |
| C | 3.83136200 | -0.30877000 | -3.78966200 | H | -1.74654900 | 5.98240700 | -0.08678500 |
| H | 5.22410700 | 0.60336800 | -2.41987900 | H | -3.96079300 | 2.95260700 | -2.18111800 |
| H | 2.33247300 | -1.38706100 | -4.89807900 | H | -3.88386600 | 5.17150100 | -1.07028700 |
| H | 4.19277300 | 0.24128700 | -4.65358500 | C | 2.71075700 | -0.19390400 | 1.64306100 |
| C | -3.04341100 | 1.46402800 | 0.79411000 | C | 4.05693700 | 0.30110300 | 1.20648900 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -4.52759000 | 1.25367700 | 0.67506700 | C | 3.89389300 | 1.70435400 | 0.80979700 |
| C | -5.06061000 | 2.17231900 | -0.34348800 | N | 3.76198000 | 2.81918700 | 0.51928800 |
| N | -5.49574000 | 2.86647400 | -1.16104600 | H | 2.20188000 | 0.37093500 | 2.42025900 |
| H | -2.76756800 | 2.48490600 | 1.04202100 | C | 5.94128600 | -0.10584900 | -0.38411300 |
| H | -4.93781400 | 1.71066800 | 1.60130400 | C | 6.51697500 | -0.73782300 | -1.47787400 |
| C | -6.30326800 | -0.47938100 | 0.24624400 | C | 5.82488300 | -1.75813500 | -2.13695400 |
| C | -6.71776100 | -1.77516900 | -0.03128100 | C | 4.57873200 | -2.15819300 | -1.66996600 |
| C | -5.76932800 | -2.78904800 | -0.18579900 | C | 3.99044600 | -1.52606000 | -0.56855800 |
| C | -4.42022400 | -2.48959100 | -0.05532200 | C | 4.66128100 | -0.46963800 | 0.05164000 |
| C | -3.99594500 | -1.18599800 | 0.22468800 | H | 6.46469100 | 0.65211400 | 0.19354600 |
| C | -4.94339700 | -0.17010700 | 0.37316100 | H | 7.50768200 | -0.44561900 | -1.81425600 |
| H | -7.03921300 | 0.31332400 | 0.36211500 | H | 6.26820400 | -2.25250800 | -2.99645100 |
| H | -7.77666800 | -1.99689600 | -0.12608500 | H | 4.04579500 | -2.97185200 | -2.15561600 |
| H | -6.08371800 | -3.80535100 | -0.40382800 | H | 2.89024800 | -3.06857000 | 0.39430500 |
| H | -3.67141100 | -3.26892400 | -0.17443000 | H | 4.91248700 | 0.41650300 | 1.99485000 |
| F | -4.68881600 | 3.43012400 | 2.08583900 | F | 6.24515500 | 0.94304000 | 2.41134900 |
| R-5 G(M062X/6-31G(d)): -1845.98787 Number of Imaginary frequency: 0 | | | | S-5 G(M062X/6-31G(d)): -1845.99324 Number of Imaginary frequency: 0 | | | |
| C | 0.24215300 | 0.00143700 | -0.61400400 | C | -0.01708400 | -0.86574300 | -0.13642400 |
| C | -0.62396100 | 0.88814300 | 0.30568400 | C | 0.81598700 | -1.47379000 | 0.99930700 |
| C | -2.08145600 | 0.57734700 | 0.15784800 | C | 2.24945700 | -1.08040700 | 0.79242500 |
| C | -2.43411900 | -0.88084300 | 0.07417200 | C | 2.83681000 | -1.62767200 | -0.48093600 |
| C | -0.23199100 | -1.46093000 | -0.65863400 | C | 0.77498500 | -0.83948100 | -1.46449600 |
| H | -0.44425400 | 1.93538400 | 0.03110400 | H | 0.71397800 | -2.57164500 | 0.91363400 |
| H | 1.28550600 | 0.03146000 | -0.26003300 | H | -0.27863800 | 0.16273200 | 0.14875500 |
| H | 0.23789800 | -1.91848000 | -1.53525300 | H | 0.09590900 | -1.16329900 | -2.26072800 |
| H | -2.22557200 | -1.37339700 | 1.04226100 | O | 1.82527800 | -1.79524400 | -1.48632300 |
| O | -1.62507800 | -1.53052200 | -0.92182200 | C | 1.25322300 | 0.57340800 | -1.81117100 |
| C | 0.15594100 | -2.31942300 | 0.56377900 | H | 1.95669900 | 0.93823800 | -1.05406900 |
| H | 0.29538400 | -1.70784600 | 1.46336000 | H | 1.76960100 | 0.56896200 | -2.77936600 |
| H | -0.66390600 | -3.02305800 | 0.74241100 | O | 0.40003600 | -1.06201900 | 2.28514200 |
| O | -0.24548400 | 0.69553100 | 1.67655000 | O | -1.20410400 | -1.63387700 | -0.25985100 |
| O | 0.15769300 | 0.52025600 | -1.93661200 | O | 0.11043800 | 1.41208900 | -1.87579200 |
| O | 1.30044000 | -3.13000600 | 0.34630200 | C | -2.25920400 | -0.92915800 | -0.87457900 |
| C | 1.38753800 | 1.01428400 | -2.43958900 | H | -2.50514300 | -0.02845300 | -0.28976700 |
| H | 2.17517800 | 0.25078000 | -2.35437500 | H | -1.96255600 | -0.58621800 | -1.87902300 |
| H | 1.21139400 | 1.20092200 | -3.50418500 | C | -0.88529900 | -1.49282400 | 2.69236600 |
| C | 0.91751800 | 1.41580000 | 2.06272900 | H | -1.13924500 | -2.45271700 | 2.22516300 |
| H | 1.35032900 | 1.95392200 | 1.20851400 | H | -0.81756800 | -1.65614500 | 3.77533200 |
| H | 0.61722500 | 2.17059400 | 2.80350800 | C | 0.22034600 | 2.57022000 | -1.07747300 |
| C | 2.54783800 | -2.48004600 | 0.46862200 | H | 0.59905100 | 2.30307200 | -0.07751800 |
| H | 2.46175500 | -1.58542600 | 1.09969900 | H | 0.94639500 | 3.27221200 | -1.51549500 |
| H | 3.21937000 | -3.17708500 | 0.98821500 | C | -1.97722000 | -0.48198600 | 2.40883900 |
| C | 1.95992500 | 0.49982700 | 2.65765200 | C | -3.30426400 | -0.90043500 | 2.29608800 |
| C | 3.31380900 | 0.67989100 | 2.37077100 | C | -1.68162700 | 0.87698400 | 2.27865100 |
| C | 1.57832000 | -0.54020700 | 3.51137600 | C | -4.32060400 | 0.02087400 | 2.04810400 |
| C | 4.27455300 | -0.17076900 | 2.92068700 | H | -3.54068900 | -1.95942000 | 2.38099600 |
| H | 3.61708000 | 1.48643600 | 1.70578600 | C | -2.69483200 | 1.79996000 | 2.02142900 |
| C | 2.53354800 | -1.39601500 | 4.05339600 | H | -0.64850000 | 1.20460000 | 2.36045900 |
| H | 0.52431800 | -0.68429800 | 3.73463800 | C | -4.01751500 | 1.37463200 | 1.90286700 |
| C | 3.88564300 | -1.21430700 | 3.75774800 | H | -5.34681400 | -0.32257100 | 1.94892500 |
| H | 5.32507300 | -0.02166600 | 2.68652800 | H | -2.45121900 | 2.85324900 | 1.90403200 |
| H | 2.22430100 | -2.20655300 | 4.70718100 | H | -4.80533500 | 2.09411300 | 1.69724600 |
| H | 4.63036500 | -1.88351600 | 4.17851000 | C | -3.47332500 | -1.81692700 | -0.97960300 |
| C | 1.82763900 | 2.28806200 | -1.75002700 | C | -3.38836300 | -3.19775600 | -0.80189000 |
| C | 0.95942400 | 3.38479900 | -1.70494900 | C | -4.71513600 | -1.24217100 | -1.26735100 |
| C | 3.07138700 | 2.38359300 | -1.12658200 | C | -4.53020600 | -3.99297200 | -0.90933600 |
| C | 1.32737600 | 4.55296200 | -1.04512000 | H | -2.42656700 | -3.64529400 | -0.57311200 |
| H | -0.01677500 | 3.30779500 | -2.17903900 | C | -5.85348400 | -2.03479300 | -1.37827400 |
| C | 3.44755600 | 3.55671400 | -0.46778100 | H | -4.78736700 | -0.16296000 | -1.39187700 |
| H | 3.74679000 | 1.53116700 | -1.15226500 | C | -5.76411800 | -3.41603600 | -1.19785200 |
| C | 2.57491700 | 4.64056600 | -0.42280500 | H | -4.45251100 | -5.06699400 | -0.76469500 |
| H | 0.64382200 | 5.39651100 | -1.01379800 | H | -6.81291600 | -1.57452200 | -1.59694800 |
| H | 4.41921200 | 3.61865000 | 0.01458800 | H | -6.65279200 | -4.03540200 | -1.27707000 |
| H | 2.86220100 | 5.55121900 | 0.09463200 | C | -1.12257500 | 3.24005000 | -0.92562800 |
| C | 3.17130500 | -2.10752500 | -0.86170100 | C | -1.19857700 | 4.43056000 | -0.19485100 |
| C | 4.23866000 | -1.20499500 | -0.89031000 | C | -2.28952700 | 2.69347500 | -1.45851800 |
| C | 2.74332400 | -2.68631800 | -2.05757700 | C | -2.42308100 | 5.05783100 | 0.01246900 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 4.86389500 | -0.88231500 | -2.09306100 | H | -0.28901200 | 4.86183900 | 0.21861300 |
| H | 4.58197800 | -0.75453200 | 0.03961800 | C | -3.51923000 | 3.32153200 | -1.24899300 |
| C | 3.35931800 | -2.35509800 | -3.26457800 | H | -2.23332400 | 1.77619900 | -2.03508900 |
| H | 1.92468700 | -3.39950300 | -2.03643600 | C | -3.59152600 | 4.50024500 | -0.51149300 |
| C | 4.42068900 | -1.45246200 | -3.28680000 | H | -2.46750500 | 5.98080200 | 0.58353800 |
| H | 5.69259400 | -0.17933500 | -2.09950800 | H | -4.42310100 | 2.88620600 | -1.66671300 |
| H | 3.01025400 | -2.80729600 | -4.18870600 | C | -4.54915900 | 4.98642800 | -0.34961700 |
| H | 4.90241200 | -1.19692700 | -4.22605400 | C | 2.98096800 | -0.32960700 | 1.63348800 |
| C | -3.02900500 | 1.53461500 | 0.20698900 | C | 4.34994700 | 0.05579700 | 1.32854300 |
| C | -4.44332500 | 1.24474800 | 0.16584100 | C | 5.03294800 | 0.91623600 | 2.20832000 |
| C | -5.37408300 | 2.29796000 | 0.14087500 | N | 5.62973500 | 1.60611700 | 2.94027800 |
| N | -6.16533300 | 3.15946100 | 0.14596400 | H | 2.54915000 | -0.01190700 | 2.57945200 |
| H | -2.72490600 | 2.57614900 | 0.31376800 | C | 5.87679500 | 0.69173400 | -0.57784300 |
| H | -4.26767900 | 0.58621300 | 1.89289200 | C | 6.22741000 | 0.62035200 | -1.91923200 |
| C | -6.18141100 | -0.41774600 | -0.57616900 | C | 5.47103100 | -0.14756500 | -2.80752400 |
| C | -6.54115400 | -1.70215400 | -0.95672300 | C | 4.36800900 | -0.84560600 | -2.32325600 |
| C | -5.57988100 | -2.71437300 | -1.01912300 | C | 4.00828400 | -0.79135000 | -0.97649700 |
| C | -4.26240200 | -2.41099900 | -0.69124400 | C | 4.76289600 | -0.00736600 | -0.07393600 |
| C | -3.88294300 | -1.12450600 | -0.30368100 | H | 6.46354800 | 1.30766300 | 0.10002500 |
| C | -4.85003900 | -0.09649900 | -0.24198400 | H | 7.09221400 | 1.17437300 | -2.27514700 |
| H | -6.93568700 | 0.36529600 | -0.53856900 | H | 5.74057600 | -0.20416300 | -3.85784300 |
| H | -7.57659900 | -1.91577800 | -1.20891400 | H | 3.76264600 | -1.44956800 | -2.99426500 |
| H | -5.85580700 | -3.72222600 | -1.31411100 | H | 3.18663300 | -2.65841700 | -0.30917800 |
| H | -3.49755800 | -3.18209500 | -0.73867400 | H | 4.90157900 | -1.61862600 | 1.58500600 |
| F | -4.00140800 | 0.01765800 | 2.62125200 | F | 5.01520900 | -2.57714000 | 1.47605900 |
| R-6 G(M062X/6-31G(d)): -1745.59225 Number of Imaginary frequency: 0 | | | | S-6 G(M062X/6-31G(d)): -1745.59564 Number of Imaginary frequency: 0 | | | |
| C | 0.04873600 | 0.13291100 | -0.46259700 | C | 0.11158300 | -1.00126300 | 0.09910900 |
| C | -0.73327500 | 0.77755600 | 0.70812600 | C | 0.84467400 | -1.49379000 | 1.35509300 |
| C | -2.19757100 | 0.53329900 | 0.54064400 | C | 2.29493700 | -1.16374600 | 1.15333300 |
| C | -2.55284100 | -0.89054300 | 0.24881100 | C | 2.91801500 | -1.97539800 | 0.05701100 |
| C | -0.45657500 | -1.27697400 | -0.82984900 | C | 0.97392500 | -1.20858600 | -1.17206900 |
| H | -0.53167300 | 1.85603400 | 0.68987700 | H | 0.69818100 | -2.58857200 | 1.41202000 |
| H | 1.11764600 | 0.07274600 | -0.19845900 | H | -0.08393900 | 0.07300100 | 0.22939700 |
| H | -0.07340300 | -1.49417700 | -1.83286200 | H | 0.31178700 | -1.59627400 | -1.95455300 |
| H | -2.19079700 | -1.55579900 | 1.05206700 | O | 1.95803800 | -2.21459300 | -1.00741900 |
| O | -1.87016500 | -1.30877500 | -0.96214900 | C | 1.57372600 | 0.10260300 | -1.68752800 |
| C | 0.03778600 | -2.40976000 | 0.09582600 | H | 2.27279200 | 0.52379400 | -0.95603100 |
| H | 0.25558900 | -2.04595400 | 1.10711800 | H | 2.12862500 | -0.08719400 | -2.61550900 |
| H | -0.76572800 | -3.15158300 | 0.15598700 | O | 0.38480200 | -0.89289800 | 2.54984900 |
| O | -0.28953500 | 0.24002000 | 1.96199600 | O | -1.12573500 | -1.69128900 | -0.00306300 |
| O | -0.12363500 | 0.96338500 | -1.60665800 | O | 0.50724500 | 1.00491800 | -1.93540100 |
| O | 1.15830800 | -3.11519700 | -0.41592600 | C | -2.07632500 | -0.99337400 | -0.77459400 |
| C | 1.06780400 | 1.58644700 | -2.05453300 | H | -2.27304400 | -0.00568600 | -0.32643300 |
| H | 1.85070900 | 0.83564100 | -2.23890000 | H | -1.69153300 | -0.81041600 | -1.79078400 |
| H | 0.81035900 | 2.04715200 | -3.01435700 | C | -0.94260900 | -1.19418300 | 2.93297300 |
| C | 0.90703100 | 0.82882800 | 2.45237100 | H | -1.22788700 | -2.19813100 | 2.59318600 |
| H | 1.28506300 | 1.58976300 | 1.75603100 | H | -0.94195600 | -1.20328700 | 4.03049300 |
| H | 0.66825800 | 1.34148700 | 3.39508200 | C | 0.67098500 | 2.25972500 | -1.31325400 |
| C | 2.41481100 | -2.50349700 | -0.21699000 | H | 1.02228100 | 2.12558900 | -0.27769600 |
| H | 2.37453000 | -1.79382600 | 0.61991200 | H | 1.44034500 | 2.85039500 | -1.83487700 |
| H | 3.11568100 | -3.29943900 | 0.06981700 | C | -1.95800200 | -0.18169800 | 2.44502400 |
| C | 1.98227000 | -0.20384400 | 2.69281200 | C | -3.29525300 | -0.55188500 | 2.29295400 |
| C | 3.31020000 | 0.05974200 | 2.35378600 | C | -1.58272200 | 1.13393700 | 2.16354400 |
| C | 1.66044900 | -1.43691700 | 3.26914400 | C | -4.24193100 | 0.37078600 | 1.85175400 |
| C | 4.30333100 | -0.89533200 | 2.57916600 | H | -3.59366700 | -1.57736600 | 2.50207800 |
| H | 3.56670500 | 1.01580800 | 1.90116900 | C | -2.52567700 | 2.05768500 | 1.71445900 |
| C | 2.64681200 | -2.39606600 | 3.48409000 | H | -0.54187200 | 1.42525700 | 2.27858200 |
| H | 0.62666600 | -1.64673900 | 3.53202500 | C | -3.85785300 | 1.67792900 | 1.55289400 |
| C | 3.97246800 | -2.12743300 | 3.13835900 | H | -5.27615500 | 0.06290200 | 1.72244800 |
| H | 5.33285500 | -0.67791400 | 2.30818300 | H | -2.21908900 | 3.07470000 | 1.48195700 |
| H | 2.38291900 | -3.35402500 | 3.92334100 | H | -4.59005800 | 2.39619200 | 1.19438000 |
| H | 4.74179500 | -2.87586300 | 3.30403700 | C | -3.36058800 | -1.77870100 | -0.85474600 |
| C | 1.58102900 | 2.63634500 | -1.09177100 | C | -3.45625500 | -3.09056900 | -0.39107900 |
| C | 0.74050800 | 3.67914200 | -0.68433600 | C | -4.49081300 | -1.16715500 | -1.40671900 |
| C | 2.87508000 | 2.57198700 | -0.57629500 | C | -4.66656700 | -3.78084400 | -0.47790800 |
| C | 1.18547400 | 4.63364100 | 0.22482600 | H | -2.58287400 | -3.56470100 | 0.04507900 |
| H | -0.27365600 | 3.72719700 | -1.07557400 | C | -5.69621800 | -1.85541800 | -1.49701200 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 3.32876400 | 3.53197600 | 0.33136300 | H | -4.42286200 | -0.13816700 | -1.75605700 |
| H | 3.53132200 | 1.76115100 | -0.88438200 | C | -5.78796000 | -3.16832300 | -1.03088800 |
| C | 2.48329900 | 4.56110900 | 0.73653400 | H | -4.73076300 | -4.80101700 | -0.10965200 |
| H | 0.52285500 | 5.43606000 | 0.53635000 | H | -6.56684300 | -1.36778700 | -1.92637800 |
| H | 4.33940600 | 3.46826700 | 0.72530000 | H | -6.72925700 | -3.70616000 | -1.09637100 |
| H | 2.83162700 | 5.30542000 | 1.44665000 | C | -0.63416200 | 3.01633700 | -1.28918600 |
| C | 2.95029300 | -1.80838100 | -1.45286400 | C | -0.66838600 | 4.27126000 | -0.67188700 |
| C | 4.02539400 | -0.92273700 | -1.33132900 | C | -1.80505000 | 2.49764800 | -1.84130500 |
| C | 2.43121600 | -2.07058200 | -2.72172400 | C | -1.85600100 | 4.99223900 | -0.59784800 |
| C | 4.56786500 | -0.30535000 | -2.45647300 | H | 0.24444000 | 4.68051100 | -0.24354200 |
| H | 4.43931200 | -0.71650300 | -0.34564300 | C | -2.99866400 | 3.21904100 | -1.76312600 |
| C | 2.96582500 | -1.44528800 | -3.84850800 | H | -1.77903400 | 1.52819500 | -2.32863500 |
| H | 1.60698000 | -2.77019600 | -2.82108600 | C | -3.02947900 | 4.46383900 | -1.14037500 |
| C | 4.03459900 | -0.56057800 | -3.72012700 | H | -1.86889900 | 5.96486100 | -0.11409000 |
| H | 5.40085700 | 0.38361400 | -2.34565100 | H | -3.90656000 | 2.80437700 | -2.19300200 |
| H | 2.54691300 | -1.65356000 | -4.82911200 | H | -3.95882600 | 5.02282200 | -1.08074900 |
| H | 4.45204200 | -0.07521700 | -4.59743100 | C | 2.91897800 | -0.10994700 | 1.72564800 |
| C | -3.10824500 | 1.53118800 | 0.45813900 | C | 4.21927400 | 0.34167700 | 1.32352000 |
| C | -4.49628600 | 1.31176600 | 0.18661500 | C | 4.83397700 | 1.41275900 | 1.98125500 |
| C | -5.39104800 | 2.38664800 | 0.13361300 | N | 5.36030600 | 2.30778600 | 2.52556600 |
| N | -6.15237300 | 3.27649700 | 0.08471900 | H | 2.40220300 | 0.43408400 | 2.51410700 |
| H | -2.77326600 | 2.55923100 | 0.60324600 | C | 6.04725000 | 0.20612600 | -0.38955500 |
| C | -6.31278700 | -0.36259000 | -0.26417200 | C | 6.60438300 | -0.37323300 | -1.51721600 |
| C | -6.73072300 | -1.67169800 | -0.43555700 | C | 5.97401400 | -1.45415900 | -2.14499100 |
| C | -5.81338800 | -2.72722900 | -0.36297100 | C | 4.78240100 | -1.93268000 | -1.61086900 |
| C | -4.47671000 | -2.42937700 | -0.12613600 | C | 4.20585800 | -1.36663300 | -0.47100700 |
| C | -4.03233100 | -1.11598800 | 0.04468500 | C | 4.83604300 | -0.26781600 | 0.16760400 |
| C | -4.95662800 | -0.04289100 | -0.01656300 | H | 6.54174900 | 1.05359400 | 0.08031100 |
| H | -7.03874600 | 0.44581300 | -0.32058100 | H | 7.53631300 | 0.02022300 | -1.91539600 |
| H | -7.78162800 | -1.87652600 | -0.62422500 | H | 6.40754800 | -1.91148000 | -3.02912100 |
| H | -6.13874900 | -3.75512200 | -0.49064200 | H | 4.27083500 | -2.76784100 | -2.08494400 |
| H | -3.74143900 | -3.23107100 | -0.07510100 | H | 3.11404400 | -3.00515600 | 0.40101500 |
| R-TS3 | | | | S-TS3 | | | |
| G(M062X/6-31G(d)): -1745.56300 | | | | G(M062X/6-31G(d)): -1745.56659 | | | |
| Number of Imaginary frequency: -224.58 | | | | Number of Imaginary frequency: -246.06 | | | |
| -1 | | | | -1 | | | |
| C | -0.17415100 | 0.70189000 | -1.08668300 | C | 0.09256000 | -1.04036300 | -0.06481400 |
| C | -0.64822800 | 0.27826600 | 0.31912000 | C | 0.84576000 | -1.52003700 | 1.18281300 |
| C | -2.14459900 | 0.12777900 | 0.38469800 | C | 2.28311800 | -1.10171400 | 1.03024000 |
| C | -2.73052200 | -0.95316100 | -0.26992800 | C | 3.13556600 | -1.95517000 | 0.32310700 |
| C | -0.74478600 | -0.09013400 | -2.30776000 | C | 0.87223500 | -1.32126900 | -1.40410000 |
| H | -0.34519500 | 1.07500000 | 1.01228400 | H | 0.77228000 | -2.61782300 | 1.21898500 |
| H | 0.92471100 | 0.61685200 | -1.10463600 | H | -0.09333800 | 0.03801100 | 0.05788900 |
| H | -0.38056300 | 0.54806700 | -3.16380500 | H | 0.04844500 | -1.55889100 | -2.12041200 |
| H | -2.12995700 | -1.81143300 | -0.54246800 | O | 1.79148800 | -2.31559300 | -1.36369700 |
| O | -2.07871100 | -0.29031900 | -2.32031100 | C | 1.48308000 | -0.01644100 | -1.95435600 |
| C | 0.00902400 | -1.42392300 | -2.51315100 | H | 2.29907100 | 0.33386400 | -1.30871600 |
| H | -0.11267500 | -2.08757200 | -1.64567200 | H | 1.91606500 | -0.23782300 | -2.93875900 |
| H | -0.46180300 | -1.91328300 | -3.37423700 | O | 0.36932600 | -0.96546600 | 2.40329400 |
| O | -0.03332300 | -0.94656900 | 0.72176100 | O | -1.17537600 | -1.70490800 | -0.07470600 |
| O | -0.53898600 | 2.07847100 | -1.23618100 | O | 0.49485000 | 1.00035600 | -2.11217500 |
| O | 1.39240800 | -1.25921100 | -2.82151000 | C | -2.15289300 | -0.98866100 | -0.78724000 |
| C | 0.56251700 | 2.96714400 | -1.23149000 | H | -2.33842300 | -0.01404500 | -0.30565400 |
| H | 1.30398200 | 2.65991800 | -1.98527400 | H | -1.80685000 | -0.77176400 | -1.81014500 |
| H | 0.15890600 | 3.94103300 | -1.52908200 | C | -0.94763400 | -1.29508500 | 2.79327600 |
| C | 1.14755000 | -0.73155100 | 1.46226400 | H | -1.24498500 | -2.27091900 | 2.39041200 |
| H | 1.85734200 | -0.11144300 | 0.88991600 | H | -0.92620000 | -1.37896300 | 3.88800300 |
| H | 0.91742500 | -0.17734200 | 2.38691500 | C | 0.71811200 | 2.15399800 | -1.34202400 |
| C | 2.28523600 | -1.54359300 | -1.77423900 | H | 1.04081500 | 1.88216500 | -0.32335100 |
| H | 1.75614300 | -1.55958500 | -0.81441800 | H | 1.52929400 | 2.76277100 | -1.77448700 |
| H | 2.72059100 | -2.54758400 | -1.90956500 | C | -1.96520600 | -0.24702200 | 2.39602400 |
| C | 1.80638800 | -2.04482100 | 1.80008400 | C | -3.31712700 | -0.58235800 | 2.30274600 |
| C | 2.98843200 | -2.03111900 | 2.54914900 | C | -1.57398200 | 1.06706200 | 2.13157000 |
| C | 1.29210400 | -3.26527400 | 1.36271800 | C | -4.26173200 | 0.37253000 | 1.93128500 |
| C | 3.64757300 | -3.21828600 | 2.85221600 | H | -3.62940200 | -1.60643100 | 2.49857500 |
| H | 3.39336600 | -1.07896300 | 2.88853200 | C | -2.51485900 | 2.02356000 | 1.75376400 |
| C | 1.95343400 | -4.45646400 | 1.66663000 | H | -0.52228100 | 1.33165500 | 2.20126600 |
| H | 0.37555300 | -3.27728900 | 0.78105700 | C | -3.86175700 | 1.67820200 | 1.64601900 |
| C | 3.13128100 | -4.43739300 | 2.40855500 | H | -5.30801800 | 0.09141900 | 1.84508800 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | 4.56510300 | -3.19432700 | 3.43305100 | H | -2.19429000 | 3.03880400 | 1.53240700 |
| H | 1.54599300 | -5.40105100 | 1.31747700 | H | -4.59258100 | 2.42147300 | 1.33869700 |
| H | 3.64660800 | -5.36458600 | 2.64134800 | C | -3.43893500 | -1.77309900 | -0.84902700 |
| C | 1.23067200 | 3.07164700 | 0.12344100 | C | -3.51530500 | -3.10183300 | -0.43192100 |
| C | 0.54657400 | 3.66058700 | 1.19329700 | C | -4.59012300 | -1.14710900 | -1.33824400 |
| C | 2.49632900 | 2.52982600 | 0.34824300 | C | -4.72569100 | -3.79400700 | -0.50253400 |
| C | 1.11534300 | 3.70060100 | 2.46254900 | H | -2.62432700 | -3.58714300 | -0.04677300 |
| H | -0.44156700 | 4.08446800 | 1.02535800 | C | -5.79594800 | -1.83654600 | -1.41243100 |
| C | 3.07182300 | 2.56704100 | 1.62000600 | H | -4.53736100 | -0.10563800 | -1.65177400 |
| H | 3.03298600 | 2.06640800 | -0.47755200 | C | -5.86762400 | -3.16651600 | -0.99314000 |
| C | 2.38075300 | 3.14911900 | 2.67949000 | H | -4.77342300 | -4.82797600 | -0.17195400 |
| H | 0.57643600 | 4.16283400 | 3.28469700 | H | -6.68249300 | -1.33692900 | -1.79290100 |
| H | 4.05691600 | 2.13523700 | 1.77824200 | H | -6.80886900 | -3.70581500 | -1.04663900 |
| H | 2.82440100 | 3.17948200 | 3.67052200 | C | -0.54525200 | 2.97675000 | -1.24668500 |
| C | 3.39767400 | -0.52280400 | -1.70361100 | C | -0.50605200 | 4.21591300 | -0.59812000 |
| C | 4.30148900 | -0.57728100 | -0.63692100 | C | -1.75732200 | 2.52197100 | -1.76648000 |
| C | 3.54808400 | 0.47219000 | -2.67065300 | C | -1.65894100 | 4.98428000 | -0.46695900 |
| C | 5.33833200 | 0.34623700 | -0.53748400 | H | 0.43747800 | 4.57854000 | -0.19467800 |
| H | 4.18680000 | -1.35163500 | 0.12026000 | C | -2.91532500 | 3.29058400 | -1.63280900 |
| C | 4.59214200 | 1.39498400 | -2.57566100 | H | -1.78613200 | 1.56512700 | -2.27734900 |
| H | 2.83980200 | 0.51992400 | -3.49191900 | C | -2.87164600 | 4.52103100 | -0.98243600 |
| C | 5.48806100 | 1.33687300 | -1.51049600 | H | -1.61270300 | 5.94528600 | 0.03772400 |
| H | 6.03037200 | 0.29447200 | 0.29859700 | H | -3.85382900 | 2.92452300 | -2.04051200 |
| H | 4.70104800 | 2.16411100 | -3.33533900 | H | -3.77300200 | 5.11857000 | -0.88036000 |
| H | 6.29612100 | 2.05859500 | -1.43489400 | C | 2.67871100 | 0.19901300 | 1.32341800 |
| C | -2.94619700 | 1.13122000 | 0.91532100 | C | 3.93523200 | 0.67997600 | 0.94938000 |
| C | -4.34024900 | 1.05703500 | 0.85458200 | C | 4.30277100 | 2.01715000 | 1.27523100 |
| C | -5.12768800 | 2.09461500 | 1.43283700 | N | 4.60492800 | 3.10970200 | 1.53222100 |
| N | -5.77678900 | 2.93686100 | 1.90144800 | H | 1.99286400 | 0.85676500 | 1.85203000 |
| H | -2.48107500 | 1.99346800 | 1.38778800 | C | 6.13472400 | 0.26337800 | -0.17660700 |
| C | -6.38694300 | -0.21500200 | 0.16265700 | C | 6.98134400 | -0.59739300 | -0.83373900 |
| C | -6.94142500 | -1.32597300 | -0.42510500 | C | 6.58639700 | -1.92713200 | -1.10985400 |
| C | -6.12024200 | -2.34403800 | -0.96744200 | C | 5.34037000 | -2.35992500 | -0.72277000 |
| C | -4.75414800 | -2.21876400 | -0.90657600 | C | 4.44029800 | -1.49629400 | -0.05075600 |
| C | -4.14881300 | -1.08642200 | -0.30458300 | C | 4.84426800 | -0.16169500 | 0.23367200 |
| C | -4.97650800 | -0.06378000 | 0.23851200 | H | 6.44766100 | 1.28276700 | 0.03561000 |
| H | -7.02622800 | 0.56122700 | 0.57593200 | H | 7.96438900 | -0.25408800 | -1.14314300 |
| H | -8.02203700 | -1.42526100 | -0.47514800 | H | 7.26657400 | -2.59743000 | -1.62646400 |
| H | -6.57425500 | -3.21515300 | -1.42966100 | H | 5.01659700 | -3.37622700 | -0.93511400 |
| H | -4.10670600 | -2.98523700 | -1.32602200 | H | 2.95301800 | -3.02122500 | 0.31220900 |
| R-7 G(M062X/6-31G(d)): -1745.57297 Number of Imaginary frequency: 0 | | | | S-7 G(M062X/6-31G(d)): -1745.57524 Number of Imaginary frequency: 0 | | | |
| C | -0.12134600 | -1.31388100 | 0.54631400 | C | -0.09963400 | -1.00014000 | -0.36350100 |
| C | -0.78833900 | -0.25451600 | -0.36540300 | C | 0.73381400 | -1.51108400 | 0.81794500 |
| C | -2.28401700 | -0.08576400 | -0.20861900 | C | 2.19070300 | -1.11481800 | 0.70011200 |
| C | -2.88014900 | 1.14469300 | -0.17235600 | C | 3.14587800 | -1.98070200 | 0.22036100 |
| C | -0.66247300 | -1.40966100 | 1.99902100 | C | 0.48987100 | -1.49573300 | -1.73157500 |
| H | -0.62794800 | -0.61123800 | -1.39486700 | H | 0.65009800 | -2.60502000 | 0.80401100 |
| H | 0.95415800 | -1.07816000 | 0.56287900 | H | -0.17358500 | 0.09913000 | -0.30421700 |
| H | -0.05328800 | -2.27707200 | 2.40946200 | H | -0.42687900 | -1.49558800 | -2.39528500 |
| H | -2.26790700 | 2.04144300 | -0.17314100 | O | 1.13040300 | -2.66719000 | -1.67069200 |
| O | -1.98765300 | -1.54533000 | 2.08402400 | C | 1.35250400 | -0.37997400 | -2.37580200 |
| C | -0.18567400 | -0.20045400 | 2.84146400 | H | 2.26031900 | -0.18478700 | -1.78908100 |
| H | -0.49885800 | 0.74454600 | 2.37123000 | H | 1.67444100 | -0.74529300 | -3.35987400 |
| H | -0.70712800 | -0.28268000 | 3.80190700 | O | 0.33891800 | -0.99960100 | 2.09196700 |
| O | -0.16515000 | 1.01436700 | -0.23110200 | O | -1.41411500 | -1.54257700 | -0.17875600 |
| O | -0.29371400 | -2.58739900 | -0.09133000 | O | 0.61651200 | 0.82981500 | -2.57341900 |
| O | 1.20986900 | -0.17681600 | 3.14015600 | C | -2.41957200 | -0.77841100 | -0.79097200 |
| C | 0.92575000 | -3.20669700 | -0.45104200 | H | -2.51839400 | 0.20087200 | -0.29375000 |
| H | 1.58797300 | -3.28852400 | 0.42461600 | H | -2.16376800 | -0.57437600 | -1.84233500 |
| H | 0.66263300 | -4.22132100 | -0.76995700 | C | -0.94444600 | -1.32374700 | 2.57939600 |
| C | 0.94864400 | 1.16868600 | -1.08629300 | H | -1.31480300 | -2.25650900 | 2.14043900 |
| H | 1.66684000 | 0.34499100 | -0.94224900 | H | -0.82569300 | -1.48654800 | 3.65952300 |
| H | 0.62000000 | 1.12859100 | -2.13693600 | C | 1.02900400 | 1.91717700 | -1.78745600 |
| C | 2.01507200 | 0.60264500 | 2.29213300 | H | 1.45954700 | 1.56920400 | -0.83733500 |
| H | 1.45552100 | 0.90613700 | 1.40077300 | H | 1.82216500 | 2.48808600 | -2.29843500 |
| H | 2.31390100 | 1.52983500 | 2.80870800 | C | -1.94946900 | -0.21375500 | 2.35644300 |
| C | 1.64432500 | 2.47781400 | -0.80972300 | C | -3.31837400 | -0.47852100 | 2.43305100 |

| | | | | | | | |
|----------------------------------|-------------|-------------|-------------|----------------------------------|-------------|-------------|-------------|
| C | 2.79212500 | 2.79663500 | -1.54389000 | C | -1.52710700 | 1.09044800 | 2.09227100 |
| C | 1.20009600 | 3.35971000 | 0.17531400 | C | -4.25053300 | 0.53739400 | 2.22973600 |
| C | 3.48619900 | 3.97624500 | -1.29382400 | H | -3.65806700 | -1.49374300 | 2.62991600 |
| H | 3.14661100 | 2.10611900 | -2.30749000 | C | -2.45683500 | 2.10933600 | 1.88772300 |
| C | 1.89810900 | 4.54179000 | 0.42832200 | H | -0.46335300 | 1.30132000 | 2.02862500 |
| H | 0.31411600 | 3.11210200 | 0.75188700 | C | -3.82263400 | 1.83530200 | 1.94882700 |
| C | 3.04139000 | 4.85300700 | -0.30236100 | H | -5.31261900 | 0.31101200 | 2.27325500 |
| H | 4.37731600 | 4.21148800 | -1.86866700 | H | -2.11205200 | 3.11775000 | 1.67433600 |
| H | 1.54498400 | 5.21868200 | 1.20115000 | H | -4.54814800 | 2.62629000 | 1.78044900 |
| H | 3.58476200 | 5.77188800 | -0.10268900 | C | -3.73781100 | -1.50819500 | -0.73686900 |
| C | 1.64875800 | -2.47339300 | -1.56320900 | C | -3.81653900 | -2.86208900 | -0.41103700 |
| C | 0.98311900 | -2.20399600 | -2.76425300 | C | -4.91389100 | -0.81097800 | -1.03267000 |
| C | 2.95628900 | -2.01718200 | -1.39781200 | C | -5.05325500 | -3.50875100 | -0.38081900 |
| C | 1.61110300 | -1.48545100 | -3.77728700 | H | -2.90484900 | -3.40261000 | -0.17770900 |
| H | -0.03929900 | -2.55239800 | -2.89475800 | C | -6.14656300 | -1.45507600 | -1.00718000 |
| C | 3.59251200 | -1.29936900 | -2.41280000 | H | -4.85780100 | 0.24927400 | -1.27433900 |
| H | 3.47730300 | -2.21513000 | -0.46326600 | C | -6.22050200 | -2.81016900 | -0.67879800 |
| C | 2.91906700 | -1.02761600 | -3.60174400 | H | -5.10197600 | -4.56305200 | -0.12232100 |
| H | 1.08284200 | -1.27988400 | -4.70407600 | H | -7.05164500 | -0.90008100 | -1.23747000 |
| H | 4.61025200 | -0.94645500 | -2.26842500 | H | -7.18207700 | -3.31458300 | -0.65300000 |
| H | 3.41002800 | -0.46587100 | -4.39134900 | C | -0.13256800 | 2.83276300 | -1.47428000 |
| C | 3.26064100 | -0.14662400 | 1.86957500 | C | 0.09637300 | 3.99182600 | -0.72474700 |
| C | 4.19206000 | 0.48080900 | 1.03468600 | C | -1.43013200 | 2.54435600 | -1.89651000 |
| C | 3.50786000 | -1.44980400 | 2.30266200 | C | -0.95204000 | 4.85100700 | -0.40917600 |
| C | 5.35379300 | -0.18166700 | 0.64640500 | H | 1.10694900 | 4.21979900 | -0.38976900 |
| H | 4.00676500 | 1.49974000 | 0.69702500 | C | -2.48459400 | 3.40178300 | -1.57440900 |
| C | 4.67624000 | -2.11201100 | 1.92084200 | H | -1.60565100 | 1.64617500 | -2.47948600 |
| H | 2.78055900 | -1.93390800 | 2.94661000 | C | -2.24969900 | 4.55764700 | -0.83461800 |
| C | 5.60211200 | -1.48163300 | 1.09234700 | H | -0.75801300 | 5.74966200 | 0.16982500 |
| H | 6.06927000 | 0.31735000 | -0.00168600 | H | -3.49183100 | 3.16335000 | -1.90621500 |
| H | 4.86058600 | -3.12404600 | 2.27114700 | H | -3.07012500 | 5.22491600 | -0.58632200 |
| H | 6.51082200 | -1.99716900 | 0.79520000 | C | 2.57671000 | 0.19101100 | 1.07433200 |
| C | -3.09856900 | -1.25558300 | -0.22372200 | C | 3.88573900 | 0.61048400 | 0.93282000 |
| C | -4.46803200 | -1.14471400 | -0.21245400 | C | 4.22310100 | 1.96020400 | 1.28593800 |
| C | -5.26240100 | -2.33759200 | -0.24443800 | N | 4.49555200 | 3.05244300 | 1.56172900 |
| N | -5.91763000 | -3.29384300 | -0.27491700 | H | 1.83450000 | 0.87838900 | 1.46949900 |
| H | -2.62364100 | -2.22756600 | -0.26649000 | C | 6.25771700 | 0.11540900 | 0.29051700 |
| C | -6.53104900 | 0.28181600 | -0.10769100 | C | 7.18248200 | -0.78335600 | -0.18037900 |
| C | -7.10022600 | 1.53522000 | -0.05043800 | C | 6.79600600 | -2.10235500 | -0.52504500 |
| C | -6.28581500 | 2.68754500 | -0.03083700 | C | 5.48812700 | -2.49367900 | -0.39225600 |
| C | -4.91518100 | 2.56389800 | -0.06865600 | C | 4.50422500 | -1.58915800 | 0.09184200 |
| C | -4.30216900 | 1.28885300 | -0.12491900 | C | 4.90002300 | -0.26756500 | 0.43992700 |
| C | -5.12629600 | 0.13447000 | -0.14649700 | H | 6.55806700 | 1.12590800 | 0.55507300 |
| H | -7.15960800 | -0.60495500 | -0.12207800 | H | 8.22010500 | -0.48282000 | -0.29062700 |
| H | -8.18080300 | 1.63767300 | -0.01914400 | H | 7.54036000 | -2.79967700 | -0.89700200 |
| H | -6.74386100 | 3.67102400 | 0.01579700 | H | 5.17885700 | -3.50134500 | -0.65738100 |
| H | -4.27948000 | 3.44572100 | -0.05358900 | H | 2.83685400 | -2.96312400 | -0.11676700 |
| 3a from R | | | | 3a from S | | | |
| G(M062X/6-31G(d)): -1746.09309 | | | | G(M062X/6-31G(d)): -1746.08729 | | | |
| Number of Imaginary frequency: 0 | | | | Number of Imaginary frequency: 0 | | | |
| C | 0.26317700 | -0.89538300 | 1.34865200 | C | -0.20226800 | -1.23270300 | 0.66737000 |
| C | -0.27561400 | -0.42985700 | -0.01805800 | C | -0.76992000 | -0.28078800 | -0.42395100 |
| C | -1.78082100 | -0.54679800 | -0.21236600 | C | -2.25846500 | -0.00362300 | -0.34404700 |
| C | -2.55252800 | 0.56541800 | -0.45744200 | C | -3.15898000 | -1.02238100 | -0.57163000 |
| C | -0.29830900 | -0.19954700 | 2.59406100 | C | -0.70371600 | -1.09513300 | 2.11212400 |
| H | 0.21117600 | -1.08638000 | -0.75408800 | H | -0.59147500 | -0.80671000 | -1.37109100 |
| H | 1.34213300 | -0.69848200 | 1.31393400 | H | 0.88238800 | -1.04582800 | 0.69077700 |
| H | 0.20279000 | -0.66160800 | 3.45368300 | H | -0.18005300 | -1.87583500 | 2.67801200 |
| H | -2.08480900 | 1.54603500 | -0.49839600 | O | -2.08009800 | -1.38972200 | 2.26085500 |
| O | -1.67931100 | -0.44226200 | 2.78915200 | C | -0.35915700 | 0.23757400 | 2.78630800 |
| C | -0.02890800 | 1.30077000 | 2.63021000 | H | -0.64432600 | 1.09421700 | 2.15799600 |
| H | -0.58911000 | 1.79000600 | 1.82294400 | H | -0.94356900 | 0.28882200 | 3.71095700 |
| H | -0.39144200 | 1.69976200 | 3.59029500 | O | -0.06873400 | 0.95076900 | -0.44460200 |
| O | 0.14161500 | 0.90473000 | -0.21354100 | O | -0.44780200 | -2.56909100 | 0.24539900 |
| O | 0.02844700 | -2.29294000 | 1.45261700 | O | 1.00496500 | 0.30050500 | 3.15423800 |
| O | 1.35835800 | 1.52441000 | 2.50077300 | C | 0.73924200 | -3.32097300 | 0.02714500 |
| C | 1.14071900 | -3.01594400 | 1.94885400 | H | 1.35816300 | -3.32530500 | 0.93649100 |
| H | 1.52873100 | -2.55405300 | 2.86770700 | H | 0.40204400 | -4.34509600 | -0.16055200 |
| H | 0.75200800 | -4.00414300 | 2.21795200 | C | 1.07438400 | 0.89195800 | -1.28125900 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 0.61690300 | 1.16982300 | -1.52057400 | H | 1.73242000 | 0.06418500 | -0.97354400 |
| H | -0.06415100 | 0.75070400 | -2.27525600 | H | 0.75851700 | 0.68563300 | -2.31531400 |
| H | 0.59562800 | 2.26074100 | -1.62436200 | C | 1.87238300 | 0.95447500 | 2.25053900 |
| C | 1.71093100 | 2.89940800 | 2.55091600 | H | 1.35547700 | 1.16688200 | 1.30844900 |
| H | 1.19811100 | 3.37757400 | 3.39877000 | H | 2.17316500 | 1.92363300 | 2.67624600 |
| H | 2.78734800 | 2.92027700 | 2.74535700 | C | 1.85349400 | 2.17957500 | -1.22677100 |
| C | 2.02227800 | 0.64909500 | -1.73085900 | C | 3.03380200 | 2.25952500 | -1.97379400 |
| C | 2.45896100 | 0.27401600 | -3.00226500 | C | 1.46641700 | 3.26623600 | -0.44389900 |
| C | 2.90876200 | 0.57048600 | -0.65131300 | C | 3.81972600 | 3.40597200 | -1.93432100 |
| C | 3.77068400 | -0.15607200 | -3.20108500 | H | 3.33824300 | 1.40759100 | -2.57958900 |
| H | 1.76858000 | 0.31965300 | -3.84181700 | C | 2.25830300 | 4.41633200 | -0.40081700 |
| C | 4.21611500 | 0.13106400 | -0.84807500 | H | 0.55199500 | 3.21055600 | 0.13938900 |
| H | 2.56238600 | 0.86459300 | 0.33760500 | C | 3.43438600 | 4.48950100 | -1.14171500 |
| C | 4.65199000 | -0.22781500 | -2.12408500 | H | 4.73537500 | 3.45390500 | -2.51654400 |
| H | 4.09973200 | -0.44500400 | -4.19518900 | H | 1.95146100 | 5.25644600 | 0.21561600 |
| H | 4.89699100 | 0.06631100 | -0.00345500 | H | 4.04828200 | 5.38450900 | -1.10608600 |
| H | 5.67117200 | -0.57257800 | -2.27484600 | C | 1.54995500 | -2.79956300 | -1.14022400 |
| C | 2.25430800 | -3.15315300 | 0.93084400 | C | 0.95816000 | -2.68383700 | -2.40303600 |
| C | 1.95382600 | -3.29152600 | -0.42754100 | C | 2.86960700 | -2.38123100 | -0.96897300 |
| C | 3.58983400 | -3.17811300 | 1.33580200 | C | 1.67210300 | -2.15072400 | -3.47194400 |
| C | 2.97154100 | -3.45560900 | -1.36382700 | H | -0.07221200 | -3.00529100 | -2.54108200 |
| H | 0.91491800 | -3.27626700 | -0.74693800 | C | 3.59139700 | -1.84997800 | -2.03931400 |
| C | 4.61036300 | -3.35931900 | 0.40217600 | H | 3.33296300 | -2.46300200 | 0.01179700 |
| H | 3.83167100 | -3.05760700 | 2.38956300 | C | 2.99127500 | -1.72873300 | -3.29097600 |
| C | 4.30309600 | -3.49740000 | -0.95008800 | H | 1.20224100 | -2.06099000 | -4.44719300 |
| H | 2.72602000 | -3.55454900 | -2.41764300 | H | 4.61675100 | -1.52240300 | -1.88932200 |
| H | 5.64553500 | -3.38050100 | 0.73091800 | H | 3.54732300 | -1.30938300 | -4.12475500 |
| H | 5.09641800 | -3.62711000 | -1.68061100 | C | 3.10658600 | 0.12680900 | 1.97115500 |
| C | 1.40940500 | 3.64928600 | 1.27209900 | C | 4.06588600 | 0.62555300 | 1.08254800 |
| C | 2.39280700 | 3.78434400 | 0.28783900 | C | 3.32160200 | -1.11005700 | 2.58047000 |
| C | 0.15431600 | 4.22616900 | 1.05233300 | C | 5.21896300 | -0.10226800 | 0.80465200 |
| C | 2.12851400 | 4.47096100 | -0.89605000 | H | 3.90825700 | 1.59606800 | 0.61507300 |
| H | 3.37808500 | 3.35574600 | 0.45666400 | C | 4.48614500 | -1.83345000 | 2.31361200 |
| C | -0.11950700 | 4.90458300 | -0.13394300 | H | 2.57933900 | -1.49623800 | 3.27193500 |
| H | -0.60862700 | 4.15662000 | 1.82480400 | C | 5.43556100 | -1.33529200 | 1.42410300 |
| C | 0.86890600 | 5.02978000 | -1.11060400 | H | 5.95248900 | 0.29530200 | 0.10853600 |
| H | 2.90564800 | 4.57334100 | -1.64827100 | H | 4.64725600 | -2.79130600 | 2.80071600 |
| H | -1.09840700 | 5.34918700 | -0.28943400 | H | 6.33865200 | -1.90062700 | 1.21315400 |
| H | 0.66037800 | 5.56835900 | -2.03060000 | C | -2.74074400 | 1.28991200 | -0.04554800 |
| C | -2.40326200 | -1.82193500 | -0.17383100 | C | -4.09971500 | 1.52518000 | 0.02947700 |
| C | -3.76058500 | -1.93932700 | -0.36959600 | C | -4.55768200 | 2.85380100 | 0.32940600 |
| C | -4.35996300 | -3.24503700 | -0.31937800 | N | -4.93591600 | 3.92142500 | 0.57093100 |
| N | -4.85275500 | -4.29226200 | -0.27893100 | H | -2.03969500 | 2.10194000 | 0.11342500 |
| H | -1.80410600 | -2.70521000 | 0.01997700 | C | -6.45805000 | 0.69590800 | -0.11788200 |
| C | -5.98570400 | -0.89069400 | -0.84587800 | C | -7.32205100 | -0.34570000 | -0.34316500 |
| C | -6.71960200 | 0.24270800 | -1.09877400 | C | -6.83057400 | -1.63958600 | -0.65042000 |
| C | -6.09319100 | 1.51120200 | -1.14392000 | C | -5.48090800 | -1.86559400 | -0.72653900 |
| C | -4.74131500 | 1.62226800 | -0.93367400 | C | -4.55718500 | -0.80867200 | -0.49824800 |
| C | -3.95528700 | 0.47014000 | -0.66975100 | C | -5.05625900 | 0.48791300 | -0.18966200 |
| C | -4.58887800 | -0.80014000 | -0.62786300 | H | -6.83820300 | 1.68641200 | 0.11720500 |
| H | -6.46880900 | -1.86354100 | -0.81242200 | H | -8.39346300 | -0.17991300 | -0.28642400 |
| H | -7.78949200 | 0.16697700 | -1.26702500 | H | -7.53146700 | -2.44998500 | -0.82466900 |
| H | -6.68792900 | 2.39610500 | -1.34852000 | H | -5.09142300 | -2.85272600 | -0.96061400 |
| H | -4.24891500 | 2.59055000 | -0.96713900 | H | -2.79345200 | -2.02220500 | -0.79630900 |
| H | -2.16703700 | 0.02171700 | 2.08868100 | H | -2.59089300 | -0.64854400 | 1.89903000 |
| R-TS4 | | | | S-TS4 | | | |
| G(M062X/6-31G(d)): -1745.90467 | | | | G(M062X/6-31G(d)): -1745.90794 | | | |
| Number of Imaginary frequency: -130.76 | | | | Number of Imaginary frequency: -162.21 | | | |
| O 1 | | | | O 1 | | | |
| C | 0.04346500 | 0.80088900 | -1.05527100 | C | -1.05807100 | 0.00909800 | -0.00968000 |
| C | 0.16310900 | -0.13414500 | 0.14878000 | C | 0.03506000 | 0.41174100 | -0.99231000 |
| C | -0.85833800 | -1.24024800 | 0.03270000 | C | 0.56881600 | 1.77672000 | -0.62826100 |
| C | -1.17803600 | -1.66824900 | -1.23152300 | C | 0.57242700 | 2.11858500 | 0.70177800 |
| C | 0.13047300 | 0.02541600 | -2.35975700 | C | -0.59168300 | 0.12867900 | 1.44156900 |
| H | 0.00414400 | 0.42990700 | 1.07630000 | H | -0.38386800 | 0.43427100 | -2.00873700 |
| H | 0.86429300 | 1.52647500 | -1.03478500 | H | -1.34836200 | -1.02631900 | -0.21522500 |
| H | -0.27557800 | 0.67109100 | -3.14441200 | H | -1.47840000 | 0.12998200 | 2.08423500 |
| H | -1.76398200 | -2.55636000 | -1.43991900 | H | 0.86897000 | 3.09682000 | 1.06399100 |
| O | -0.70579200 | -1.15147300 | -2.36783400 | O | 0.03021300 | 1.40851400 | 1.68973000 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 1.52961800 | -0.44007300 | -2.78221300 | C | 0.35655500 | -0.94906600 | 1.98794100 |
| H | 1.91564300 | -1.17140800 | -2.06735600 | H | 1.23778800 | -1.06135700 | 1.34816800 |
| H | 1.42559200 | -0.92983100 | -3.75735300 | H | 0.68013400 | -0.60830000 | 2.97651700 |
| O | 1.49292100 | -0.63998300 | 0.13324500 | O | 1.01659200 | -0.61017300 | -0.89252500 |
| O | -1.20087300 | 1.47427800 | -1.06846400 | O | -2.15314200 | 0.87600600 | -0.23544500 |
| O | 2.40860200 | 0.65477200 | -2.93752700 | O | -0.29818800 | -2.18214800 | 2.19455800 |
| C | -1.31484500 | 2.55169700 | -0.14556000 | C | -3.39800900 | 0.26544600 | 0.04109400 |
| H | -0.33571900 | 3.03074100 | -0.00108000 | H | -3.53525600 | -0.61439300 | -0.60857600 |
| H | -1.97840900 | 3.27802600 | -0.62742700 | H | -3.42826900 | -0.09901800 | 1.07910800 |
| C | 1.89218400 | -1.21138900 | 1.36785700 | C | 2.09214700 | -0.51420200 | -1.81712800 |
| H | 1.93683600 | -0.43589400 | 2.14729300 | H | 1.70368100 | -0.60713400 | -2.84219900 |
| H | 1.15744100 | -1.96599300 | 1.68638400 | H | 2.59678800 | 0.45525200 | -1.72240700 |
| C | 3.45366600 | 0.79147900 | -1.97955900 | C | -0.37529900 | -3.05478400 | 1.07905900 |
| H | 3.56024100 | -0.12418000 | -1.38642300 | H | 0.23254100 | -2.67796600 | 0.24615700 |
| H | 4.38093500 | 0.93528700 | -2.54845100 | H | 0.05260100 | -4.01841800 | 1.38617400 |
| C | 3.23918000 | -1.85659100 | 1.17699500 | C | 3.05591000 | -1.62158700 | -1.48633500 |
| C | 4.32206500 | -1.52448900 | 1.99126400 | C | 2.73303600 | -2.95075100 | -1.77561800 |
| C | 3.41110300 | -2.80764700 | 0.16504500 | C | 4.24820700 | -1.33739500 | -0.81966000 |
| C | 5.56165100 | -2.13736400 | 1.80360700 | C | 3.59302000 | -3.98049600 | -1.40323900 |
| H | 4.19426200 | -0.78038900 | 2.77412300 | H | 1.80376400 | -3.17439400 | -2.29531700 |
| C | 4.64821200 | -3.41507800 | -0.02806600 | C | 5.11224000 | -2.36618600 | -0.44674600 |
| H | 2.56563000 | -3.07006400 | -0.46699600 | H | 4.49894200 | -0.30275700 | -0.59522000 |
| C | 5.72687900 | -3.08087800 | 0.79300700 | C | 4.78421300 | -3.68892300 | -0.73672500 |
| H | 6.39826800 | -1.87133400 | 2.44296400 | H | 3.33744800 | -5.01064400 | -1.63386300 |
| H | 4.77232700 | -4.15324600 | -0.81495900 | H | 6.03728000 | -2.13294900 | 0.07323900 |
| H | 6.69210400 | -3.55576700 | 0.64371900 | H | 5.45422900 | -4.49293500 | -0.44627700 |
| C | -1.89873300 | 2.13768100 | 1.18782000 | C | -4.51859800 | 1.24981800 | -0.17835400 |
| C | -1.19903600 | 2.33958300 | 2.37902500 | C | -5.83789300 | 0.79684900 | -0.07748700 |
| C | -3.15444000 | 1.52516100 | 1.23129800 | C | -4.27826000 | 2.59292700 | -0.46457300 |
| C | -1.73722600 | 1.92401600 | 3.59698400 | C | -6.90169400 | 1.67486100 | -0.25629600 |
| H | -0.21874900 | 2.81186200 | 2.34772500 | H | -6.02689500 | -0.25251300 | 0.14177800 |
| C | -3.69108700 | 1.10121600 | 2.44443700 | C | -5.34594400 | 3.47311800 | -0.64659500 |
| H | -3.70806700 | 1.37557400 | 0.30723400 | H | -3.25542100 | 2.94598600 | -0.54514100 |
| C | -2.98256100 | 1.29879200 | 3.63050000 | C | -6.65801400 | 3.01926900 | -0.54234600 |
| H | -1.18260400 | 2.08406700 | 4.51713000 | H | -7.92183400 | 1.31070000 | -0.17536800 |
| H | -4.66410400 | 0.61720500 | 2.46412400 | H | -5.14773800 | 4.51753700 | -0.87031500 |
| H | -3.40062700 | 0.96751800 | 4.57666900 | H | -7.48674200 | 3.70664600 | -0.68420600 |
| C | 3.22913400 | 1.97350300 | -1.06320600 | C | -1.80553000 | -3.26034700 | 0.62551800 |
| C | 3.37717600 | 1.84787600 | 0.31825100 | C | -2.06669700 | -3.70198300 | -0.67499600 |
| C | 2.83124400 | 3.20346500 | -1.59612900 | C | -2.87470200 | -3.01398800 | 1.48805400 |
| C | 3.11890100 | 2.92949000 | 1.16020900 | C | -3.37701800 | -3.89035700 | -1.10812300 |
| H | 3.68240100 | 0.89127900 | 0.73528200 | H | -1.23674100 | -3.88547800 | -1.35482200 |
| C | 2.56941900 | 4.28504200 | -0.75888600 | C | -4.18745400 | -3.20288300 | 1.05595700 |
| H | 2.70389200 | 3.30160500 | -2.67139000 | H | -2.67330000 | -2.65888200 | 2.49424300 |
| C | 2.70782700 | 4.14880800 | 0.62393800 | C | -4.44288600 | -3.63868900 | -0.24299300 |
| H | 3.23096200 | 2.81640000 | 2.23519600 | H | -3.56734500 | -4.22506500 | -2.12391800 |
| H | 2.25290000 | 5.23417800 | -1.18211800 | H | -5.01215900 | -3.00352100 | 1.73490600 |
| H | 2.49755600 | 4.99013000 | 1.27807700 | H | -5.46521900 | -3.78030300 | -0.58135600 |
| C | -1.51599700 | -1.69613700 | 1.21883500 | C | 1.17580800 | 2.56576500 | -1.64841000 |
| C | -2.42988400 | -2.68882400 | 1.40434700 | C | 1.92503400 | 3.70370000 | -1.56301100 |
| C | -2.71344300 | -3.71807800 | 0.45676200 | C | 1.98744000 | 4.57880500 | -0.43609400 |
| N | -2.91886000 | -4.58620500 | -0.28608100 | N | 2.01210700 | 5.33398600 | 0.44515100 |
| H | -1.30972700 | -1.09071600 | 2.10242300 | H | 1.12370700 | 2.13231200 | -2.64621300 |
| H | -2.88065400 | -2.82708200 | 2.38175400 | H | 2.37824500 | 4.10424800 | -2.46435500 |
| C | -5.58950400 | -0.85277800 | -0.03950200 | C | 5.15642700 | 2.36176400 | 0.04038200 |
| C | -5.97604700 | 0.11746000 | -0.98132000 | C | 5.66990900 | 1.57525600 | 1.08775000 |
| C | -5.11842800 | 0.55432400 | -2.00789500 | C | 4.83600000 | 0.89612400 | 1.99200400 |
| C | -3.81261000 | 0.05408900 | -2.15792300 | C | 3.43355400 | 0.95517200 | 1.90513000 |
| C | -3.53342300 | -0.86995700 | -1.16970200 | C | 3.02664000 | 1.73149100 | 0.83304200 |
| C | -4.28326600 | -1.27853100 | -0.24535100 | C | 3.76928000 | 2.34700000 | 0.01752500 |
| H | -6.26179900 | -1.19455100 | 0.74146100 | H | 5.80460600 | 2.89831100 | -0.64547600 |
| H | -6.97406100 | 0.54355000 | -0.91472600 | H | 6.74787300 | 1.49581300 | 1.20477700 |
| H | -5.47763500 | 1.30390300 | -2.70846800 | H | 5.28899800 | 0.31329700 | 2.79000600 |
| H | -3.14096200 | 0.38348600 | -2.94355300 | H | 2.78757600 | 0.45237100 | 2.61813000 |
| R-8 G(M062X/6-31G(d)): -1746.06937 Number of Imaginary frequency: 0 | | | | S-8 G(M062X/6-31G(d)): -1746.06398 Number of Imaginary frequency: 0 | | | |
| C | -0.31659100 | -1.08056300 | 0.58543600 | C | 0.24266500 | -1.43529700 | 0.33752600 |
| C | 0.39597500 | 0.14152500 | 0.00096700 | C | 0.72483600 | -0.18740800 | 1.11289600 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 1.88467700 | 0.02634500 | 0.20598800 | C | 2.20809400 | 0.08666000 | 0.92957000 |
| C | 2.45338700 | -1.29551600 | -0.23286000 | C | 3.12697800 | -1.04375100 | 0.50590800 |
| C | 0.35884400 | -2.40196500 | 0.20063600 | C | 1.22046200 | -1.83302900 | -0.76110200 |
| H | 0.01286900 | 1.04474600 | 0.49303100 | H | 0.51772600 | -0.37857100 | 2.17698200 |
| H | -1.35354800 | -1.08572000 | 0.22385500 | H | -0.73528700 | -1.21169200 | -0.11002900 |
| H | -0.01716600 | -3.15560400 | 0.90203500 | H | 0.88887600 | -2.79169900 | -1.17558200 |
| H | 2.30708600 | -1.39516700 | -1.32054300 | O | 2.48580200 | -2.10748100 | -0.18176900 |
| O | 1.76245300 | -2.36115800 | 0.42803000 | C | 1.29647700 | -0.84048900 | -1.92664900 |
| C | 0.02839200 | -2.90964300 | -1.20785100 | H | 1.52752200 | 0.17929800 | -1.58946400 |
| H | 0.32096500 | -2.19871100 | -1.98648200 | H | 2.09869600 | -1.15998600 | -2.60128200 |
| H | 0.58049900 | -3.84277700 | -1.36744400 | O | 0.04548400 | 0.98531600 | 0.70039000 |
| O | 0.08224400 | 0.16127800 | -1.38793800 | O | 0.13674600 | -2.52590100 | 1.24190700 |
| O | -0.28718500 | -0.95663300 | 1.99985200 | O | 0.07628700 | -0.87696900 | -2.64403700 |
| O | -1.35658000 | -3.19920100 | -1.27923400 | C | -1.11184300 | -3.19803800 | 1.18233700 |
| C | -1.58236600 | -0.93488400 | 2.58157800 | H | -1.35488600 | -3.47421300 | 0.14588100 |
| H | -2.16462200 | -1.80863400 | 2.25357300 | H | -0.97387200 | -4.12133500 | 1.75431000 |
| H | -1.41874400 | -1.02132100 | 3.66035300 | C | -1.26865800 | 1.11076100 | 1.20988200 |
| C | 0.63837900 | 1.24754500 | -2.11557500 | H | -1.87277700 | 0.22253100 | 0.97355000 |
| H | 1.73536100 | 1.20581400 | -2.10250400 | H | -1.23174100 | 1.19777000 | 2.30701500 |
| H | 0.30942900 | 1.08479500 | -3.14685900 | C | -0.80221000 | 0.21073500 | -2.42741300 |
| C | -2.14412900 | -2.26142600 | -1.98881700 | H | -0.56505600 | 0.71780100 | -1.48349500 |
| H | -1.64460400 | -1.28561300 | -2.03166900 | H | -0.67813400 | 0.95128700 | -3.23206100 |
| H | -2.27657400 | -2.60564700 | -3.02598700 | C | -1.92782400 | 2.32230400 | 0.59882200 |
| C | 0.17195700 | 2.59800100 | -1.62123400 | C | -3.29642300 | 2.52009700 | 0.80739800 |
| C | 1.08011300 | 3.64736400 | -1.47480000 | O | -1.22239600 | 3.22658000 | -0.19484800 |
| C | -1.17577900 | 2.81231800 | -1.31564900 | C | -3.95149900 | 3.60055200 | 0.22530300 |
| C | 0.64842500 | 4.90424100 | -1.05128100 | H | -3.85174700 | 1.81008300 | 1.41745800 |
| H | 2.13329400 | 3.47694300 | -1.69010100 | C | -1.88061000 | 4.30759600 | -0.78428600 |
| C | -1.60800200 | 4.06634100 | -0.89175100 | H | -0.16076400 | 3.07531700 | -0.36258300 |
| H | -1.88292100 | 1.98927900 | -1.40305400 | C | -3.24499700 | 4.49630800 | -0.57971300 |
| C | -0.69749000 | 5.11593800 | -0.76117400 | H | -5.01608900 | 3.73983200 | 0.39102000 |
| H | 1.36509700 | 5.71287400 | -0.94125700 | H | -1.32205800 | 5.00128400 | -1.40639300 |
| H | -2.65698200 | 4.22560500 | -0.65931100 | C | -3.75631500 | 5.33498700 | -1.04286100 |
| H | -1.03723000 | 6.09236500 | -0.42856300 | H | -2.22608600 | -2.36278900 | 1.77292100 |
| C | -2.33604500 | 0.33658600 | 2.26111100 | C | -2.07393600 | -1.81938100 | 3.05297000 |
| C | -1.77662900 | 1.57527700 | 2.59582100 | C | -3.38251900 | -2.07961100 | 1.04622600 |
| C | -3.57349900 | 0.30098000 | 1.61964700 | C | -3.06187900 | -1.00271500 | 3.59443100 |
| C | -2.45381100 | 2.75606900 | 2.31005700 | H | -1.17004700 | -2.03373700 | 3.61861900 |
| H | -0.80333900 | 1.60562600 | 3.08128600 | C | -4.37400500 | -1.25749700 | 1.58375200 |
| C | -4.25974500 | 1.48419800 | 1.33763900 | H | -3.50277000 | -2.49449500 | 0.04843200 |
| H | -4.00634500 | -0.65875200 | 1.34267100 | C | -4.21331300 | -0.71587000 | 2.85796500 |
| C | -3.70318900 | 2.71156800 | 1.68565000 | H | -2.93535300 | -0.58414000 | 4.58886100 |
| H | -2.01113800 | 3.71299900 | 2.57257400 | H | -5.26455500 | -1.03352100 | 1.00255900 |
| H | -5.22656100 | 1.44125300 | 0.84331100 | H | -4.98120700 | -0.07231500 | 3.27789600 |
| H | -4.23553500 | 3.63328800 | 1.46838200 | C | -2.23805600 | -0.25839800 | -2.38268100 |
| C | -3.49498900 | -2.10236700 | -1.32987200 | C | -3.24464200 | 0.67832800 | -2.11977200 |
| C | -4.33234600 | -1.05877200 | -1.73729400 | C | -2.58832700 | -1.59322600 | -2.58783400 |
| C | -3.93446700 | -2.97721500 | -0.33497100 | C | -4.57655900 | 0.28357700 | -2.04712900 |
| C | -5.59342100 | -0.89944300 | -1.16957100 | H | -2.97921900 | 1.72361500 | -1.96978800 |
| H | -3.99070700 | -0.36788400 | -2.50567200 | C | -3.92779600 | -1.98542200 | -2.53617500 |
| C | -5.19972500 | -2.81895100 | 0.23383000 | H | -1.80916500 | -2.32129700 | -2.79027600 |
| H | -3.28188700 | -3.78115000 | -0.01014600 | C | -4.92381000 | -1.05273400 | -2.25797100 |
| C | -6.03260200 | -1.78195500 | -0.18110300 | H | -5.34549300 | 1.02047200 | -1.83078100 |
| H | -6.23295100 | -0.08365400 | -1.49491400 | H | -4.18917100 | -3.02658400 | -2.70539500 |
| H | -5.53294300 | -3.50782200 | 1.00512500 | H | -5.96429100 | -1.36083500 | -2.20962200 |
| H | -7.01576300 | -1.65834900 | 0.26357100 | C | 2.70010400 | 1.30190800 | 1.16522000 |
| C | 2.61324900 | 1.02763500 | 0.68722300 | C | 4.16854400 | 1.62509200 | 0.99233600 |
| C | 4.11491100 | 0.96488800 | 0.81713000 | C | 4.86152800 | 1.45869800 | 2.28584500 |
| C | 4.69251300 | 1.95139700 | -0.11713600 | N | 5.39600800 | 1.31512900 | 3.30134500 |
| N | 5.12011500 | 2.72389600 | -0.86401600 | H | 2.05338300 | 2.10610300 | 1.50023900 |
| H | 2.14194300 | 1.96453300 | 0.97919500 | C | 5.91488100 | 1.21873900 | -0.79301200 |
| C | 6.06582400 | -0.61776900 | 0.81004500 | C | 6.49585200 | 0.42011100 | -1.77311900 |
| C | 6.64439900 | -1.86148600 | 0.59670300 | C | 5.97847300 | -0.84990900 | -2.02516400 |
| C | 5.86083300 | -2.91654500 | 0.12424300 | C | 4.88743400 | -1.31751100 | -1.29793700 |
| C | 4.51141100 | -2.71396700 | -0.13125300 | C | 4.30276700 | -0.52197200 | -0.31125000 |
| C | 3.92213900 | -1.46126400 | 0.07529700 | C | 4.82243300 | 0.74938900 | -0.06401200 |
| C | 4.70666400 | -0.41148500 | 0.55241700 | H | 6.30155400 | 2.21506700 | -0.59348300 |
| H | 6.66635600 | 0.20929600 | 1.18239500 | H | 7.34405700 | 0.78919000 | -2.34166000 |
| H | 7.70021900 | -2.01122000 | 0.80041600 | H | 6.42391500 | -1.47722100 | -2.79163200 |
| H | 6.30462600 | -3.89346200 | -0.04207500 | H | 4.47499300 | -2.30179900 | -1.49283800 |

| | | | | | | | |
|----------------------------------|-------------|-------------|-------------|----------------------------------|-------------|-------------|-------------|
| H | 3.89127700 | -3.52994500 | -0.49155400 | H | 3.53226000 | -1.50012300 | 1.42176800 |
| H | 4.40866500 | 1.29245300 | 1.82342800 | H | 4.28558200 | 2.67896000 | 0.71583300 |
| R-9 | | | | S-9 | | | |
| G(M062X/6-31G(d)): -1845.96941 | | | | G(M062X/6-31G(d)): -1845.97269 | | | |
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| C | 2.22473661 | 0.13030901 | 0.95302702 | C | 1.70137900 | -0.12697800 | 0.06002400 |
| C | 3.13017967 | -1.01346582 | 0.52479998 | C | 2.16511000 | -1.48952700 | -0.38843700 |
| C | 1.20983232 | -1.78540305 | -0.72502886 | C | -0.00746600 | -2.43786300 | 0.05994300 |
| H | 0.54854543 | -0.34269395 | 2.21907780 | H | -0.07922800 | 1.01576200 | 0.43343900 |
| H | -0.73721250 | -1.11754386 | -0.08104925 | H | -1.61440600 | -0.99751200 | 0.18489100 |
| H | 0.86298056 | -2.73774221 | -1.14215244 | H | -0.42777300 | -3.18401000 | 0.74462900 |
| O | 2.46327688 | -2.08293221 | -0.13271683 | H | 2.01374300 | -1.56898100 | -1.47772900 |
| C | 1.31982890 | -0.79815812 | -1.89441843 | O | 1.39688100 | -2.51005400 | 0.26050900 |
| H | 1.55753473 | 0.22031874 | -1.55889194 | C | -0.40099000 | -2.87909700 | -1.35610000 |
| H | 2.13131219 | -1.13337331 | -2.54926978 | H | -0.10272200 | -2.15428400 | -2.11939400 |
| O | 0.05886940 | 1.04419617 | 0.77004592 | H | 0.10802500 | -3.82734800 | -1.56153800 |
| O | 0.09019040 | -2.46067492 | 1.26589321 | O | -0.14842500 | 0.16474700 | -1.46287300 |
| O | 0.12153395 | -0.81956008 | -2.64740210 | O | -0.46998600 | -0.99295900 | 1.91554400 |
| C | -1.15622067 | -3.12872113 | 1.15140159 | O | -1.79612800 | -3.11965200 | -1.40276500 |
| H | -1.37171694 | -3.37380900 | 0.10112085 | C | -1.73312600 | -0.88758000 | 2.55422100 |
| H | -1.03689983 | -4.06808207 | 1.70051360 | H | -2.38634300 | -1.71991200 | 2.25270100 |
| C | -1.24332729 | 1.16454506 | 1.30806363 | H | -1.52723900 | -0.98861200 | 3.62427600 |
| H | -1.83593762 | 0.25738157 | 1.12148630 | C | 0.46984800 | 1.20597400 | -2.20327700 |
| H | -1.18217039 | 1.29386425 | 2.40027088 | H | 1.55958100 | 1.07591900 | -2.22856900 |
| C | -0.79229658 | 0.22952692 | -2.38958023 | H | 0.09468400 | 1.07829100 | -3.22371200 |
| H | -0.57054038 | 0.71314565 | -1.42972954 | C | -2.58250800 | -2.09838700 | -1.98543800 |
| H | -0.69396194 | 1.00093537 | -3.16839580 | H | -2.03824000 | -1.14593400 | -2.00145800 |
| C | -1.94383695 | 2.33693018 | 0.66686784 | H | -2.80618900 | -2.36104400 | -3.03049600 |
| C | -3.31113918 | 2.51442320 | 0.90160390 | C | 0.13166600 | 2.58788300 | -1.69063400 |
| C | -1.27809013 | 3.22095331 | -0.18258128 | C | 1.11840600 | 3.57213000 | -1.61288900 |
| C | -4.00543503 | 3.55223072 | 0.28808928 | C | -1.17570900 | 2.89856300 | -1.30369000 |
| H | -3.83351658 | 1.82134848 | 1.55799123 | C | 0.80186000 | 4.85922900 | -1.17891400 |
| C | -1.97567193 | 4.25952358 | -0.80246461 | H | 2.14175900 | 3.32635300 | -1.89004000 |
| H | -0.21757164 | 3.08592769 | -0.36972729 | C | -1.49286400 | 4.18296600 | -0.86892600 |
| C | -3.33918463 | 4.42612963 | -0.57343637 | H | -1.94157600 | 2.12569700 | -1.33757500 |
| H | -5.06858315 | 3.67523730 | 0.47397991 | C | -0.50535000 | 5.16732500 | -0.80847400 |
| H | -1.44907655 | 4.93760006 | -1.46796565 | H | 1.57783300 | 5.61710200 | -1.12318300 |
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| C | -2.28335240 | -2.30704872 | 1.73695528 | H | -0.75479300 | 6.16819900 | -0.46876100 |
| C | -2.17545570 | -1.83224889 | 3.04861127 | C | -2.41718900 | 0.43115000 | 2.26725600 |
| C | -3.40333772 | -1.96542852 | 0.97870523 | C | -1.76515800 | 1.63276900 | 2.56933500 |
| C | -3.17396848 | -1.03058943 | 3.59316453 | C | -3.68055900 | 0.47285600 | 1.67845800 |
| H | -1.29700027 | -2.08772761 | 3.63660043 | C | -2.37675200 | 2.85335800 | 2.30194500 |
| C | -4.40755854 | -1.16198482 | 1.52150931 | H | -0.77195500 | 1.60301900 | 3.01208500 |
| H | -3.48569113 | -2.32040546 | -0.04610065 | C | -4.30020500 | 1.69609700 | 1.41429800 |
| C | -4.29331501 | -0.69278855 | 2.82870282 | H | -4.18565100 | -0.45825800 | 1.42923000 |
| H | -3.08212338 | -0.66640943 | 4.61236118 | C | -3.65097300 | 2.88671700 | 1.72859200 |
| H | -5.27233347 | -0.89726147 | 0.91900502 | H | -1.86287700 | 3.78089800 | 2.53815700 |
| H | -5.07185631 | -0.06456649 | 3.25215296 | H | -5.28680100 | 1.71347100 | 0.95940800 |
| C | -2.21138248 | -0.29181942 | -2.36785363 | H | -4.13069800 | 3.83987800 | 1.52516100 |
| C | -3.25145022 | 0.58314580 | -2.03349295 | C | -3.87670900 | -1.92808100 | -1.22151400 |
| C | -2.51215079 | -1.61890788 | -2.67781536 | C | -4.73785800 | -0.87849700 | -1.55925300 |
| C | -4.56869528 | 0.13501576 | -2.00057986 | C | -4.24157200 | -2.80212000 | -0.19614800 |
| H | -3.02489650 | 1.62269463 | -1.80343486 | C | -5.94900400 | -0.71369500 | -0.89291200 |
| C | -3.83590586 | -2.06347449 | -2.66330189 | H | -4.45566000 | -0.18947800 | -2.35291300 |
| H | -1.70617167 | -2.29812712 | -2.93553571 | C | -5.45695800 | -2.63836900 | 0.47159500 |
| C | -4.86664550 | -1.19180829 | -2.31933290 | H | -3.57160700 | -3.61215900 | 0.07233800 |
| H | -5.36454780 | 0.82334546 | -1.72897938 | C | -6.31449500 | -1.59662800 | 0.12539900 |
| H | -4.05861849 | -3.09687582 | -2.91429070 | H | -6.60838100 | 0.10514500 | -1.16655800 |
| H | -5.89517561 | -1.54016655 | -2.30062358 | H | -5.73136800 | -3.32753900 | 1.26530600 |
| C | 2.73546820 | 1.34158290 | 1.17945843 | H | -7.25957400 | -1.46939200 | 0.64506300 |
| C | 4.19676872 | 1.65486810 | 0.96980195 | C | 2.52569800 | 0.83688100 | 0.46368500 |
| C | 4.92638932 | 1.49885164 | 2.23508997 | C | 4.02081600 | 0.68135400 | 0.48588900 |
| N | 5.50982790 | 1.40395675 | 3.23151668 | C | 4.57279200 | 1.48557700 | -0.61607100 |
| H | 2.09188684 | 2.14702983 | 1.52080772 | N | 4.98466600 | 2.13273900 | -1.48397800 |
| C | 5.86963342 | 1.25235890 | -0.86512769 | H | 2.12557300 | 1.81109500 | 0.74235300 |
| C | 6.42531718 | 0.44925225 | -1.85712771 | C | 5.80633300 | -1.05835200 | 0.69764400 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 5.91828186 | -0.83119385 | -2.08316383 | C | 6.27210300 | -2.36284300 | 0.59095000 |
| C | 4.85036970 | -1.30582046 | -1.32453549 | C | 5.41630600 | -3.37643200 | 0.15121900 |
| C | 4.29011327 | -0.50900754 | -0.32399089 | C | 4.09560500 | -3.07998300 | -0.16354100 |
| C | 4.81382862 | 0.76323639 | -0.09303777 | C | 3.61556100 | -1.76899400 | -0.06500700 |
| H | 6.18262842 | 2.27788344 | -0.66909517 | C | 4.48277800 | -0.75877900 | 0.35267800 |
| H | 7.24586086 | 0.82331794 | -2.46307470 | H | 6.40438300 | -0.23015200 | 1.08023800 |
| H | 6.34751629 | -1.45868221 | -2.85910598 | H | 7.29863600 | -2.59719100 | 0.85865900 |
| H | 4.43875056 | -2.29311078 | -1.50777334 | H | 5.77599900 | -4.39786400 | 0.06710300 |
| H | 3.55006874 | -1.46369125 | 1.43720796 | H | 3.41622500 | -3.86623400 | -0.47971300 |
| H | 4.43187896 | 2.72081500 | 0.67814795 | H | 4.56319000 | 1.12597100 | 1.35994700 |
| F | 5.49861163 | 3.91309424 | 0.31100196 | F | 6.12541400 | 1.61383700 | 1.83118900 |
| R-TS5 | | | | S-TS5 | | | |
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| C | 0.38880300 | 0.57656100 | -0.05473100 | C | 0.77973500 | 0.36714600 | -1.00866100 |
| C | 1.88408100 | 0.65976700 | -0.19450300 | C | 2.22844300 | -0.01224900 | -0.91616000 |
| C | 2.44030900 | -0.49886500 | -0.96030800 | C | 3.05151300 | 1.02641500 | -0.22136800 |
| C | 0.97267900 | -1.91494100 | 0.45335100 | C | 1.32277700 | 0.64071500 | 1.54611200 |
| H | -0.02632400 | 1.43877900 | 0.48371400 | H | 0.56958700 | 1.10011600 | -1.80085000 |
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| H | 1.06143300 | -2.54706600 | 1.34233300 | H | 1.18946400 | 1.38951500 | 2.33141300 |
| H | 1.83909800 | -0.83249900 | -1.80627500 | O | 2.76771500 | 0.66552400 | 1.25244700 |
| O | 2.35739600 | -1.61412200 | 0.08462500 | C | 0.96338100 | -0.72914000 | 2.13076500 |
| C | 0.35148300 | -2.74783900 | -0.66471800 | H | 1.00773100 | -1.52013500 | 1.37293900 |
| H | -0.04058600 | -2.09909800 | -1.45908600 | H | 1.68242900 | -0.97341600 | 2.92160800 |
| H | 1.10438500 | -3.42308500 | -1.09393800 | O | -0.00018600 | -0.79178700 | -1.19148400 |
| O | -0.28207800 | 0.36737300 | -1.28225200 | O | 0.56753300 | 2.48012300 | 0.19806700 |
| O | 0.38003800 | -0.31677200 | 2.15721300 | O | -0.32131300 | -0.63762400 | 2.70321400 |
| O | -0.69033500 | -3.48259900 | -0.05496200 | C | -0.62881300 | 3.19929900 | 0.48603200 |
| C | -0.52050600 | -0.92061400 | 3.07197900 | H | -0.98753200 | 2.94846400 | 1.49432400 |
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| H | -0.07185300 | -0.78290100 | 4.06103300 | C | -1.29501900 | -0.51194400 | -1.69379300 |
| C | -0.24921800 | 1.48632200 | -2.14634400 | H | -1.79003900 | 0.25725500 | -1.08079900 |
| H | 0.77651500 | 1.87264700 | -2.23641600 | H | -1.21540400 | -0.11247600 | -2.71597800 |
| H | -0.54831100 | 1.10590100 | -3.12892800 | C | -1.35197100 | -1.27197200 | 1.96442600 |
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| C | -1.91476100 | 4.89821200 | -1.89108600 | H | -3.83127200 | -0.70407600 | -2.50851300 |
| H | -0.17063900 | 4.10072400 | -2.87039500 | C | -2.53652400 | -4.07777400 | -1.12530300 |
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| H | -4.00837900 | 3.12223400 | 0.11134700 | H | -4.51511900 | -4.83237900 | -1.51941700 |
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| H | -2.92365000 | -2.12002700 | 3.52088200 | C | -3.65406900 | 2.33783100 | -2.46211500 |
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| H | -5.17383200 | -1.08119600 | 3.52380000 | H | -4.40681500 | 2.10687100 | -3.21062000 |
| H | -5.42768600 | 1.33897100 | 3.01743800 | C | -2.65339100 | -0.52668000 | 2.13437600 |
| C | -2.61590600 | -2.68766300 | -1.29765800 | C | -3.75260100 | -0.90347900 | 1.35482300 |
| C | -3.25200300 | -2.00283500 | -0.25523100 | C | -2.78806400 | 0.52399900 | 3.04273100 |
| C | -2.79844600 | -2.25103400 | -2.60852000 | C | -4.96620200 | -0.23328200 | 1.47676400 |
| C | -4.05460700 | -0.89840500 | -0.51991800 | H | -3.65478300 | -1.73019500 | 0.65347300 |
| H | -3.10726800 | -2.33950000 | 0.76966000 | C | -4.01011800 | 1.18632900 | 3.17482000 |
| C | -3.60624800 | -1.14406200 | -2.87947900 | H | -1.93580900 | 0.81836400 | 3.64630700 |
| H | -2.30039500 | -2.77433200 | -3.42162000 | C | -5.09935700 | 0.81522200 | 2.38958200 |

| | | | | | | | |
|---------------------------------------|-------------|-------------|-------------|---------------------------------------|-------------|-------------|-------------|
| C | -4.23227800 | -0.46625700 | -1.83706100 | H | -5.80969500 | -0.52995600 | 0.85923400 |
| H | -4.53938700 | -0.37130500 | 0.29842700 | H | -4.10699800 | 1.99785500 | 3.89056400 |
| H | -3.73858600 | -0.80910900 | -3.90424900 | H | -6.04778800 | 1.33511800 | 2.48865600 |
| H | -4.85192300 | 0.40124900 | -2.04623000 | C | 2.64867900 | -1.26759300 | -0.65766300 |
| C | 2.64026900 | 0.98174200 | 0.87936300 | C | 3.87215200 | -1.43401800 | 0.14067800 |
| C | 3.89592800 | 0.25011900 | 1.08355500 | C | 4.23520800 | -2.75535800 | 0.53300000 |
| C | 4.62709100 | 0.49658500 | 2.28286100 | N | 4.53046300 | -3.82208300 | 0.88847000 |
| N | 5.22852800 | 0.65910100 | 3.26407900 | H | 2.01180100 | -2.12883200 | -0.84019600 |
| H | 2.24084500 | 1.57920800 | 1.69519100 | C | 6.33354300 | -0.73352400 | -0.11050700 |
| C | 6.06724900 | -0.02297200 | -0.26473600 | C | 7.23234200 | 0.29198500 | -0.38802500 |
| C | 6.65157700 | -0.30127500 | -1.49740700 | C | 6.78555600 | 1.58679800 | -0.66867400 |
| C | 5.86779700 | -0.60794100 | -2.61299400 | C | 5.42206400 | 1.86550700 | -0.64762300 |
| C | 4.48169700 | -0.66186700 | -2.48922400 | C | 4.52058900 | 0.84064700 | -0.37424100 |
| C | 3.89596700 | -0.38231600 | -1.25887500 | C | 4.96043600 | -0.46792100 | -0.12160300 |
| C | 4.67529900 | -0.04385200 | -0.14189300 | H | 6.69292600 | -1.73813400 | 0.09702500 |
| H | 6.68564500 | 0.22615500 | 0.59368600 | H | 8.29741900 | 0.07832500 | -0.39234000 |
| H | 7.73324700 | -0.27084000 | -1.59247400 | H | 7.50006700 | 2.37489100 | -0.88390200 |
| H | 6.33866200 | -0.81767400 | -3.56814900 | H | 5.05490000 | 2.87195200 | -0.83161500 |
| H | 3.85673100 | -0.92764400 | -3.33783600 | H | 2.71981200 | 2.05728700 | -0.33379300 |
| H | 3.02142700 | -1.04601900 | 0.89640100 | H | 3.21856800 | -0.42537900 | 1.15579600 |
| R-TS6 | | | | S-TS6 | | | |
| G(M062X/6-31G(d)): -1845.96558 | | | | G(M062X/6-31G(d)): -1845.96776 | | | |
| Number of Imaginary frequency: -79.34 | | | | Number of Imaginary frequency: -50.39 | | | |
| -1 1 | | | | -1 1 | | | |
| C | 0.22261800 | -0.11671700 | -0.22045000 | C | 0.25887600 | 1.11623000 | -0.16013200 |
| C | -0.64456800 | 0.92856100 | 0.50615200 | C | 0.69847000 | -0.29254300 | -0.63441800 |
| C | -2.10153500 | 0.61777900 | 0.28156900 | C | 2.16224400 | -0.52225900 | -0.33724900 |
| C | -2.45136100 | -0.80695000 | 0.62028400 | C | 2.96735900 | 0.74891000 | -0.32508500 |
| C | -0.22386700 | -1.55332300 | 0.09067900 | C | 1.10673300 | 1.62808200 | 0.99952100 |
| H | -0.39751000 | 1.92297800 | 0.11449900 | H | 0.55315800 | -0.30750600 | -1.72651300 |
| H | 1.27580300 | 0.01799800 | 0.06392500 | H | -0.78766000 | 1.06522100 | 0.17075300 |
| H | 0.23700600 | -2.20245700 | -0.66132800 | H | 0.81696600 | 2.67073700 | 1.18561800 |
| H | -2.25506400 | -0.97152500 | 1.69333500 | O | 2.49740400 | 1.64416200 | 0.69945000 |
| O | -1.62171300 | -1.69964200 | -0.13472800 | C | 0.88888800 | 0.85648200 | 2.30576700 |
| C | 0.19622900 | -2.09593600 | 1.47451800 | H | 1.01875700 | -0.22418800 | 2.15991900 |
| H | 0.37279700 | -1.28911300 | 2.19491000 | H | 1.64834300 | 1.19337500 | 3.01867100 |
| H | -0.62165800 | -2.72347800 | 1.84413300 | O | -0.06560700 | -1.32407900 | -0.04277000 |
| O | -0.44284600 | 0.89471100 | 1.91703000 | O | 0.38688900 | 2.03145200 | -1.24188200 |
| O | 0.04881500 | 0.10841500 | -1.61417600 | O | -0.38019200 | 1.15588800 | 2.85708100 |
| O | 1.32934100 | -2.94735600 | 1.41884200 | C | -0.81962600 | 2.71362700 | -1.55494500 |
| C | 1.25968700 | 0.23563600 | -2.33653400 | H | -1.22365800 | 3.20776200 | -0.65926300 |
| H | 1.94218000 | -0.59854900 | -2.11177500 | H | -0.53767400 | 3.48879500 | -2.27446600 |
| H | 0.97944400 | 0.15853200 | -3.39292100 | C | -1.30899400 | -1.53529300 | -0.68764900 |
| C | 0.42978500 | 1.88401100 | 2.44945500 | H | -1.85167900 | -0.58580200 | -0.80962200 |
| H | 0.34251400 | 2.81064400 | 1.86645800 | H | -1.13426300 | -1.94094200 | -1.69632600 |
| H | 0.06539500 | 2.08142200 | 3.46244200 | C | -1.39581700 | 0.20048700 | 2.62392300 |
| C | 2.56687600 | -2.29336900 | 1.22764200 | H | -1.09449000 | -0.49563000 | 1.83243000 |
| H | 2.49245700 | -1.22626500 | 1.48242700 | H | -1.55190200 | -0.39812400 | 3.53442900 |
| H | 3.28091600 | -2.73728000 | 1.93468000 | C | -2.16129900 | -2.47852300 | 0.12312400 |
| C | 1.87259700 | 1.43941100 | 2.50920700 | C | -3.48412900 | -2.69477700 | -0.27657000 |
| C | 2.77724800 | 1.79573500 | 1.50593900 | C | -1.68581500 | -3.10636000 | 1.27402100 |
| C | 2.31494400 | 0.64916400 | 3.57500200 | C | -4.32316500 | -3.51632900 | 0.46935100 |
| C | 4.10290400 | 1.36684000 | 1.56650200 | H | -3.85787900 | -2.20136600 | -1.17203400 |
| H | 2.44254800 | 2.42051600 | 0.67815300 | C | -2.52977800 | -3.92498000 | 2.02708400 |
| C | 3.63935600 | 0.22195300 | 3.64092300 | H | -0.65950100 | -2.94193200 | 1.58733600 |
| H | 1.61470100 | 0.37671700 | 4.36210800 | C | -3.84864000 | -4.12972800 | 1.63050900 |
| C | 4.53605200 | 0.58091500 | 2.63463600 | H | -5.35015500 | -3.67208400 | 0.15125100 |
| H | 4.79882900 | 1.65342900 | 0.78226400 | H | -2.15139800 | -4.40145000 | 2.92708900 |
| H | 3.97216500 | -0.38638300 | 4.47705000 | H | -4.50390100 | -4.76424100 | 2.21996600 |
| H | 5.57072000 | 0.25342000 | 2.68383000 | C | -1.85633200 | 1.78412900 | -2.14584800 |
| C | 1.94904200 | 1.55947500 | -2.07752400 | C | -1.52811800 | 1.00874000 | -3.26329600 |
| C | 1.18798400 | 2.72530600 | -1.94409100 | C | -3.11813600 | 1.64491300 | -1.56722000 |
| C | 3.33862600 | 1.64388000 | -1.98735800 | C | -2.44692500 | 0.10656300 | -3.79099600 |
| C | 1.80583000 | 3.95106000 | -1.70933800 | H | -0.54245000 | 1.11118800 | -3.71162300 |
| H | 0.10547300 | 2.66290000 | -2.02233800 | C | -4.04346200 | 0.74243300 | -2.09500700 |
| C | 3.96206500 | 2.87266800 | -1.76571000 | H | -3.37541700 | 2.23637600 | -0.69143900 |
| H | 3.93508500 | 0.74025100 | -2.08640900 | C | -3.70743600 | -0.03032300 | -3.20487800 |
| C | 3.19680100 | 4.02744500 | -1.61792200 | H | -2.18267800 | -0.49189400 | -4.65808600 |
| H | 1.20384100 | 4.84924000 | -1.60331100 | H | -5.02060000 | 0.63672100 | -1.63123200 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 5.04534800 | 2.92416900 | -1.69786800 | H | -4.42372500 | -0.73712500 | -3.61404300 |
| H | 3.67997800 | 4.98310400 | -1.43654700 | C | -2.69394800 | 0.86667800 | 2.22957600 |
| C | 3.11135800 | -2.44823200 | -0.17858400 | C | -3.80077900 | 0.06419700 | 1.92887000 |
| C | 4.20170800 | -1.67096300 | -0.57958900 | C | -2.81988500 | 2.25446100 | 2.15846400 |
| C | 2.58203700 | -3.38252000 | -1.07071400 | C | -5.01131300 | 0.64115100 | 1.55698100 |
| C | 4.74983900 | -1.82051500 | -1.85156600 | H | -3.71132100 | -1.01896000 | 1.99593700 |
| H | 4.62139300 | -0.94303900 | 0.11197200 | C | -4.03963600 | 2.83377200 | 1.80265400 |
| C | 3.12006600 | -3.52278900 | -2.35037400 | H | -1.96090900 | 2.87523000 | 2.39290900 |
| H | 1.74260400 | -3.99582500 | -0.75784700 | C | -5.13620800 | 2.03110100 | 1.49610500 |
| C | 4.20462400 | -2.74242900 | -2.74556500 | H | -5.86037600 | 0.00620500 | 1.31822300 |
| H | 5.59896500 | -1.21058500 | -2.14795800 | H | -4.12895900 | 3.91584700 | 1.75940700 |
| H | 2.69275300 | -4.24743100 | -3.03770100 | H | -6.08286600 | 2.48229800 | 1.21294000 |
| H | 4.62604100 | -2.85384800 | -3.74019700 | C | 2.67622400 | -1.73106800 | -0.11575700 |
| C | -2.98551900 | 1.51981600 | -0.14020300 | C | 4.13544300 | -1.97965000 | 0.11890200 |
| C | -4.44418700 | 1.22546100 | -0.31996900 | C | 4.64574900 | -2.84747800 | -0.94856000 |
| C | -5.22262700 | 2.04508800 | 0.60837200 | N | 5.04953700 | -3.56014900 | -1.76797200 |
| N | -5.85881700 | 2.71927100 | 1.30478400 | H | 2.02224900 | -2.59962900 | -0.13063200 |
| H | -2.65843500 | 2.53669700 | -0.35546300 | C | 6.31517700 | -0.84991800 | 0.58906900 |
| C | -6.08951100 | -0.64401700 | -0.52706800 | C | 7.13209900 | 0.26986400 | 0.66125500 |
| C | -6.47455500 | -1.97001300 | -0.38524700 | C | 6.61059100 | 1.53324800 | 0.36725100 |
| C | -5.56547800 | -2.91038700 | 0.10828600 | C | 5.26927100 | 1.66328500 | 0.03154100 |
| C | -4.27438300 | -2.51400700 | 0.43285000 | C | 4.43741300 | 0.53957300 | -0.04779900 |
| C | -3.88029600 | -1.17728000 | 0.30266900 | C | 4.97419200 | -0.72287000 | 0.20297000 |
| C | -4.80221900 | -0.23436400 | -0.15498700 | H | 6.65203500 | -1.84388400 | 0.87506900 |
| H | -6.74018200 | 0.10563600 | -0.97019400 | H | 8.17216500 | 0.16570800 | 0.95749300 |
| H | -7.47642800 | -2.27780200 | -0.67112100 | H | 7.24527200 | 2.41315400 | 0.41798700 |
| H | -5.85980600 | -3.94977300 | 0.22141500 | H | 4.84631200 | 2.64596000 | -0.16185500 |
| H | -3.54926800 | -3.24263000 | 0.78608900 | H | 2.83743600 | 1.25849800 | -1.29240200 |
| H | -4.94438800 | 1.56084300 | -1.33539600 | H | 4.42867400 | -2.61786200 | 1.03468800 |
| F | -6.07136300 | 1.84391300 | -2.22132200 | F | 5.49271000 | -3.45067200 | 1.78376300 |
| R-10 G(M062X/6-31G(d)): -1845.98846 Number of Imaginary frequency: 0 | | | | S-10 G(M062X/6-31G(d)): -1845.99500 Number of Imaginary frequency: 0 | | | |
| C | 0.11404100 | 0.07332500 | -0.10107700 | C | 0.16499100 | -1.32148500 | -0.10107100 |
| C | -0.70398200 | 0.99874900 | 0.82735000 | C | 0.62673000 | -0.25461700 | 0.93338200 |
| C | -2.16160000 | 0.73009700 | 0.61078400 | C | 2.09703000 | 0.01081900 | 0.75322400 |
| C | -2.51389400 | -0.71991200 | 0.74504200 | C | 2.84795000 | -1.18945300 | 0.26550800 |
| C | -0.36152000 | -1.39123100 | -0.05014900 | C | 1.04061800 | -1.35031200 | -1.35619400 |
| H | -0.45744100 | 2.03802000 | 0.57280200 | H | 0.42047900 | -0.68518200 | 1.92796800 |
| H | 1.17784100 | 0.12331400 | 0.17204300 | H | -0.86449600 | -1.09154200 | -0.40890300 |
| H | 0.06618700 | -1.89421500 | -0.92518000 | H | 0.71425900 | -2.21246300 | -1.95530800 |
| H | -2.20740700 | -1.09144700 | 1.73761100 | O | 2.42178900 | -1.54152200 | -1.07785700 |
| O | -1.76831800 | -1.48306900 | -0.23275500 | C | 0.87339000 | -0.10804700 | -2.23767800 |
| C | 0.10071900 | -2.17954900 | 1.19778100 | H | 1.02668400 | 0.81576500 | -1.66800700 |
| H | 0.35353300 | -1.51257100 | 2.03081900 | H | 1.64166000 | -0.14785300 | -3.01632000 |
| H | -0.72890200 | -2.82365500 | 1.50711500 | O | -0.09201900 | 0.95961100 | 0.79742700 |
| O | -0.40194900 | 0.75710900 | 2.20471500 | O | 0.20802800 | -2.61031100 | 0.50498800 |
| O | -0.07439600 | 0.56255800 | -1.42499300 | O | -0.39257200 | -0.12234000 | -2.87700300 |
| O | 1.18118700 | -3.06338900 | 0.94326400 | C | -1.03138100 | -3.30009600 | 0.46729400 |
| C | 1.12332400 | 0.68660700 | -2.16522400 | H | -1.41536700 | -3.34728300 | -0.56259100 |
| H | 1.71844700 | -0.23890900 | -2.11719500 | H | -0.80744900 | -4.32134100 | 0.79219800 |
| H | 0.81367800 | 0.82444700 | -3.20745300 | C | -1.36204500 | 0.92918800 | 1.41656900 |
| C | 0.61009100 | 1.57495200 | 2.77415500 | H | -1.93723000 | 0.04961800 | 1.08876400 |
| H | 0.61259700 | 2.56079100 | 2.28907600 | H | -1.24166300 | 0.84661400 | 2.50845000 |
| H | 0.32303200 | 1.71460500 | 3.82213200 | C | -1.38148000 | 0.70336100 | -2.29905800 |
| C | 2.43944100 | -2.44826300 | 0.76544600 | H | -1.08485700 | 1.01011300 | -1.28912300 |
| H | 2.43282400 | -1.41658900 | 1.14471400 | H | -1.48758800 | 1.62439100 | -2.89355600 |
| H | 3.16441400 | -3.00331800 | 1.37703700 | C | -2.14508200 | 2.16916500 | 1.06555900 |
| C | 1.99653700 | 0.97274700 | 2.71683300 | C | -3.46118300 | 2.28047000 | 1.52684600 |
| C | 2.93957200 | 1.42374300 | 1.79048700 | C | -1.61899800 | 3.17867800 | 0.26020600 |
| C | 2.35363100 | -0.04654100 | 3.60627600 | C | -4.24339000 | 3.37672800 | 1.17858100 |
| C | 4.21751300 | 0.86566300 | 1.75144500 | H | -3.87545400 | 1.49076300 | 2.15116400 |
| H | 2.67324700 | 2.22365400 | 1.10066600 | C | -2.40541300 | 4.27678200 | -0.09440800 |
| C | 3.62940000 | -0.60430800 | 3.57313500 | H | -0.59859000 | 3.09601300 | -0.10123900 |
| H | 1.62552200 | -0.39625200 | 4.33547400 | C | -3.71790500 | 4.37800400 | 0.35920300 |
| C | 4.56508500 | -0.14781000 | 2.64352100 | H | -5.26535700 | 3.44831300 | 1.53990000 |
| H | 4.94249300 | 1.23047600 | 1.02838900 | H | -1.98768700 | 5.05304500 | -0.72934600 |
| H | 3.89613200 | -1.39213000 | 4.27199000 | H | -4.32844600 | 5.23172900 | 0.08033400 |
| H | 5.56225700 | -0.57824200 | 2.61688100 | C | -2.06331200 | -2.66438400 | 1.37294300 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 1.96211300 | 1.86575400 | -1.71459600 | C | -1.75523600 | -2.43969100 | 2.71896800 |
| C | 1.34091800 | 3.05569500 | -1.32227800 | C | -3.30176200 | -2.25316700 | 0.88020900 |
| C | 3.35538700 | 1.79362600 | -1.70232000 | C | -2.67056800 | -1.80981200 | 3.55649500 |
| C | 2.10084000 | 4.14967600 | -0.91449000 | H | -0.78775300 | -2.75502100 | 3.10294400 |
| H | 0.25586400 | 3.11648100 | -1.33854500 | C | -4.22345200 | -1.62192700 | 1.71736600 |
| C | 4.12021800 | 2.89103200 | -1.30506400 | H | -3.54198900 | -2.41651400 | -0.16814800 |
| H | 3.84405200 | 0.87049200 | -2.00440800 | C | -3.90725500 | -1.39662900 | 3.05564900 |
| C | 3.49441200 | 4.06936500 | -0.90321300 | H | -2.42252600 | -1.63755400 | 4.60000000 |
| H | 1.60632400 | 5.06771000 | -0.60941100 | H | -5.18204000 | -1.29801400 | 1.32055200 |
| H | 5.20456600 | 2.82069100 | -1.30106000 | H | -4.62097800 | -0.90291300 | 3.70922200 |
| H | 4.08759200 | 4.92233200 | -0.58669900 | C | -2.71416400 | -0.00669300 | -2.22926600 |
| C | 2.90658700 | -2.46342400 | -0.67636500 | C | -3.79613000 | 0.64201400 | -1.62285100 |
| C | 4.04360100 | -1.73353700 | -1.03510800 | C | -2.89695600 | -1.28667400 | -2.75465700 |
| C | 2.25562800 | -3.22383200 | -1.64896100 | C | -5.03763800 | 0.01881800 | -1.53904800 |
| C | 4.51621700 | -1.75567300 | -2.34528000 | H | -3.66242000 | 1.64498600 | -1.22080400 |
| H | 4.55936900 | -1.14257900 | -0.28022100 | C | -4.14727200 | -1.90477000 | -2.68678300 |
| C | 2.72091500 | -3.23816400 | -2.96413300 | H | -2.05755300 | -1.78999900 | -3.22371300 |
| H | 1.38008500 | -3.80128800 | -1.36887500 | C | -5.21923300 | -1.25804100 | -2.07550500 |
| C | 3.85087400 | -2.50371000 | -3.31714200 | H | -5.86567600 | 0.53135700 | -1.05669000 |
| H | 5.40000900 | -1.18149200 | -2.61000400 | H | -4.27951800 | -2.89745200 | -3.10848600 |
| H | 2.19962300 | -3.82757200 | -3.71322100 | H | -6.18967200 | -1.74237100 | -2.01583500 |
| H | 4.21352300 | -2.51558300 | -4.34067400 | C | 2.66912400 | 1.22764300 | 0.83779100 |
| C | -3.04242300 | 1.65059900 | 0.17482000 | C | 4.06446000 | 1.45858600 | 0.53473700 |
| C | -4.41469500 | 1.33377300 | -0.15324200 | C | 4.63986500 | 2.70926200 | 0.83034100 |
| C | -5.34050300 | 2.37156400 | -0.36664000 | N | 5.12466400 | 3.75310100 | 1.03719700 |
| N | -6.11244900 | 3.22236500 | -0.58667400 | H | 2.05535500 | 2.08397700 | 1.10916500 |
| H | -2.71091900 | 2.67981900 | 0.03459300 | C | 6.32401200 | 0.40447200 | 0.19535000 |
| C | -6.23239100 | -0.40266600 | -0.10550800 | C | 7.11614600 | -0.71591100 | 0.00140200 |
| C | -6.65861200 | -1.70069300 | 0.12621500 | C | 6.53858700 | -1.98805300 | -0.07512600 |
| C | -5.75751900 | -2.67390100 | 0.57156500 | C | 5.15851200 | -2.10304000 | 0.03770000 |
| C | -4.43021000 | -2.31389600 | 0.76912600 | C | 4.34162900 | -0.98466800 | 0.22324000 |
| C | -3.98028600 | -1.01170500 | 0.53670000 | C | 4.92159900 | 0.30139500 | 0.31377700 |
| C | -4.88835600 | -0.02215100 | 0.09721200 | H | 6.78639100 | 1.38664600 | 0.26503600 |
| H | -6.94317300 | 0.34443900 | -0.45206000 | H | 8.19359100 | -0.60039000 | -0.08381900 |
| H | -7.70166600 | -1.95793900 | -0.03887700 | H | 7.15658500 | -2.86880500 | -0.22076200 |
| H | -6.08847500 | -3.69077600 | 0.75916500 | H | 4.68768500 | -3.08237800 | -0.02524700 |
| H | -3.70995400 | -3.05508800 | 1.11115700 | H | 2.61672800 | -2.06396300 | 0.89335500 |
| H | -4.18830800 | 1.04093300 | -1.92421300 | H | 3.60871600 | 1.77806900 | -1.18619100 |
| F | -4.18982600 | 0.84924500 | -2.87014600 | F | 3.29033400 | 1.92966000 | -2.08666100 |
| R-11 G(M062X/6-31G(d)): -1745.59089 Number of Imaginary frequency: 0 | | | | S-11 G(M062X/6-31G(d)): -1745.59486 Number of Imaginary frequency: 0 | | | |
| C | -0.04730700 | 0.13840400 | -0.22024600 | C | 0.31324100 | -1.25240700 | -0.04134800 |
| C | -0.91315100 | 1.13850100 | 0.57607800 | C | 0.77926700 | -0.08726400 | 0.87725400 |
| C | -2.36067900 | 0.84066800 | 0.34618900 | C | 2.23844700 | 0.18954000 | 0.63689600 |
| C | -2.71673200 | -0.59825400 | 0.55684800 | C | 3.00328900 | -1.02943200 | 0.23037100 |
| C | -0.52893000 | -1.31845200 | -0.07888500 | C | 1.15193400 | -1.37748200 | -1.31569100 |
| H | -0.66838700 | 2.14887400 | 0.22208900 | H | 0.60009500 | -0.42713600 | 1.91238500 |
| H | 0.99722800 | 0.21379700 | 0.11498700 | H | -0.72999700 | -1.07272700 | -0.33676900 |
| H | -0.05256700 | -1.88972100 | -0.88465600 | H | 0.82618000 | -2.29701200 | -1.82382700 |
| H | -2.45781900 | -0.91154700 | 1.58375000 | O | 2.54428800 | -1.51081300 | -1.06852200 |
| O | -1.92251600 | -1.42673200 | -0.33021300 | C | 0.92755000 | -0.22508100 | -2.30140100 |
| C | -0.13778200 | -2.00272600 | 1.25213400 | H | 1.06730800 | 0.74877300 | -1.81540100 |
| H | 0.09045400 | -1.26957200 | 2.03577700 | H | 1.67807800 | -0.31866800 | -3.09330400 |
| H | -0.99130800 | -2.60581300 | 1.57766500 | O | 0.02529300 | 1.09375700 | 0.64860300 |
| O | -0.63976700 | 1.05321000 | 1.98104400 | O | 0.40184400 | -2.48093400 | 0.67532500 |
| O | -0.14523300 | 0.51723900 | -1.59007400 | O | -0.35015400 | -0.31927400 | -2.90817000 |
| O | 0.93601100 | -2.92150300 | 1.12362500 | C | -0.81880700 | -3.20248600 | 0.71939900 |
| C | 1.09628700 | 0.52381100 | -2.26469200 | H | -1.21666100 | -3.35062800 | -0.29552800 |
| H | 1.64486400 | -0.41647700 | -2.09571700 | H | -0.56410300 | -4.18462000 | 1.13083400 |
| H | 0.85530500 | 0.57445400 | -3.33264500 | C | -1.22400000 | 1.09169100 | 1.30920500 |
| C | 0.40242600 | 1.89249500 | 2.45743000 | H | -1.77848700 | 0.16395500 | 1.09958100 |
| H | 0.49465700 | 2.78007900 | 1.81628500 | H | -1.06755500 | 1.13218500 | 2.39904100 |
| H | 0.08475400 | 2.22819800 | 3.45129700 | C | -1.34759800 | 0.52460100 | -2.37151300 |
| C | 2.21452400 | -2.34376900 | 0.97019500 | H | -1.04072700 | 0.90824500 | -1.39138600 |
| H | 2.20438700 | -1.27930200 | 1.24388400 | H | -1.48424600 | 1.39847500 | -3.02765000 |
| H | 2.88892900 | -2.84325200 | 1.67997300 | C | -2.05965500 | 2.26172000 | 0.85436900 |
| C | 1.74733400 | 1.20906600 | 2.57783900 | C | -3.37501800 | 2.36525200 | 1.31922600 |
| C | 2.79566600 | 1.51835600 | 1.70898600 | C | -1.57828900 | 3.21505100 | -0.04282100 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 1.96120500 | 0.26562300 | 3.58930900 | C | -4.20009000 | 3.39788900 | 0.88579500 |
| C | 4.03800600 | 0.89741100 | 1.84705800 | H | -3.75427600 | 1.61960400 | 2.01565500 |
| H | 2.64129700 | 2.25741400 | 0.92423600 | C | -2.40772900 | 4.24845300 | -0.48292500 |
| C | 3.19920900 | -0.35584200 | 3.73132700 | H | -0.55844300 | 3.13780800 | -0.40700400 |
| H | 1.15052900 | 0.02776700 | 4.27509700 | C | -3.71901000 | 4.34195300 | -0.02393400 |
| C | 4.24206600 | -0.03940000 | 2.85925600 | H | -5.22096100 | 3.46408300 | 1.25124000 |
| H | 4.84711200 | 1.15244000 | 1.16717900 | H | -2.02418700 | 4.98080200 | -1.18766600 |
| H | 3.35321800 | -1.08375500 | 4.52272000 | H | -4.36353200 | 5.14524200 | -0.36872100 |
| H | 5.21039300 | -0.51906900 | 2.97080300 | C | -1.85306800 | -2.51275100 | 1.58232800 |
| C | 1.96178100 | 1.70540700 | -1.87231500 | C | -1.52628100 | -2.15578800 | 2.89509600 |
| C | 1.37196000 | 2.93963800 | -1.58285300 | C | -3.10938200 | -2.17655800 | 1.07854700 |
| C | 3.35151500 | 1.59029800 | -1.81529900 | C | -2.44166300 | -1.47285800 | 3.68976700 |
| C | 2.15786500 | 4.03522100 | -1.23125700 | H | -0.54347000 | -2.40862900 | 3.28646500 |
| H | 0.29094500 | 3.03621600 | -1.63706700 | C | -4.03067600 | -1.49102500 | 1.87228700 |
| C | 4.14224700 | 2.68778400 | -1.47300200 | H | -3.36454100 | -2.44309600 | 0.05520900 |
| H | 3.81711600 | 0.63330000 | -2.03765500 | C | -3.69652700 | -1.13570700 | 3.17782500 |
| C | 3.54675500 | 3.91162900 | -1.17324400 | H | -2.17877300 | -1.19981000 | 4.70780700 |
| H | 1.68625100 | 4.98796200 | -1.00702200 | H | -5.00334800 | -1.22668800 | 1.46545000 |
| H | 5.22295700 | 2.58248500 | -1.43204400 | H | -4.41014700 | -0.59851100 | 3.79629500 |
| H | 4.15943900 | 4.76519800 | -0.89843200 | C | -2.66197700 | -0.20757200 | -2.22791600 |
| C | 2.77333300 | -2.50749600 | -0.42899700 | C | -3.75320300 | 0.46380300 | -1.66484900 |
| C | 3.95116000 | -1.83863300 | -0.77344100 | C | -2.81710000 | -1.53048800 | -2.64337400 |
| C | 2.16583000 | -3.33825700 | -1.37160100 | C | -4.97720800 | -0.18086100 | -1.51247800 |
| C | 4.50651500 | -1.98790000 | -2.04213900 | H | -3.64025800 | 1.50033000 | -1.35063800 |
| H | 4.43048200 | -1.19141200 | -0.04090400 | C | -4.05031000 | -2.17155700 | -2.50729600 |
| C | 2.71529500 | -3.48105400 | -2.64644000 | H | -1.96974500 | -2.04950000 | -3.07999000 |
| H | 1.25791600 | -3.86851900 | -1.10117400 | C | -5.13116200 | -1.50249800 | -1.93744200 |
| C | 3.88523400 | -2.80576200 | -2.98649000 | H | -5.81324400 | 0.34935400 | -1.06404800 |
| H | 5.42020400 | -1.45761000 | -2.29691900 | H | -4.16217000 | -3.19900000 | -2.84294100 |
| H | 2.22825800 | -4.12506300 | -3.37334100 | H | -6.08837000 | -2.00347400 | -1.82526700 |
| H | 4.31349800 | -2.91746500 | -3.97818700 | C | 2.79746400 | 1.42193800 | 0.63144000 |
| C | -3.24708700 | 1.74094400 | -0.13634900 | C | 4.18444800 | 1.64962600 | 0.35305500 |
| C | -4.61510700 | 1.42383500 | -0.42040200 | C | 4.70791700 | 2.94789700 | 0.36773600 |
| C | -5.49214400 | 2.40730200 | -0.89116300 | N | 5.15997400 | 4.02932900 | 0.37276100 |
| N | -6.23870800 | 3.22002500 | -1.28642600 | H | 2.16808700 | 2.28190000 | 0.85362300 |
| H | -2.90989400 | 2.76150000 | -0.32262400 | C | 6.43984200 | 0.63022500 | -0.07236700 |
| C | -6.40904100 | -0.33209700 | -0.43441100 | C | 7.24473600 | -0.48297400 | -0.24463700 |
| C | -6.82882900 | -1.62997500 | -0.19656500 | C | 6.69368400 | -1.77048700 | -0.22129400 |
| C | -5.93452900 | -2.58789900 | 0.29700700 | C | 5.32242600 | -1.90264500 | -0.03804500 |
| C | -4.61885700 | -2.20745900 | 0.53411500 | C | 4.48884100 | -0.79307100 | 0.12274200 |
| C | -4.17253800 | -0.90554300 | 0.29568100 | C | 5.04303100 | 0.51236400 | 0.12339200 |
| C | -5.07416600 | 0.07265800 | -0.19455500 | H | 6.88431500 | 1.62321900 | -0.08149000 |
| H | -7.11663200 | 0.40051500 | -0.81666600 | H | 8.31395800 | -0.35111300 | -0.39123300 |
| H | -7.86313900 | -1.90070000 | -0.39403000 | H | 7.32357100 | -2.64602300 | -0.34580000 |
| H | -6.26122000 | -3.60494800 | 0.49103400 | H | 4.86926100 | -2.89264300 | -0.02740800 |
| H | -3.90223700 | -2.93505500 | 0.91158300 | H | 2.81224100 | -1.85795300 | 0.93088300 |
| R-TS7 | | | | S-TS7 | | | |
| G(M062X/6-31G(d)): -1745.55645 | | | | G(M062X/6-31G(d)): -1745.56385 | | | |
| Number of Imaginary frequency: -226.31 | | | | Number of Imaginary frequency: -206.53 | | | |
| -1 1 | | | | -1 1 | | | |
| C | -0.05328300 | -0.21150400 | -0.25671000 | C | 0.28092500 | -1.31397800 | -0.23396100 |
| C | -0.84611800 | 0.41990800 | 0.90907300 | C | 0.77352500 | -0.18420100 | 0.71313000 |
| C | -2.32717100 | 0.39777800 | 0.61867600 | C | 2.25093600 | 0.09844800 | 0.56689200 |
| C | -2.98625400 | -0.82250000 | 0.76150900 | C | 3.10043200 | -1.00217500 | 0.46595900 |
| C | -0.44377300 | -1.67481700 | -0.64292800 | C | 1.01279300 | -1.48319300 | -1.59777700 |
| H | -0.50314000 | 1.45957200 | 1.00520100 | H | 0.57555700 | -0.53964300 | 1.73770800 |
| H | 1.01422200 | -0.16309100 | 0.01140400 | H | -0.78350200 | -1.11636700 | -0.43155000 |
| H | 0.12929200 | -1.82914600 | -1.59880800 | H | 0.42698300 | -2.32651100 | -2.06842300 |
| H | -2.54497100 | -1.60569200 | 1.36301600 | O | 2.33750100 | -1.72269200 | -1.51913100 |
| O | -1.77333800 | -1.86930900 | -0.79849800 | C | 0.73369300 | -0.27556500 | -2.52492800 |
| C | 0.18430600 | -2.71172600 | 0.34235100 | H | 0.98276600 | 0.67406200 | -2.02516500 |
| H | 0.27141100 | -2.31197700 | 1.36257700 | H | 1.41406000 | -0.39094100 | -3.37566200 |
| H | -0.51792200 | -3.55102800 | 0.35525500 | O | 0.05906100 | 1.02674700 | 0.51277400 |
| O | -0.61893400 | -0.27315100 | 2.13368300 | O | 0.39324600 | -2.55071800 | 0.48272000 |
| O | -0.28561900 | 0.63875400 | -1.38591800 | O | -0.58366100 | -0.22793300 | -3.06720200 |
| O | 1.43362600 | -3.28558300 | -0.04831500 | C | -0.83250100 | -3.24214400 | 0.61398800 |
| C | 0.88936800 | 1.12955200 | -1.98984300 | H | -1.30734000 | -3.37901000 | -0.36982500 |
| H | 1.62119700 | 0.32204300 | -2.15224900 | H | -0.57577300 | -4.23354800 | 1.00387400 |
| H | 0.58699900 | 1.49990000 | -2.97708300 | C | -1.17842400 | 1.05969300 | 1.19124500 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.17300000 | 0.40109800 | 3.09728200 | H | -1.80205400 | 0.19699800 | 0.90840100 |
| H | -0.01990700 | 1.48170100 | 3.05525500 | H | -1.00901000 | 0.99273000 | 2.27773200 |
| H | -0.16544800 | 0.03434900 | 4.07182800 | C | -1.52023900 | 0.56150400 | -2.37556600 |
| C | 2.57139800 | -2.47772500 | 0.11935700 | H | -1.11033000 | 0.90159900 | -1.41792900 |
| H | 2.35908100 | -1.61355500 | 0.76495700 | H | -1.74338400 | 1.46671100 | -2.96369700 |
| H | 3.33401000 | -3.07512500 | 0.64168500 | C | -1.92667000 | 2.32551000 | 0.85987300 |
| C | 1.65143100 | 0.12781800 | 2.94335600 | C | -3.18462000 | 2.52714900 | 1.43884200 |
| C | 2.47216600 | 0.98358800 | 2.20377000 | C | -1.42713300 | 3.27546100 | -0.03058300 |
| C | 2.21198800 | -1.01086400 | 3.53060300 | C | -3.93331000 | 3.65745500 | 1.12826000 |
| C | 3.82991800 | 0.70348300 | 2.05316600 | H | -3.57935800 | 1.78272700 | 2.12835100 |
| H | 2.04682200 | 1.88043100 | 1.75409500 | C | -2.18020400 | 4.40852100 | -0.34547300 |
| C | 3.56892200 | -1.29130200 | 3.38717700 | H | -0.45316000 | 3.12162900 | -0.48513500 |
| H | 1.57701000 | -1.67556100 | 4.11274400 | C | -3.43297400 | 4.60260700 | 0.22992000 |
| C | 4.38070800 | -0.43262900 | 2.64648000 | H | -4.90938200 | 3.80086400 | 1.58301800 |
| H | 4.45986300 | 1.37667300 | 1.47761500 | H | -1.78322700 | 5.13923200 | -1.04439700 |
| H | 3.99379200 | -2.17575000 | 3.85331300 | H | -4.01792600 | 5.48344700 | -0.01759800 |
| H | 5.44025200 | -0.64500700 | 2.53409400 | C | -1.79707400 | -2.54125900 | 1.54905400 |
| C | 1.53268900 | 2.25533200 | -1.20237500 | C | -1.38004200 | -2.18478700 | 2.83596400 |
| C | 0.72955500 | 3.23069500 | -0.60263900 | C | -3.08569400 | -2.20208100 | 1.13664400 |
| C | 2.91873700 | 2.35756800 | -1.08239800 | C | -2.23445400 | -1.49573500 | 3.69157400 |
| C | 1.29977700 | 4.27907800 | 0.11482200 | H | -0.37381900 | -2.44289900 | 3.15856200 |
| H | -0.35022400 | 3.15626700 | -0.70134000 | C | -3.94662700 | -1.51069000 | 1.99094800 |
| C | 3.49580100 | 3.41309000 | -0.37412900 | H | -3.41398000 | -2.46866300 | 0.13435000 |
| H | 3.55090400 | 1.60322800 | -1.54461800 | C | -3.52038100 | -1.15193900 | 3.26813100 |
| C | 2.68788000 | 4.37185300 | 0.23301400 | H | -1.89958200 | -1.22127300 | 4.68796400 |
| H | 0.66264200 | 5.02730900 | 0.57818100 | H | -4.94467500 | -1.24422500 | 1.65286600 |
| H | 4.57723300 | 3.47947000 | -0.28991400 | H | -4.18597700 | -0.60910800 | 3.93350900 |
| H | 3.13561100 | 5.18912200 | 0.79108400 | C | -2.81075000 | -0.19127600 | -2.13253600 |
| C | 3.15731100 | -2.00041700 | -1.19634500 | C | -3.86038400 | 0.44514200 | -1.45969300 |
| C | 4.21179000 | -1.08273000 | -1.19189200 | C | -2.98874000 | -1.50003600 | -2.58276300 |
| C | 2.69456100 | -2.48956500 | -2.41928300 | C | -5.06740300 | -0.21450700 | -1.24540000 |
| C | 4.78282200 | -0.65018600 | -2.38697300 | H | -3.73160300 | 1.46987500 | -1.11467600 |
| H | 4.58479300 | -0.70177700 | -0.24292700 | C | -4.20372300 | -2.15786500 | -2.37993900 |
| C | 3.25839300 | -2.05073200 | -3.61764100 | H | -2.17186500 | -1.99149400 | -3.10158100 |
| H | 1.88444700 | -3.21137900 | -2.42085600 | C | -5.24586400 | -1.51919500 | -1.71084300 |
| C | 4.30161800 | -1.12753700 | -3.60662300 | H | -5.87299000 | 0.29206200 | -0.72064900 |
| H | 5.59964000 | 0.06667200 | -2.36617200 | H | -4.33330600 | -3.17306700 | -2.74533100 |
| H | 2.88146100 | -2.43402000 | -4.56181200 | H | -6.19066000 | -2.03104800 | -1.55189200 |
| H | 4.73972600 | -0.78400100 | -4.53919400 | C | 2.76183300 | 1.38413700 | 0.42371400 |
| C | -2.98407000 | 1.47729400 | 0.04503300 | C | 4.12883800 | 1.59941400 | 0.22674000 |
| C | -4.31758000 | 1.38097600 | -0.36801600 | C | 4.61933400 | 2.93200800 | 0.10039900 |
| C | -4.96439300 | 2.51453800 | -0.93863500 | N | 5.03020400 | 4.01376000 | -0.00520100 |
| N | -5.50205900 | 3.43229900 | -1.40725700 | H | 2.08727100 | 2.23359600 | 0.46399300 |
| H | -2.45743000 | 2.41886200 | -0.09043400 | C | 6.43766200 | 0.65023500 | -0.01470600 |
| C | -6.39182400 | -0.00666000 | -0.59560800 | C | 7.26190300 | -0.44818700 | -0.04676700 |
| C | -7.03894100 | -1.20152200 | -0.39401000 | C | 6.73399700 | -1.75403200 | 0.10239300 |
| C | -6.36941000 | -2.29469100 | 0.20809100 | C | 5.38274500 | -1.92439300 | 0.27769100 |
| C | -5.05695600 | -2.15978700 | 0.58991100 | C | 4.50376400 | -0.81217900 | 0.31533200 |
| C | -4.35812800 | -0.94152000 | 0.39400500 | C | 5.03669000 | 0.49894100 | 0.16644900 |
| C | -5.03526500 | 0.15746200 | -0.20714100 | H | 6.85239800 | 1.64849900 | -0.13042300 |
| H | -6.91428900 | 0.82688100 | -1.05833200 | H | 8.33065800 | -0.31442600 | -0.18809400 |
| H | -8.07589100 | -1.30978300 | -0.69938300 | H | 7.39875300 | -2.61182800 | 0.07433800 |
| H | -6.89461000 | -3.23235000 | 0.36191100 | H | 4.95752800 | -2.91948500 | 0.38382100 |
| H | -4.52388000 | -2.99120800 | 1.04516900 | H | 2.73518700 | -1.99089800 | 0.71341900 |
| R-12 G(M062X/6-31G(d)): -1745.56657 Number of Imaginary frequency: 0 | | | | S-12 G(M062X/6-31G(d)): -1745.56971 Number of Imaginary frequency: 0 | | | |
| C | 0.19316500 | 0.59713700 | -0.46525600 | C | 0.13487000 | -1.28616700 | -0.57405900 |
| C | -0.82922400 | -0.53488500 | -0.25870500 | C | 0.76717000 | -0.19231300 | 0.32173100 |
| C | -2.30498700 | -0.15258000 | -0.23675700 | C | 2.26517700 | 0.01348500 | 0.19543300 |
| C | -3.24891000 | -1.11914400 | -0.48576100 | C | 3.11552200 | -1.07485300 | 0.17635600 |
| C | -0.00038600 | 1.34709100 | -1.81850900 | C | 0.60683500 | -1.38947900 | -2.05458900 |
| H | -0.61137100 | -0.95375500 | 0.73550700 | H | 0.58984100 | -0.52617600 | 1.35517800 |
| H | 1.18956900 | 0.13724800 | -0.38069900 | H | -0.95166500 | -1.10238300 | -0.55051500 |
| H | 0.58005700 | 2.30522900 | -1.65428400 | H | -0.03011700 | -2.26486300 | -2.41881300 |
| H | -2.93361000 | -2.10898500 | -0.80549000 | O | 1.91941400 | -1.51989000 | -2.21969100 |
| O | -1.29309400 | 1.49909900 | -2.12794900 | C | 0.07400600 | -0.19633100 | -2.89346900 |
| C | 0.76061300 | 0.63623800 | -2.97999800 | H | 0.38180000 | 0.76185300 | -2.44611300 |
| H | 0.63797900 | -0.45464100 | -2.92167600 | H | 0.57256500 | -0.28474400 | -3.86505600 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | 0.26731500 | 0.98997000 | -3.89106900 | O | 0.11331600 | 1.05898300 | 0.15004700 |
| O | -0.64879000 | -1.55955400 | -1.22659500 | O | 0.39325400 | -2.54208900 | 0.07240700 |
| O | 0.03907400 | 1.52138200 | 0.62408300 | O | -1.32746500 | -0.19405700 | -3.16854700 |
| O | 2.14290600 | 0.95713700 | -3.16826200 | C | -0.77621600 | -3.21320300 | 0.49640000 |
| C | 1.15925200 | 1.65378600 | 1.46989100 | H | -1.47137900 | -3.34642300 | -0.34718600 |
| H | 2.08518600 | 1.75382500 | 0.88556400 | H | -0.44810500 | -4.20666500 | 0.82226300 |
| H | 1.01237000 | 2.59502600 | 2.01426500 | C | -0.99432000 | 1.21707500 | 1.01259200 |
| C | -0.17598200 | -2.80473000 | -0.73633700 | H | -1.70589900 | 0.38416400 | 0.88742200 |
| H | -0.59997200 | -3.00613800 | 0.25674300 | H | -0.65692600 | 1.19560100 | 2.06096000 |
| H | -0.55608200 | -3.56214200 | -1.42998200 | C | -2.14085500 | 0.51876400 | -2.27193300 |
| C | 3.06357900 | 0.35162800 | -2.29788100 | H | -1.55840900 | 0.85654400 | -1.40820800 |
| H | 2.61380700 | -0.49374000 | -1.75689400 | H | -2.52821900 | 1.42568300 | -2.76477100 |
| H | 3.87819200 | -0.06954600 | -2.90685800 | C | -1.70206600 | 2.51688300 | 0.72254500 |
| C | 1.33202300 | -2.87307500 | -0.68500400 | C | -2.84634900 | 2.83892600 | 1.46093200 |
| C | 2.02706500 | -2.53318300 | 0.47891500 | C | -1.26697100 | 3.39062300 | -0.27371300 |
| C | 2.05272600 | -3.24449700 | -1.82418800 | C | -3.54536000 | 4.01428800 | 1.20444100 |
| C | 3.42049000 | -2.56461800 | 0.50288800 | H | -3.19280300 | 2.15523500 | 2.23426400 |
| H | 1.47067800 | -2.25510300 | 1.37349500 | C | -1.96922500 | 4.56898600 | -0.53207600 |
| C | 3.44524100 | -3.28269000 | -1.80260700 | H | -0.38411800 | 3.14008100 | -0.85370300 |
| H | 1.51329600 | -3.50992400 | -2.73091300 | C | -3.10839100 | 4.88386000 | 0.20334200 |
| C | 4.13120200 | -2.94207200 | -0.63706000 | H | -4.43355900 | 4.25218600 | 1.78267700 |
| H | 3.95218000 | -2.30119100 | 1.41354800 | H | -1.62281200 | 5.23991800 | -1.31308700 |
| H | 3.99525500 | -3.57830400 | -2.69148500 | H | -3.65515400 | 5.79978000 | -0.00060400 |
| H | 5.21699600 | -2.97329800 | -0.61474500 | C | -1.49024000 | -2.49848000 | 1.62654900 |
| C | 1.30012700 | 0.51490500 | 2.46071200 | C | -0.80261000 | -2.20118600 | 2.80854800 |
| C | 0.16419400 | -0.06918800 | 3.02995600 | C | -2.81656900 | -2.08797900 | 1.49506300 |
| C | 2.56006000 | 0.05341200 | 2.84372400 | C | -1.42836700 | -1.50091600 | 3.83583400 |
| C | 0.28630100 | -1.10584900 | 3.95226900 | H | 0.23479400 | -2.51248700 | 2.91256700 |
| H | -0.81923900 | 0.02787800 | 2.73271500 | C | -3.45060000 | -1.38835900 | 2.52410300 |
| C | 2.68748600 | -0.97605700 | 3.77713900 | H | -3.35552100 | -2.31013200 | 0.57611900 |
| H | 3.44799600 | 0.50069400 | 2.40260000 | C | -2.75583800 | -1.08939900 | 3.69389100 |
| C | 1.55046100 | -1.56293900 | 4.32874900 | H | -0.88327500 | -1.27356400 | 4.74761700 |
| H | -0.60477200 | -1.55485400 | 4.38207700 | H | -4.48359600 | -1.07194200 | 2.40543100 |
| H | 3.67538300 | -1.32473000 | 4.06581200 | H | -3.24487400 | -0.54228600 | 4.49480500 |
| H | 1.64701600 | -2.36922700 | 5.05000200 | C | -3.31239100 | -0.31463000 | -1.79670900 |
| C | 3.66430300 | 1.32975300 | -1.30603900 | C | -4.25618200 | 0.25003100 | -0.93098500 |
| C | 4.50663600 | 0.86206800 | -0.29282200 | C | -3.48559000 | -1.63294600 | -2.22014600 |
| C | 3.41968300 | 2.70026400 | -1.40107700 | C | -5.35847500 | -0.48738700 | -0.50640100 |
| C | 5.08032000 | 1.74605200 | 0.61834700 | H | -4.12902800 | 1.27970300 | -0.59884400 |
| H | 4.71091400 | -0.20413900 | -0.21714900 | C | -4.59337800 | -2.37158500 | -1.80007900 |
| C | 3.98493300 | 3.58659100 | -0.48315200 | H | -2.75007200 | -2.06709400 | -2.88986200 |
| H | 2.77700800 | 3.06132800 | -2.19688100 | C | -5.53401700 | -1.80177500 | -0.94450800 |
| C | 4.81293400 | 3.11308900 | 0.53203000 | H | -6.08532300 | -0.03579100 | 0.16337100 |
| H | 5.73222300 | 1.36704200 | 1.40114000 | H | -4.72036900 | -3.39435900 | -2.14458400 |
| H | 3.77786200 | 4.65019000 | -0.56415000 | H | -6.39773800 | -2.37521700 | -0.62050800 |
| H | 5.25209900 | 3.80262600 | 1.24709900 | C | 2.81553300 | 1.30648000 | 0.19174100 |
| C | -2.75505300 | 1.13924100 | 0.15828800 | C | 4.19014500 | 1.49340700 | 0.15684600 |
| C | -4.09897900 | 1.39890200 | 0.30445600 | C | 4.70958200 | 2.82953100 | 0.14693100 |
| C | -4.50588000 | 2.71477500 | 0.70824600 | N | 5.13777400 | 3.90695200 | 0.13868500 |
| N | -4.84639700 | 3.77289200 | 1.03748800 | H | 2.15668600 | 2.16769400 | 0.21046300 |
| H | -2.02987200 | 1.92103300 | 0.32866500 | C | 6.50396600 | 0.52978300 | 0.11061600 |
| C | -6.49035600 | 0.63646300 | 0.20581400 | C | 7.31032700 | -0.57946700 | 0.09725600 |
| C | -7.39584300 | -0.36779800 | -0.04946800 | C | 6.74789800 | -1.88267000 | 0.11143200 |
| C | -6.94993200 | -1.64309000 | -0.46421800 | C | 5.38784300 | -2.04384200 | 0.13804600 |
| C | -5.60557000 | -1.88971700 | -0.61434200 | C | 4.51936200 | -0.91525500 | 0.15369100 |
| C | -4.64770600 | -0.87566300 | -0.35680800 | C | 5.09027300 | 0.38947800 | 0.14006800 |
| C | -5.10286800 | 0.40231800 | 0.05838000 | H | 6.93907500 | 1.52590300 | 0.09779200 |
| H | -6.83430300 | 1.61709100 | 0.52490800 | H | 8.38960200 | -0.46211500 | 0.07444900 |
| H | -8.45902700 | -0.18044800 | 0.06754800 | H | 7.40211200 | -2.74895600 | 0.09971700 |
| H | -7.67424900 | -2.42757600 | -0.66199900 | H | 4.94456100 | -3.03639200 | 0.14601500 |
| H | -5.25357600 | -2.86775000 | -0.93293900 | H | 2.69837800 | -2.07526400 | 0.15188400 |
| R-TS8 G(M062X/6-31G(d)): -1807.22938 Number of Imaginary frequency: -193.38 | | | | S-TS8 G(M062X/6-31G(d)): -1807.22919 Number of Imaginary frequency: -201.27 | | | |
| 0 1 | | | | 0 1 | | | |
| C | -0.28194100 | 0.70156900 | 0.06876300 | C | -1.20086300 | -0.03788400 | 0.14958900 |
| C | -1.12799600 | -0.49381200 | -0.36919700 | C | -0.01564300 | 0.51027200 | -0.64305400 |
| C | -0.71624300 | -1.71139600 | 0.43200400 | C | 0.61439700 | 1.66774300 | 0.09865600 |
| C | -0.36413400 | -1.46852600 | 1.73762200 | C | 0.50752600 | 1.66277400 | 1.46085700 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -0.39888800 | 0.96145900 | 1.57117400 | C | -0.83918900 | -0.32289300 | 1.60888400 |
| H | -0.94918300 | -0.63475800 | -1.44062500 | H | -0.39216200 | 0.82332700 | -1.62526900 |
| H | -0.60399700 | 1.59499600 | -0.48276200 | H | -1.53650800 | -0.95945100 | -0.33759800 |
| H | 0.48823000 | 1.51479700 | 1.90342900 | H | -1.76863300 | -0.47341200 | 2.16925400 |
| H | -0.31914900 | -2.24697500 | 2.49291100 | H | 0.86201900 | 2.48178500 | 2.07681500 |
| O | -0.41641700 | -0.25854800 | 2.33809300 | O | -0.23673400 | 0.83467900 | 2.20803400 |
| C | -1.62569500 | 1.76572200 | 2.03262900 | C | 0.07459700 | -1.51866800 | 1.92644600 |
| H | -2.52347500 | 1.46245300 | 1.48398100 | H | 0.96768100 | -1.51412600 | 1.29289600 |
| H | -1.77008400 | 1.52981700 | 3.09099100 | H | 0.38195900 | -1.39544500 | 2.96965900 |
| O | -2.48653800 | -0.14435000 | -0.15583200 | O | 0.84806400 | -0.61345600 | -0.78952800 |
| O | 1.02855100 | 0.33714200 | -0.30590900 | O | -2.22117300 | 0.93995600 | 0.09100200 |
| O | -1.44222900 | 3.16488200 | 1.97417000 | O | -0.59058000 | -2.76357000 | 1.87131700 |
| C | 1.97065300 | 1.38204900 | -0.37354500 | C | -3.52102400 | 0.39325600 | 0.17847800 |
| H | 1.59948000 | 2.18264800 | -1.03358400 | H | -3.66168200 | -0.36724800 | -0.60687900 |
| H | 2.14077100 | 1.83277100 | 0.61494900 | H | -3.66554800 | -0.11705400 | 1.14310700 |
| C | -3.40146800 | -1.04909200 | -0.74148500 | C | 2.01635100 | -0.42637100 | -1.57263200 |
| H | -3.17251600 | -1.16130000 | -1.81369200 | H | 1.73361500 | -0.21505300 | -2.61509400 |
| H | -3.31373900 | -2.04463900 | -0.28372300 | H | 2.60826300 | 0.41649600 | -1.19847700 |
| C | -1.64043300 | 3.77762000 | 0.71435100 | C | -0.79175600 | -3.31133800 | 0.58065400 |
| H | -2.22872700 | 3.12890300 | 0.05003100 | H | -0.16446200 | -2.79944400 | -0.16146700 |
| H | -2.23793700 | 4.68083600 | 0.89320900 | H | -0.46221300 | -4.35807300 | 0.61827600 |
| C | -4.80543200 | -0.52526300 | -0.56888800 | C | 2.83030300 | -1.68892500 | -1.47185200 |
| C | -5.88359500 | -1.41142800 | -0.63532800 | C | 2.32787800 | -2.89926400 | -1.96069500 |
| C | -5.05357500 | 0.83582200 | -0.38333600 | C | 4.07733100 | -1.67021200 | -0.84782100 |
| C | -7.19076000 | -0.94509500 | -0.52146600 | C | 3.06435400 | -4.07265300 | -1.82513300 |
| H | -5.69506000 | -2.47373900 | -0.77405600 | H | 1.35587100 | -2.91675800 | -2.44918700 |
| C | -6.36176100 | 1.30238500 | -0.26023300 | C | 4.81929600 | -2.84365100 | -0.71316100 |
| H | -4.21764000 | 1.52710600 | -0.33146200 | H | 4.46618500 | -0.72961700 | -0.46231000 |
| C | -7.43352600 | 0.41502600 | -0.33112000 | C | 4.31253900 | -4.04624800 | -1.20017100 |
| H | -8.01967400 | -1.64515700 | -0.57350200 | H | 2.66842400 | -5.00862500 | -2.20847200 |
| H | -6.54301100 | 2.36290800 | -0.11011900 | H | 5.78838900 | -2.81638300 | -0.22252200 |
| H | -8.45192100 | 0.77994400 | -0.23567400 | H | 4.88615600 | -4.96261900 | -1.09510300 |
| C | 3.27427800 | 0.82785700 | -0.89621000 | C | -4.54978800 | 1.48570800 | 0.02796600 |
| C | 3.36171400 | -0.45603800 | -1.43640500 | C | -4.19375900 | 2.83285500 | -0.02211300 |
| C | 4.42338100 | 1.62160000 | -0.83080800 | C | -5.90017200 | 1.13200200 | -0.05398900 |
| C | 4.58668200 | -0.94197000 | -1.89489700 | C | -5.17744400 | 3.81440000 | -0.15268300 |
| H | 2.47357300 | -1.07926700 | -1.47326500 | H | -3.14644200 | 3.11013500 | 0.03799600 |
| C | 5.64356600 | 1.13920500 | -1.29515300 | C | -6.88054500 | 2.11066800 | -0.18209500 |
| H | 4.35782500 | 2.62181500 | -0.40634500 | H | -6.18051600 | 0.08070900 | -0.01982900 |
| C | 5.72915500 | -0.14798100 | -1.82720200 | C | -6.52082500 | 3.45831300 | -0.23279700 |
| H | 4.64699100 | -1.94784300 | -2.30153100 | H | -4.88908400 | 4.86111300 | -0.19188300 |
| H | 6.52983900 | 1.76459100 | -1.23725500 | H | -7.92605200 | 1.82285000 | -0.24554000 |
| H | 6.68172700 | -0.52859900 | -2.18382900 | H | -7.28454500 | 4.22350300 | -0.33582700 |
| C | -0.34092600 | 4.17573000 | 0.04626500 | C | -2.24698000 | -3.26151100 | 0.16032700 |
| C | -0.28392000 | 4.32925300 | -1.34213800 | C | -2.58841100 | -3.38294000 | -1.19059300 |
| C | 0.79735400 | 4.44483000 | 0.80797900 | C | -3.26140500 | -3.10369100 | 1.10567600 |
| C | 0.89308600 | 4.74495000 | -1.96065400 | C | -3.92194800 | -3.34253200 | -1.58980600 |
| H | -1.16692700 | 4.11432000 | -1.94058000 | H | -1.80124300 | -3.49770200 | -1.93350800 |
| C | 1.97727800 | 4.85845700 | 0.19043600 | C | -4.59793700 | -3.06383800 | 0.70757200 |
| H | 0.75497300 | 4.32174000 | 1.88634900 | H | -2.99700800 | -3.00228100 | 2.15390500 |
| C | 2.02947500 | 5.00819700 | -1.19463700 | C | -4.93255100 | -3.18081000 | -0.64005800 |
| H | 0.92635100 | 4.85588900 | -3.04074100 | H | -4.17338000 | -3.43019600 | -2.64301700 |
| H | 2.85811000 | 5.06533900 | 0.79237300 | H | -5.37828700 | -2.93739500 | 1.45302600 |
| H | 2.94968000 | 5.32805900 | -1.67517800 | H | -5.97280900 | -3.14583500 | -0.95066700 |
| C | -0.56024300 | -3.02647100 | -0.15655800 | C | 1.44962200 | 2.65115700 | -0.56183200 |
| C | -0.77861700 | -3.24944600 | -1.53937200 | C | 1.53024700 | 2.72385200 | -1.97496000 |
| C | -0.09676600 | -4.12707600 | 0.60459500 | C | 2.31797300 | 3.50320000 | 0.17440600 |
| C | -0.57001700 | -4.49023700 | -2.11338900 | C | 2.39938600 | 3.58907200 | -2.60924900 |
| H | -1.12503900 | -2.44196600 | -2.17474700 | H | 0.89304500 | 2.09164200 | -2.58415900 |
| C | 0.08668200 | -5.38684800 | 0.01768600 | C | 3.17420600 | 4.40744000 | -0.48766400 |
| H | -0.00085800 | -4.05025100 | 1.68086000 | H | 2.17864000 | 3.64711900 | 1.23913500 |
| C | -0.13470800 | -5.57268300 | -1.33594700 | C | 3.24094900 | 4.43520600 | -1.86529700 |
| H | -0.75226100 | -4.62401300 | -3.17571800 | H | 2.42600800 | 3.61817800 | -3.69471400 |
| H | 0.40895800 | -6.21653300 | 0.64020600 | H | 3.78984100 | 5.07554300 | 0.10820400 |
| H | 0.01583900 | -6.54706600 | -1.79091900 | H | 3.91555700 | 5.11840800 | -2.37250600 |
| C | 3.59983900 | -3.30880400 | 1.05498000 | C | 5.02978600 | 1.82670700 | 0.94041200 |
| C | 4.45319300 | -2.32430000 | 1.57970800 | C | 5.63874900 | 0.75241200 | 1.61447400 |
| C | 3.95739100 | -1.12352200 | 2.11690500 | C | 4.88318800 | -0.20773400 | 2.30770600 |
| C | 2.58286100 | -0.84002800 | 2.14744300 | C | 3.47950400 | -0.15222300 | 2.36041000 |
| C | 1.83483000 | -1.86214300 | 1.58971500 | C | 2.94000900 | 0.92503800 | 1.66480500 |

| | | | | | | | |
|---|------------|-------------|------------|---|------------|-------------|------------|
| C | 2.25405300 | -2.95773600 | 1.10072900 | C | 3.65367400 | 1.77801400 | 1.04833500 |
| H | 3.99305400 | -4.23965200 | 0.65441300 | H | 5.60136700 | 2.58396300 | 0.41014600 |
| H | 5.52720500 | -2.49446200 | 1.57121800 | H | 6.72225600 | 0.66457600 | 1.59974100 |
| H | 4.65698300 | -0.39489100 | 2.51889900 | H | 5.40052600 | -1.01667400 | 2.81792400 |
| H | 2.18571300 | 0.07812900 | 2.57121400 | H | 2.90841100 | -0.89694000 | 2.90936600 |

| R-13 G(M062X/6-31G(d)): -1807.34554 Number of Imaginary frequency: 0 | | | | S-13 G(M062X/6-31G(d)): -1807.34936 Number of Imaginary frequency: 0 | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.47467500 | -0.68054900 | 0.55081600 | C | -0.69853800 | -0.49866000 | -1.60579700 |
| C | -0.93434200 | -0.15249800 | 0.81173900 | C | -0.07763900 | -0.42354700 | -0.20695700 |
| C | -1.14266200 | 1.24143200 | 0.26118400 | C | 1.39320700 | -0.72514900 | -0.34636100 |
| C | -0.41336300 | 1.59254600 | -1.02585300 | C | 2.03330700 | -0.17097500 | -1.60535600 |
| C | 0.92670500 | -0.43220700 | -0.89340300 | C | -0.06108300 | 0.55481800 | -2.52434900 |
| H | -1.09031800 | -0.17427600 | 1.89697000 | H | -0.56859800 | -1.14120500 | 0.46098000 |
| H | 0.47827600 | -1.75187000 | 0.78023300 | H | -1.77697200 | -0.31047000 | -1.54649000 |
| H | 1.99690200 | -0.66536400 | -0.96625600 | H | -0.06156400 | 0.11423800 | -3.53198900 |
| H | -1.05683400 | 1.31272100 | -1.88238700 | H | 2.11364500 | -0.99375000 | -2.34339300 |
| O | 0.85067500 | 0.95852400 | -1.15933700 | O | 1.27431300 | 0.88657200 | -2.15526200 |
| C | 0.22042300 | -1.21873900 | -2.01477600 | C | -0.78410400 | 1.91234600 | -2.54066500 |
| H | -0.86009300 | -1.27883600 | -1.84621400 | H | -0.40823700 | 2.49702800 | -1.69652800 |
| H | 0.39795500 | -0.65414600 | -2.93571500 | H | -0.52015200 | 2.43954600 | -3.46541400 |
| O | -1.81613300 | -1.09310600 | 0.19393100 | O | -0.33727300 | 0.89969600 | 0.24018200 |
| O | 1.30468400 | 0.00690100 | 1.46991100 | O | -0.45255800 | -1.77433200 | -2.18076700 |
| O | 0.75383400 | -2.50638100 | -2.26206000 | O | -2.19006700 | 1.78347300 | -2.48279600 |
| C | 2.60166600 | -0.53515500 | 1.63454600 | C | -1.53004100 | -2.69410400 | -2.06192900 |
| H | 2.78843000 | -0.59708500 | -2.71460400 | H | -2.45272200 | -2.24012300 | -2.45041400 |
| H | 2.64758400 | -1.56111600 | 1.24265700 | H | -1.26072100 | -3.53560900 | -2.70709800 |
| C | -3.15269000 | -1.01786500 | 0.63958100 | C | -0.06172100 | 1.11387400 | 1.61039600 |
| H | -3.18692300 | -1.06910500 | 1.73846000 | H | -0.78650900 | 0.57511600 | 2.23980300 |
| H | -3.60289400 | -0.05803500 | 0.34553700 | H | 0.94169000 | 0.73288000 | 1.85265900 |
| C | 0.51816500 | -3.47881200 | -1.26225100 | C | -2.79723900 | 2.27238600 | -1.29227900 |
| H | -0.36257500 | -3.21727600 | -0.65887200 | H | -2.03730900 | 2.53106000 | -0.54818100 |
| H | 0.28563000 | -4.41680000 | -1.78281900 | H | -3.35199700 | 3.18795800 | -1.54244400 |
| C | -3.96046000 | -2.15127700 | 0.05739400 | C | -0.12231500 | 2.59738500 | 1.86307300 |
| C | -5.20763900 | -2.43573300 | 0.62190000 | C | -0.84890300 | 3.12795700 | 2.92805000 |
| C | -3.52197300 | -2.90112300 | -1.03421800 | C | 0.57359400 | 3.46066500 | 1.00910100 |
| C | -6.00583800 | -3.45042200 | 0.10440100 | C | -0.87479500 | 4.50634000 | 3.14639500 |
| H | -5.55035100 | -1.85566200 | 1.47618100 | H | -1.39827600 | 2.46078500 | 3.58842100 |
| C | -4.32018000 | -3.92317300 | -1.55026400 | C | 0.54243000 | 4.83525300 | 1.22155100 |
| H | -2.55462700 | -2.68897300 | -1.48013600 | H | 1.13486000 | 3.03824600 | 0.17806100 |
| C | -5.56211900 | -4.20081500 | -0.98510600 | C | -0.18194100 | 5.36114300 | 2.29326400 |
| H | -6.97174700 | -3.65985700 | 0.55503700 | H | -1.44322400 | 4.91070000 | 3.97907200 |
| H | -3.96781300 | -4.50333700 | -2.39849300 | H | 1.08509000 | 5.49883600 | 0.55426900 |
| H | -6.18127000 | -4.99668500 | -1.38844900 | H | -0.20556400 | 6.43407400 | 2.45990100 |
| C | 3.68258100 | 0.30842700 | 0.99274100 | C | -1.74330600 | -3.16129700 | -0.64273400 |
| C | 3.40978000 | 1.57706100 | 0.48164100 | C | -0.77950200 | -3.96221000 | -0.02269800 |
| C | 4.99177100 | -0.18085300 | 0.94704100 | C | -2.85018500 | -2.73425900 | 0.09069300 |
| C | 4.43334300 | 2.34320100 | -0.07701200 | C | -0.92508700 | -4.33617000 | 1.31014300 |
| H | 2.38886300 | 1.94389600 | 0.50213200 | H | 0.09275600 | -4.28262900 | -0.58873800 |
| C | 6.01359700 | 0.58494000 | 0.39276900 | C | -2.99771400 | -3.10312300 | 1.42799700 |
| H | 5.20682000 | -1.16907800 | 1.34977100 | H | -3.59589200 | -2.10161700 | -0.38734500 |
| C | 5.73612400 | 1.85158900 | -0.12300800 | C | -2.03506800 | -3.90437000 | 2.03917200 |
| H | 4.20907900 | 3.32942500 | -0.47604900 | H | -0.16991900 | -4.95661000 | 1.78478100 |
| H | 7.02636800 | 0.19333800 | 0.36009800 | H | -3.86358100 | -2.76457300 | 1.99083600 |
| H | 6.53167700 | 2.44926100 | -0.55852500 | H | -2.14752200 | -4.19332800 | 3.08017500 |
| C | 1.72611200 | -3.69383600 | -0.37174100 | C | -3.74760400 | 1.26276700 | -0.69480400 |
| C | 1.57332000 | -4.23847800 | 0.90676700 | C | -3.72680900 | 1.00959600 | 0.67816800 |
| C | 3.00736800 | -3.37439400 | -0.82536400 | C | -4.69242600 | 0.61004400 | -1.49318700 |
| C | 2.68239400 | -4.45414300 | 1.72158000 | C | -4.66159900 | 0.14918500 | 1.25502900 |
| H | 0.57652900 | -4.48326000 | 1.26849700 | H | -2.97872900 | 1.50250600 | 1.29666900 |
| C | 4.11888000 | -3.59039200 | -0.01168100 | C | -5.62077700 | -0.25693400 | -0.92127800 |
| H | 3.12591500 | -2.94580000 | -1.81588600 | H | -4.70337600 | 0.79418000 | -2.56457100 |
| C | 3.95978100 | -4.12794300 | 1.26520700 | C | -5.61417100 | -0.48145800 | 0.45700800 |
| H | 2.54927500 | -4.87088500 | 2.71584600 | H | -4.64150700 | -0.03174200 | 2.32618600 |
| H | 5.11062900 | -3.33444300 | -0.37432500 | H | -6.35599800 | -0.75287900 | -1.54880800 |
| H | 4.82520200 | -4.29234100 | 1.90087200 | H | -6.34259800 | -1.15288700 | 0.90289000 |

| | | | | | | | |
|--|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -2.04608500 | 2.11597200 | 0.75674100 | C | 2.14530000 | -1.47865300 | 0.47910300 |
| C | -2.75051600 | 1.93683000 | 2.02546800 | C | 1.66580500 | -2.05394600 | 1.73206300 |
| C | -2.37843900 | 3.35752400 | -0.07421300 | C | 3.59465700 | -1.74026500 | 0.06136800 |
| C | -3.60569300 | 2.86133200 | 2.50140500 | C | 2.48470900 | -2.73889100 | 2.55295500 |
| H | -2.53889100 | 1.05466600 | 2.62063600 | H | 0.62912200 | -1.89138200 | 2.01392600 |
| C | -3.31581200 | 4.33130900 | 0.58330300 | C | 4.41555300 | -2.47448000 | 1.08419000 |
| H | -2.91576300 | 2.98076200 | -0.96467700 | H | 3.54426500 | -2.40098900 | -0.82491800 |
| C | -3.89776600 | 4.08687900 | 1.76290200 | C | 3.89332400 | -2.94763300 | 2.22217000 |
| H | -4.08649600 | 2.70830200 | 3.46327000 | H | 2.10501700 | -3.14081700 | 3.48797300 |
| H | -3.55582000 | 5.23359000 | 0.02721900 | H | 5.45756900 | -2.66154000 | 0.83798700 |
| H | -4.60162500 | 4.79602400 | 2.18860900 | H | 4.51120100 | -3.50660800 | 2.91922200 |
| C | -0.83869700 | 5.34387000 | -0.63353700 | C | 5.49189400 | 0.00118400 | -0.10460500 |
| C | 0.35940500 | 5.82930900 | -1.15530400 | C | 5.98048700 | 1.20373900 | -0.61757900 |
| C | 1.30943600 | 4.94368700 | -1.65654300 | C | 5.19333600 | 1.96997500 | -1.47211100 |
| C | 1.06429900 | 3.57186800 | -1.62603800 | C | 3.91121100 | 1.53760600 | -1.81094200 |
| C | -0.13363200 | 3.08477200 | -1.10301500 | C | 3.42476400 | 0.33816700 | -1.29837100 |
| C | -1.09542900 | 3.97327800 | -0.61330000 | C | 4.21603800 | -0.44191800 | -0.44590500 |
| H | -1.56500900 | 6.04223400 | -0.23030300 | H | 6.11026300 | -0.57936600 | 0.57318400 |
| H | 0.54999700 | 6.89850200 | -1.16189900 | H | 6.97494200 | 1.54092000 | -0.34015600 |
| H | 2.24489600 | 5.31694800 | -2.06335100 | H | 5.57129800 | 2.90732000 | -1.86966300 |
| H | 1.80562700 | 2.87251100 | -1.99683300 | H | 3.28162000 | 2.13112800 | -2.46559800 |
| R-14 G(M062X/6-31G(d)): -1907.261363 Number of Imaginary frequency: 0 | | | | S-14 G(M062X/6-31G(d)): -1907.35660 Number of Imaginary frequency: 0 | | | |
| C | 0.53455576 | -0.64650805 | 0.70101126 | C | -1.05974000 | -0.56292800 | -1.46140900 |
| C | -0.84426521 | -0.14735846 | 1.12990797 | C | -0.52509400 | -0.57007700 | -0.02071900 |
| C | -1.13564330 | 1.24191375 | 0.61728350 | C | 0.95258400 | -0.75250900 | -0.00997700 |
| C | -0.64893524 | 1.54370755 | -0.78634591 | C | 1.64354600 | -0.30016100 | -1.26633800 |
| C | 0.79748589 | -0.39987851 | -0.79367787 | C | -0.31938300 | 0.47329400 | -2.32852500 |
| H | -0.88858119 | -0.18150806 | 2.22560890 | H | -1.03478200 | -1.36636800 | 0.54584700 |
| H | 0.58825375 | -1.71737067 | 0.92898387 | H | -2.12742600 | -0.30165200 | -1.44082400 |
| H | 1.86182946 | -0.59475916 | -0.98345287 | H | -0.21759500 | 0.02784700 | -3.33161500 |
| H | -1.42247226 | 1.16431031 | -1.47825356 | H | 1.62632300 | -1.09082000 | -2.04895600 |
| O | 0.63076406 | 0.97975208 | -1.06787627 | O | 0.95800600 | 0.82546000 | -1.82550700 |
| C | 0.01223719 | -1.23045361 | -1.82915718 | C | -1.08159000 | 1.78485100 | -2.43089500 |
| H | -1.04134274 | -1.33753010 | -1.55314443 | H | -1.26032900 | 2.15688900 | -1.41548300 |
| H | 0.07554468 | -0.67002557 | -2.76742989 | H | -0.47045500 | 2.52188300 | -2.97382700 |
| O | -1.73488596 | -1.12477324 | 0.58352415 | O | -1.00058200 | 0.69682900 | 0.49135200 |
| O | 1.47139834 | 0.05697278 | 1.49963897 | O | -0.90335500 | -1.82383700 | -2.09641900 |
| O | 0.57815856 | -2.49744951 | -2.11492105 | O | -2.29750500 | 1.55510300 | -3.11630100 |
| C | 2.75902066 | -0.52240921 | 1.57365759 | C | -1.69139200 | -2.86766800 | -1.55566900 |
| H | 3.03947661 | -0.55925368 | 2.63462798 | H | -2.53896200 | -2.46453600 | -0.98434400 |
| H | 2.73734559 | -1.56031196 | 1.21300436 | H | -2.11085400 | -3.41500900 | -2.41021400 |
| C | -3.12954545 | -0.82948146 | 0.62674619 | C | -0.69391300 | 0.93809600 | 1.84182800 |
| H | -3.47266653 | -0.82180470 | 1.67312075 | H | -1.39995900 | 0.41606100 | 2.50856100 |
| H | -3.32969643 | 0.13731929 | 0.15179802 | H | 0.31572600 | 0.56419100 | 2.06725900 |
| O | 0.42670152 | -3.47889983 | -1.10927617 | H | -3.23923600 | 2.59721200 | -2.91168000 |
| H | -0.40774050 | -3.22826559 | -0.43912817 | C | -2.79396900 | 3.57078600 | -3.16446500 |
| H | 0.16435116 | -4.41682442 | -1.61605350 | H | -4.05348100 | 2.40045800 | -3.61588800 |
| C | -3.82622885 | -1.90608686 | -0.16527254 | C | -0.74473600 | 2.42642500 | 2.07924500 |
| C | -4.31520464 | -1.60424917 | -1.44017721 | C | -1.35121700 | 2.96995400 | 3.21113000 |
| C | -3.95137559 | -3.20580929 | 0.33340004 | C | -0.15961800 | 3.28135000 | 1.13892000 |
| C | -4.93285141 | -2.59695524 | -2.20163814 | C | -1.37428400 | 4.35164400 | 3.40651700 |
| H | -4.19576708 | -0.57983122 | -1.79739834 | H | -1.81502800 | 2.30918000 | 3.94022900 |
| C | -4.56562330 | -4.19613130 | -0.42943911 | C | -0.19118000 | 4.66038500 | 1.32634500 |
| H | -3.56713062 | -3.43800903 | 1.32446431 | H | 0.31150700 | 2.84326800 | 0.26134000 |
| C | -5.05892408 | -3.89127894 | -1.69919530 | C | -0.79967900 | 5.19978900 | 2.46179500 |
| H | -5.31672852 | -2.36118143 | -3.19057101 | H | -1.84990600 | 4.76523300 | 4.29144500 |
| H | -4.66377922 | -5.20384465 | -0.03564952 | H | 0.26053300 | 5.31843700 | 0.58904500 |
| H | -5.54126467 | -4.66235377 | -2.29327964 | H | -0.82441600 | 6.27582500 | 2.60806400 |
| C | 3.81193057 | 0.25781237 | 0.81370265 | C | -0.89328400 | -3.83067400 | -0.70212800 |
| C | 3.50640709 | 1.44819301 | 0.15429717 | C | 0.43709400 | -4.11293700 | -1.02178100 |
| C | 5.12773008 | -0.21706141 | 0.79332108 | C | -1.48602000 | -4.48754100 | 0.37761900 |
| C | 4.50341349 | 2.14975328 | -0.52577922 | C | 1.16030800 | -5.04263500 | -0.27869800 |
| H | 2.48013892 | 1.80177449 | 0.15605369 | H | 0.91365700 | -3.58469800 | -1.84129600 |
| C | 6.12192189 | 0.48375948 | 0.11649362 | C | -0.76886200 | -5.43091900 | 1.11458500 |
| H | 5.37069209 | -1.14265643 | 1.31219649 | H | -2.51690300 | -4.26077600 | 0.64228000 |
| C | 5.81156268 | 1.67223306 | -0.54707106 | C | 0.55503800 | -5.71360500 | 0.78517300 |
| H | 4.25308944 | 3.07406121 | -1.03995818 | H | 2.20025000 | -5.23323300 | -0.52806000 |

| | | | | | | | |
|---------------------------------------|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | 7.13948638 | 0.10360815 | 0.10565553 | H | -1.24315600 | -5.93543200 | 1.95170900 |
| H | 6.58610573 | 2.21950155 | -1.07636834 | H | 1.11935600 | -6.43886600 | 1.36481600 |
| C | 1.70150797 | -3.68879787 | -0.31586364 | C | -3.75584500 | 2.61306300 | -1.49058400 |
| C | 1.65203381 | -4.24646106 | 0.96509414 | C | -3.45331400 | 3.65858300 | -0.61742700 |
| C | 2.94159345 | -3.35180563 | -0.86240214 | C | -4.47524500 | 1.51384500 | -1.01058600 |
| C | 2.82234659 | -4.45992065 | 1.69031853 | C | -3.85781400 | 3.60780500 | 0.71665300 |
| H | 0.68807262 | -4.50230657 | 1.40046611 | H | -2.88022900 | 4.50974700 | -0.97975100 |
| C | 4.11455580 | -3.56668108 | -0.13899257 | C | -4.87888400 | 1.45768900 | 0.32041100 |
| H | 2.97940509 | -2.91120484 | -1.85393520 | H | -4.70778200 | 0.69398500 | -1.68707200 |
| C | 4.05852692 | -4.11880431 | 1.14016713 | C | -4.56502900 | 2.50479100 | 1.18900200 |
| H | 2.76940880 | -4.88521580 | 2.68839021 | H | -3.60299800 | 4.42270100 | 1.38892400 |
| H | 5.07303304 | -3.29720531 | -0.57401865 | H | -5.43426600 | 0.59725700 | 0.68293200 |
| H | 4.97144492 | -4.28102181 | 1.70591049 | H | -4.87024300 | 2.45935800 | 2.23071500 |
| C | -2.00285889 | 2.09162410 | 1.21003066 | C | 1.65562300 | -1.51402400 | 0.90622500 |
| C | -2.56252522 | 1.89056464 | 2.54400399 | C | 1.05743200 | -2.20906100 | 2.02653900 |
| C | -2.54273353 | 3.25850807 | 0.38710794 | C | 3.10362500 | -1.65839400 | 0.79212300 |
| C | -3.43194347 | 2.76424919 | 3.08987536 | C | 1.77250100 | -3.08493500 | 2.80441600 |
| H | -2.24095800 | 1.03134093 | 3.12390672 | H | 0.00243500 | -2.05480800 | 2.23931300 |
| C | -3.42673949 | 4.20721322 | 1.13298959 | C | 3.78964300 | -2.57772200 | 1.61014900 |
| H | -3.16350421 | 2.72857250 | -0.38305225 | H | 3.13547800 | -2.88196700 | -0.74954600 |
| C | -3.86747594 | 3.95897494 | 2.37400652 | C | 3.15167600 | -3.32371000 | 2.58555700 |
| H | -3.81069119 | 2.59349324 | 4.09384399 | H | 1.25977000 | -3.61400700 | 3.60608700 |
| H | -3.77159362 | 5.09073192 | 0.60141030 | H | 4.86063300 | -2.70559800 | 1.46178500 |
| H | -4.55553303 | 4.64018014 | 2.86640140 | H | 3.69723700 | -4.04285400 | 3.18730500 |
| C | -1.27015023 | 5.28033236 | -0.57027246 | C | 5.16956700 | -0.36395600 | 0.13215100 |
| C | -0.22412596 | 5.79538531 | -1.33496044 | C | 5.79268000 | 0.62145900 | -0.62211600 |
| C | 0.68607145 | 4.93202500 | -1.93816155 | C | 5.06430500 | 1.35222100 | -1.56335100 |
| C | 0.55110439 | 3.55531049 | -1.76608635 | C | 3.71300500 | 1.07144900 | -1.74263600 |
| C | -0.49755002 | 3.03696464 | -1.00530322 | C | 3.08309600 | 0.06975200 | -1.00331200 |
| C | -1.42298947 | 3.90212638 | -0.40770805 | C | 3.80689500 | -0.67283300 | -0.04343600 |
| H | -1.96003469 | 5.96589248 | -0.08812026 | H | 5.74246000 | -0.88296800 | 0.89519900 |
| H | -0.11963842 | 6.87044483 | -1.45038709 | H | 6.84554300 | 0.83595900 | -0.45948600 |
| H | 1.50398661 | 5.32613057 | -2.53452687 | H | 5.54539500 | 2.13132100 | -2.14768300 |
| H | 1.26415671 | 2.87369135 | -2.21713273 | H | 3.12631400 | 1.62623800 | -2.46882500 |
| F | -3.52484623 | 1.36811324 | -1.52578409 | F | 3.24277600 | -3.20858900 | -1.63997600 |
| R-TS9 | | | | S-TS9 | | | |
| G(M062X/6-31G(d)): -1907.24255 | | | | G(M062X/6-31G(d)): -1907.25532 | | | |
| Number of Imaginary frequency: -46.16 | | | | Number of Imaginary frequency: -208.81 | | | |
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| C | -0.55520700 | 0.70069500 | 0.66145800 | C | 0.35270500 | 1.16003900 | -0.35620400 |
| C | 0.93463600 | 0.62543900 | 1.02422600 | C | -0.89099500 | 0.90309600 | 0.51178100 |
| C | 1.53405700 | -0.65736300 | 0.50129300 | C | -1.99342300 | 0.33911800 | -0.34332100 |
| C | 1.23580800 | -0.84928900 | -0.96203100 | C | -1.53005900 | -0.62931700 | -1.41846800 |
| C | -0.82013700 | 0.37826500 | -0.81962300 | C | 0.77927700 | -0.11440100 | -1.13902300 |
| H | 1.00475800 | 0.69731000 | 2.11606200 | H | -1.18977600 | 1.85538700 | 0.96862200 |
| H | -0.91918000 | 1.71360000 | 0.89129900 | H | 1.17375400 | 1.48286400 | 0.29427000 |
| H | -1.89278100 | 0.17755900 | -0.93950500 | H | 0.98987100 | 0.19102300 | -2.17683200 |
| H | 1.65565200 | 0.00194700 | -1.52589300 | H | -1.54333200 | -0.08731200 | -2.38348600 |
| O | -0.18681600 | -0.84552100 | -1.17486300 | O | -0.22186300 | -1.12788300 | -1.13955900 |
| C | -0.46442600 | 1.50253000 | -1.82094300 | C | 2.02649200 | -0.77881900 | -0.56253800 |
| H | 0.30315300 | 2.17782300 | -1.42688300 | H | 1.88300400 | -0.97952700 | 0.50861700 |
| H | -0.07238900 | 1.01479400 | -2.72029600 | H | 2.19218700 | -1.73754100 | -1.07272800 |
| O | 1.55407200 | 1.76296400 | 0.43028100 | O | -0.43773300 | 0.01647900 | 1.55682000 |
| O | -1.17653300 | -0.25258100 | 1.50520800 | O | -0.00149000 | 2.21866200 | -1.25268900 |
| O | -1.58242900 | 2.25555800 | -2.25885800 | O | 3.12242200 | 0.10655900 | -0.76333700 |
| C | -2.57529400 | -0.10425200 | 1.66241200 | C | 1.10761600 | 2.98735300 | -1.71853100 |
| H | -2.78813600 | 0.10226500 | 2.72010100 | H | 1.93314900 | 2.33672000 | -2.03621100 |
| H | -2.93378500 | 0.75980600 | 1.08948800 | H | 0.73600300 | 3.50544700 | -2.61080100 |
| C | 2.88077600 | 1.97684800 | 0.87734700 | C | -1.37879700 | -0.17792800 | 2.60565100 |
| C | 2.88399600 | 2.24660700 | 1.94387900 | C | 1.60885000 | 4.00045700 | -0.70433600 |
| H | 3.46537500 | 1.05139500 | 0.76749200 | C | 0.70133400 | 4.79224400 | 0.01500300 |
| C | -2.01848500 | 3.26851200 | -1.37507300 | C | 2.98068400 | 4.18912000 | -0.49694600 |
| H | -1.19155600 | 3.61423000 | -0.73827500 | C | 1.15689200 | 5.75278200 | 0.91877700 |
| H | -2.32062800 | 4.11786200 | -2.00127200 | H | -0.36529400 | 4.64838800 | -0.13581200 |
| C | 3.49761800 | 3.07646400 | 0.05220100 | C | 3.44068900 | 5.15566000 | 0.40264000 |
| C | 4.26801600 | 4.07387100 | 0.65036000 | H | 3.69372200 | 3.57518100 | -1.04296500 |
| C | 3.32496100 | 3.08911300 | -1.33539500 | C | 2.52958100 | 5.93939600 | 1.11362100 |
| C | 4.86350700 | 5.06857700 | -0.12490800 | H | 0.44208800 | 6.35910300 | 1.46966400 |
| H | 4.40019800 | 4.07394600 | 1.72970600 | H | 4.50915100 | 5.28901600 | 0.55278400 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 3.91186400 | 4.08548700 | -2.11000500 | H | 2.88431300 | 6.68880100 | 1.81653800 |
| H | 2.72474500 | 2.31309300 | -1.80455000 | C | -3.31197500 | 0.67801900 | -0.32617600 |
| C | 4.68489700 | 5.07794200 | -1.50628300 | C | -3.90838600 | 1.64967300 | 0.57649600 |
| H | 5.45931600 | 5.84079900 | 0.35326600 | C | -4.21588500 | 0.02917200 | -1.37163800 |
| H | 3.76862600 | 4.08734700 | -3.18678500 | C | -5.22955800 | 1.95906700 | 0.52614600 |
| H | 5.14361100 | 5.85530700 | -2.11040100 | H | -3.27629600 | 2.12889000 | 1.31880400 |
| C | -3.33244500 | -1.33666900 | 1.22302200 | C | -5.65490500 | 0.37533000 | -1.26757600 |
| C | -2.75497500 | -2.28311900 | 0.37561300 | C | -6.12561400 | 1.31377500 | -0.41648700 |
| C | -4.65359900 | -1.51270500 | 1.64653700 | H | -5.63771400 | 2.69539600 | 1.21528100 |
| C | -3.49660200 | -3.38670100 | -0.04924600 | H | -6.33477100 | -0.10321300 | -1.97010700 |
| H | -1.72608500 | -2.14563600 | 0.05213300 | H | -7.17602200 | 1.59523200 | -0.42133500 |
| C | -5.39359400 | -2.61121100 | 1.21907100 | C | -4.82083800 | -2.47311500 | -1.62780800 |
| H | -5.10156400 | -0.78208500 | 2.31747200 | C | -4.41714700 | -3.80463100 | -1.77182300 |
| C | -4.81497200 | -3.55379800 | 0.36786100 | C | -3.05908600 | -4.12676500 | -1.79497800 |
| H | -3.03996000 | -4.11949900 | -0.70897800 | C | -2.10641100 | -3.11016700 | -1.67257200 |
| H | -6.41899000 | -2.73669100 | 1.55531400 | C | -2.50797900 | -1.78006000 | -1.53933900 |
| H | -5.38885100 | -4.41490100 | 0.03777200 | C | -3.87724400 | -1.44338100 | -1.51827800 |
| C | -3.19461700 | 2.84742400 | -0.51910000 | H | -5.88182000 | -2.24353000 | -1.58514200 |
| C | -3.40035500 | 3.42993300 | 0.73379500 | H | -5.16716500 | -4.58798000 | -1.85355700 |
| C | -4.11054300 | 1.90257700 | -0.98972300 | H | -2.74097900 | -5.16084200 | -1.90392400 |
| C | -4.50324500 | 3.07211700 | 1.50819000 | H | -1.04649700 | -3.34474500 | -1.68096000 |
| H | -2.68660100 | 4.16045400 | 1.10886800 | H | -3.80563100 | 0.49056000 | -2.39765500 |
| C | -5.21036200 | 1.53923200 | -0.21501700 | F | -2.96654000 | 0.92948700 | -3.53070700 |
| H | -3.94711700 | 1.44400500 | -1.96075300 | C | 4.32899500 | -0.31750500 | -0.14000100 |
| C | -5.40982400 | 2.12341800 | 1.03638900 | H | 4.98176500 | 0.56397300 | -0.15932400 |
| H | -4.64895100 | 3.52737700 | 2.48366500 | H | 4.14755800 | -0.56834000 | 0.91587400 |
| H | -5.91091400 | 0.79640200 | -0.58640500 | C | 5.01276200 | -1.48097500 | -0.83724300 |
| H | -6.26703000 | 1.83996900 | 1.64030200 | C | 5.70942100 | -2.44273800 | -0.09531400 |
| C | 2.21148100 | -1.55620700 | 1.24270200 | C | 4.99378300 | -1.58685600 | -2.23491800 |
| C | 2.38958700 | -1.43349200 | 2.69924600 | C | 6.38441600 | -3.48552000 | -0.73583600 |
| C | 2.83979300 | -2.78558300 | 0.65435400 | H | 5.72295500 | -2.37552900 | 0.99063300 |
| C | 2.51879400 | -2.54249600 | 3.45508300 | C | 5.65873000 | -2.63308300 | -2.87688100 |
| H | 2.35300500 | -0.45538200 | 3.16957200 | H | 4.44590300 | -0.84946900 | -2.81540500 |
| C | 2.59550700 | -3.99578400 | 1.51992300 | C | 6.35954500 | -3.58434000 | -2.12906700 |
| C | 2.49029400 | -3.87350600 | 2.85208600 | H | 6.92098700 | -4.22459900 | -0.14606100 |
| H | 2.60463100 | -2.45714200 | 4.53547800 | H | 5.63109400 | -2.70575400 | -3.96131800 |
| H | 2.61087200 | -4.97472000 | 1.04603400 | H | 6.87835400 | -4.39840000 | -2.62874800 |
| H | 2.40193300 | -4.74462200 | 3.49478900 | H | -2.27763400 | -0.69196300 | 2.23826800 |
| C | 3.18720600 | -4.07938200 | -1.45373200 | H | -1.70207300 | 0.80211300 | 2.99670500 |
| C | 2.95376700 | -4.33120500 | -2.79821800 | C | -0.73120500 | -0.98532200 | 3.70689300 |
| C | 2.11203600 | -3.48873500 | -3.53245500 | C | -1.38224800 | -2.09625800 | 4.25597600 |
| C | 1.55065500 | -2.37939000 | -2.91530400 | C | 0.52252900 | -0.61610300 | 4.21699400 |
| C | 1.78016400 | -2.12191600 | -1.55758600 | C | -0.79970200 | -2.82172100 | 5.29966700 |
| C | 2.56026900 | -3.00195900 | -0.80773500 | H | -2.35079300 | -2.39718600 | 3.86301900 |
| H | 3.91264500 | -4.64622500 | -0.87666100 | C | 1.11003700 | -1.34255000 | 5.25332300 |
| H | 3.44116700 | -5.17097500 | -3.28612300 | H | 1.03821200 | 0.24088400 | 3.79228200 |
| H | 1.92450700 | -3.68173800 | -4.58483300 | C | 0.44882600 | -2.44751700 | 5.80016000 |
| H | 0.92820100 | -1.69111300 | -3.48271100 | H | -1.31897900 | -3.68204700 | 5.71445400 |
| H | 3.98074700 | -2.77507400 | 0.70194800 | H | 2.08298400 | -1.04595300 | 5.63734700 |
| F | 5.37401400 | -3.64018700 | 0.47780800 | H | 0.90565800 | -3.01237000 | 6.60874300 |
| R-15 G(M062X/6-31G(d)): -1907.28408 Number of Imaginary frequency: 0 | | | | S-15 G(M062X/6-31G(d)): -1907.28469 Number of Imaginary frequency: 0 | | | |
| C | 0.91567000 | 0.52102900 | -0.58922500 | C | 1.35346900 | -0.49054100 | -0.72661300 |
| C | -0.55492000 | 0.51804700 | -1.03465100 | C | 0.37349500 | 0.08348300 | 0.31194200 |
| C | -1.27382700 | -0.69248600 | -0.53788600 | C | -0.97049900 | 0.24188000 | -0.30491600 |
| C | -1.04011100 | -0.92702200 | 0.91501000 | C | -1.25983200 | -0.74328700 | -1.40848500 |
| C | 1.09275600 | 0.16881400 | 0.89902800 | C | 0.84775700 | -1.85051000 | -1.24109300 |
| H | -0.54405600 | 0.57237000 | -2.13105600 | H | 0.76165600 | 1.03350400 | 0.70407500 |
| H | 1.34144200 | 1.51507200 | -0.78677000 | H | 2.34920200 | -0.61314000 | -0.28142900 |
| H | 2.15218000 | -0.07032200 | 1.07202300 | H | 1.18533900 | -1.91646900 | -2.28867000 |
| H | -1.39916500 | -0.07114500 | 1.52228800 | H | -0.89697500 | -0.36634500 | -2.38700000 |
| O | 0.38487900 | -1.01842300 | 1.21556800 | O | -0.56084600 | -1.97927400 | -1.17909300 |
| C | 0.73694800 | 1.29816000 | 1.89253800 | C | 1.39242300 | -3.05860300 | -0.47905700 |
| H | -0.09740900 | 1.91110200 | 1.53346300 | H | 1.00224000 | -3.05048800 | 0.54315200 |
| H | 0.43831900 | 0.80978200 | 2.82638400 | H | 1.03924500 | -3.96855900 | -0.97751300 |
| O | -1.10207700 | 1.75676400 | -0.52889100 | O | 0.44653400 | -0.87413100 | 1.40298900 |
| O | 1.55199400 | -0.43936900 | -1.42072900 | O | 1.45685100 | 0.36414600 | -1.86022000 |
| O | 1.83022200 | 2.13340400 | 2.23943400 | O | 2.80862000 | -3.07415800 | -0.49355800 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 2.96167800 | -0.36952500 | -1.46474700 | C | 2.56124300 | 1.24528700 | -1.85736300 |
| H | 3.26631600 | -0.26456100 | -2.51546800 | H | 3.48945600 | 0.69478100 | -1.64521500 |
| H | 3.32009200 | 0.52467600 | -0.93947000 | H | 2.62584500 | 1.62609900 | -2.88282000 |
| C | -2.42648500 | 1.98585700 | -0.96451300 | C | -0.30537300 | -0.51876200 | 2.53870500 |
| H | -2.45046300 | 2.13773200 | -2.05587200 | H | 0.17772100 | -1.02358900 | 3.38557300 |
| H | -3.05306400 | 1.11081600 | -0.73781100 | H | -0.23142500 | 0.56271300 | 2.72841900 |
| C | 2.17371800 | 3.12292000 | 1.29198300 | C | 3.42327200 | -2.68825200 | 0.71939100 |
| H | 1.32740500 | 3.33829400 | 0.62423000 | H | 2.74025500 | -2.06463300 | 1.31345400 |
| H | 2.38210100 | 4.04243600 | 1.85484800 | H | 3.65291800 | -3.57971200 | 1.32233200 |
| C | -2.96617000 | 3.20235000 | -0.25836000 | C | -1.76681700 | -0.92719000 | 2.50572600 |
| C | -3.53462300 | 4.26009500 | -0.96788300 | C | -2.68923000 | -0.24560500 | 3.30244400 |
| C | -2.91533300 | 3.27240000 | 1.13821300 | C | -2.20858100 | -1.99646600 | 1.72286500 |
| C | -4.05094800 | 5.36926200 | -0.29708000 | C | -4.03220300 | -0.62385800 | 3.32195700 |
| H | -3.57220700 | 4.21621200 | -2.05383300 | H | -2.35701500 | 0.59894800 | 3.90349400 |
| C | -3.42252000 | 4.38023400 | 1.81013500 | C | -3.54921100 | -2.37538400 | 1.74108100 |
| H | -2.47513700 | 2.44763700 | 1.69468200 | H | -1.50512800 | -2.48677300 | 1.05507400 |
| C | -3.99386900 | 5.43281600 | 1.09274200 | C | -4.46685900 | -1.69171200 | 2.54005900 |
| H | -4.49266200 | 6.18530000 | -0.86203500 | H | -4.73842900 | -0.07582000 | 3.93968000 |
| H | -3.37695100 | 4.42336300 | 2.89470100 | H | -3.88428500 | -3.19697800 | 1.11247300 |
| C | -4.39240400 | 6.29705900 | 1.61625700 | H | -5.51336900 | -1.98326900 | 2.54331400 |
| C | 3.62360600 | -1.59610700 | -0.87332500 | C | 2.42061000 | 2.39862600 | -0.89154300 |
| C | 2.89028400 | -2.54240800 | -0.15741500 | C | 1.26203000 | 3.18338300 | -0.90442800 |
| C | 5.00039900 | -1.78044600 | -1.03994300 | C | 3.43126900 | 2.68461100 | 0.02532400 |
| C | 3.52962100 | -3.65542300 | 0.39129100 | C | 1.13253200 | 4.25246100 | -0.02274200 |
| H | 1.82339100 | -2.38658100 | -0.02062900 | H | 0.45186800 | 2.93009600 | -1.58622100 |
| C | 5.63700200 | -2.89018000 | -0.49160700 | C | 3.30176300 | 3.75470000 | 0.91139200 |
| H | 5.57472200 | -1.04802800 | -1.60479500 | H | 4.32280200 | 2.06068700 | 0.04890000 |
| C | 4.90092300 | -3.83391200 | 0.22669700 | C | 2.15342600 | 4.54223700 | 0.88563600 |
| H | 2.95088300 | -4.38637300 | 0.94967700 | H | 0.22790800 | 4.85409100 | -0.03287600 |
| H | 6.70688000 | -3.02219800 | -0.62760300 | H | 4.09336700 | 3.96627800 | 1.62454600 |
| H | 5.39506700 | -4.70162200 | 0.65417800 | H | 2.04785800 | 5.37404500 | 1.57603400 |
| C | 3.39904300 | 2.75292500 | 0.48226000 | C | 4.69198200 | -1.91158300 | 0.45026100 |
| C | 3.58340300 | 3.27489900 | -0.80057900 | C | 5.51483000 | -1.55225600 | 1.52318300 |
| C | 4.37146400 | 1.90511800 | 1.01811400 | C | 5.04574700 | -1.51224600 | -0.83867700 |
| C | 4.71869500 | 2.94999100 | -1.54071800 | C | 6.66710300 | -0.80211500 | 1.31133300 |
| H | 2.82549600 | 3.92953000 | -1.22617900 | H | 5.24553900 | -1.86176500 | 2.53106900 |
| C | 5.50714200 | 1.57709300 | 0.27884600 | C | 6.20400200 | -0.76257900 | -1.05292500 |
| H | 4.22273700 | 1.49034200 | 2.01072000 | H | 4.40836900 | -1.79233300 | -1.67154600 |
| C | 5.68269600 | 2.09679900 | -1.00374600 | C | 7.01646900 | -0.40341600 | 0.01947300 |
| H | 4.84569800 | 3.35530200 | -2.54051600 | H | 7.29493500 | -0.52831600 | 2.15442900 |
| H | 6.25170100 | 0.90768400 | 0.70094300 | H | 6.46885700 | -0.46004700 | -2.06235700 |
| H | 6.56453800 | 1.83681800 | -1.58226200 | H | 7.91792300 | 0.17887000 | -0.14780600 |
| C | -2.14647800 | -1.46186600 | -1.29115300 | C | -1.88913500 | 1.22113700 | 0.01358700 |
| C | -2.47420900 | -1.17500700 | -2.67389700 | C | -1.63952900 | 2.33313400 | 0.90946500 |
| C | -2.85107600 | -2.60351400 | -0.71915800 | C | -3.23834600 | 1.18682300 | -0.55265700 |
| C | -3.39289000 | -1.90425200 | -3.38500900 | C | -2.53776000 | 3.35743100 | 1.07698700 |
| H | -1.98876600 | -0.33738300 | -3.16531000 | H | -0.69116000 | 2.38008700 | 1.43675800 |
| C | -3.78698800 | -3.31775400 | -1.49338300 | C | -4.11847500 | 2.26827600 | -0.35646000 |
| C | -4.08178800 | -2.99431400 | -2.80603600 | C | -3.79077700 | 3.36720400 | 0.41757400 |
| H | -3.60224500 | -1.62361200 | -4.41565300 | H | -2.27181700 | 4.18487100 | 1.73294900 |
| H | -4.32093900 | -4.14623300 | -1.03552200 | H | -5.09399300 | 2.23605400 | -0.83833800 |
| H | -4.82274300 | -3.55372500 | -3.36681800 | H | -4.48016300 | 4.19641400 | 0.53506700 |
| C | -3.03184400 | -4.17229100 | 1.25098100 | C | -5.04691000 | -0.41353500 | -1.27779600 |
| C | -2.72785800 | -4.52653600 | 2.55493800 | C | -5.45129600 | -1.64841300 | -1.76612800 |
| C | -1.89297500 | -3.71423100 | 3.32906900 | C | -4.50085200 | -2.60618800 | -2.12709100 |
| C | -1.37048700 | -2.56241800 | 2.75967600 | C | -3.15016500 | -2.30159300 | -1.99212000 |
| C | -1.66716400 | -2.19373300 | 1.44193900 | C | -2.73327400 | -1.05660200 | -1.51631700 |
| C | -2.52608900 | -2.99306300 | 0.65841000 | C | -3.68311600 | -0.07896100 | -1.14994200 |
| H | -3.66603300 | -4.83669400 | 0.67352400 | H | -5.80446100 | 0.29309200 | -0.95199200 |
| H | -3.13828100 | -5.44301200 | 2.97033800 | H | -6.51177000 | -1.87241300 | -1.84658800 |
| H | -1.65281400 | -3.98251100 | 4.35366000 | H | -4.81135600 | -3.57680600 | -2.50312500 |
| H | -0.70517900 | -1.92313700 | 3.33496100 | H | -2.39326700 | -3.03488100 | -2.25409100 |
| H | -4.31061300 | -1.24099800 | -0.61177500 | H | -2.29573700 | 1.99819500 | -2.05970000 |
| F | -4.91404000 | -0.50736900 | -0.58887700 | F | -1.75815000 | 2.18052800 | -2.82518400 |
| R-16 G(M062X/6-31G(d)): -1806.88705 Number of Imaginary frequency: 0 | | | | S-16 G(M062X/6-31G(d)): -1806.88217 Number of Imaginary frequency: 0 | | | |
| C | 0.66816400 | 0.48972600 | -0.52779000 | C | -1.01701300 | 0.15704600 | -1.14547100 |
| C | -0.81484000 | 0.42742400 | -0.92554000 | C | -0.24163400 | -0.18263700 | 0.13382400 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -1.46862500 | -0.82571500 | -0.44503800 | C | 1.09669900 | -0.74255300 | -0.20117600 |
| C | -1.14011500 | -1.14731300 | 0.97178500 | C | 1.60869000 | -0.34518700 | -1.55795600 |
| C | 0.91115600 | 0.09718200 | 0.93973400 | C | -0.20574600 | 1.10134100 | -2.04927200 |
| H | -0.83496800 | 0.50252600 | -2.02059400 | H | -0.84330800 | -0.86850000 | 0.74707900 |
| H | 1.03227400 | 1.50940400 | -0.71159000 | H | -1.95031300 | 0.66023700 | -0.88081200 |
| H | 1.99021300 | -0.06066000 | 1.08049500 | H | -0.47275200 | 0.82879300 | -3.08343200 |
| H | -1.52302400 | -0.37367200 | 1.66640100 | H | 1.17793500 | -0.97832700 | -2.36516500 |
| O | 0.30524100 | -1.15451500 | 1.21039200 | O | 1.19878700 | 0.99538400 | -1.87566700 |
| C | 0.48510100 | 1.14490700 | 1.99216600 | C | -0.51208200 | 2.58520900 | -1.82335400 |
| H | -0.43850900 | 1.65868200 | 1.70340900 | H | -0.07147300 | 2.88693600 | -0.86892300 |
| H | 0.30513400 | 0.59658000 | 2.92285300 | H | -0.02951600 | 3.16313400 | -2.62147500 |
| O | -1.39023900 | 1.64802300 | -0.39343300 | O | -0.22783100 | 1.10466500 | 0.81908800 |
| O | 1.33208600 | -0.41078000 | -1.40491800 | O | -1.33186500 | -1.01338500 | -1.89558900 |
| O | 1.48553900 | 2.09914200 | 2.31128300 | O | -1.90207000 | 2.85181500 | -1.85725800 |
| C | 2.71925400 | -0.20045900 | -1.56081800 | C | -2.63127000 | -1.52659800 | -1.70011600 |
| H | 2.92873700 | -0.11176200 | -2.63596000 | H | -3.35784100 | -0.70984200 | -1.56818800 |
| H | 3.02179600 | 0.74941800 | -1.09986900 | H | -2.89284000 | -2.04137400 | -2.63336800 |
| C | -2.68414600 | 1.88526900 | -0.88415000 | C | 0.45461300 | 1.12314900 | 2.05232400 |
| H | -2.65999700 | 2.00355000 | -1.98120100 | H | -0.26164600 | 1.08638100 | 2.88722700 |
| H | -3.33686400 | 1.02350400 | -0.67478500 | H | 1.10571200 | 0.24330000 | 2.13284900 |
| C | 1.69312900 | 3.11982900 | 1.35825000 | C | -2.49456500 | 3.21565100 | -0.61289500 |
| H | 0.81593700 | 3.23266900 | 0.70444300 | H | -1.76490900 | 3.12341100 | 0.19901500 |
| H | 1.80324500 | 4.05985300 | 1.91544400 | H | -2.80644500 | 4.26715700 | -0.67674000 |
| C | -3.26779200 | 3.12827400 | -0.25753000 | C | 1.30956900 | 2.36444900 | 2.14670500 |
| C | -4.48833100 | 3.62174400 | -0.73202000 | C | 1.36770000 | 3.12446400 | 3.31497000 |
| C | -2.63208300 | 3.79430900 | 0.79086700 | C | 2.09470100 | 2.73644200 | 1.04877200 |
| C | -5.06300600 | 4.75623800 | -0.16839000 | C | 2.20352100 | 4.23915500 | 3.39390500 |
| H | -4.98979400 | 3.10927600 | -1.55051600 | H | 0.75418200 | 2.84423700 | 4.16839500 |
| C | -3.20767000 | 4.93240400 | 1.35743100 | C | 2.92731800 | 3.84949600 | 1.12655800 |
| H | -1.68300500 | 3.41950500 | 1.16126800 | H | 2.03301000 | 2.14508500 | 0.13587400 |
| C | -4.42279900 | 5.41740900 | 0.88143200 | C | 2.98471800 | 4.60426600 | 2.29981500 |
| H | -6.01053400 | 5.12742700 | -0.54848000 | H | 2.23769900 | 4.82516900 | 4.30804300 |
| H | -2.70150600 | 5.44072400 | 2.17336400 | H | 3.53445300 | 4.13099800 | 0.27044400 |
| H | -4.86910100 | 6.30421900 | 1.32179100 | H | 3.63241300 | 5.47435400 | 2.35748400 |
| C | 3.55924400 | -1.32182500 | -0.98672400 | C | -2.75485100 | -2.50988400 | -0.55434800 |
| C | 2.99950100 | -2.32542700 | -0.19578200 | C | -1.66196300 | -3.27829500 | -0.14860000 |
| C | 4.93300100 | -1.34537400 | -1.25080200 | C | -3.99100200 | -2.70686500 | 0.06569600 |
| C | 3.80895500 | -3.33297500 | 0.33287100 | C | -1.80261400 | -4.22630500 | 0.86357100 |
| H | 1.93267300 | -2.29916300 | 0.01232100 | H | -0.69512500 | -3.10986000 | -0.61679900 |
| C | 5.73882800 | -2.34932900 | -0.72234600 | C | -4.13571900 | -3.65855500 | 1.07376100 |
| H | 5.37116600 | -0.56883200 | -1.87572600 | H | -4.84470800 | -2.10646300 | -0.24194900 |
| C | 5.17700200 | -3.34883600 | 0.07393800 | C | -3.04035000 | -4.42222700 | 1.47533900 |
| H | 3.36439200 | -4.10908900 | 0.95028700 | H | -0.94031900 | -4.80913000 | 1.17597900 |
| H | 6.80438100 | -2.35586100 | -0.93444400 | H | -5.10227200 | -3.79886600 | 1.54956500 |
| H | 5.80410000 | -4.13451300 | 0.48551800 | H | -3.14978500 | -5.16185800 | 2.26300400 |
| C | 2.94143400 | 2.89141100 | 0.52984400 | C | -3.68874500 | 2.34003400 | -0.31260000 |
| C | 3.08617700 | 3.50398000 | -0.71833100 | C | -3.69291900 | 1.50730800 | 0.80979100 |
| C | 3.97345000 | 2.08534000 | 1.01525300 | C | -4.78398400 | 2.31640700 | -1.18053900 |
| C | 4.24070200 | 3.30697400 | -1.47295100 | C | -4.77702500 | 0.66963700 | 1.06761400 |
| C | 2.28235900 | 4.12661200 | -1.10644600 | H | -2.82332200 | 1.49927800 | 1.46374000 |
| H | 5.12889300 | 1.88617400 | 0.26142000 | C | -5.86649300 | 1.47612200 | -0.92977300 |
| H | 3.85628400 | 1.60426700 | 1.98146200 | H | -4.78318100 | 2.95579400 | -2.06023300 |
| C | 5.26501200 | 2.49433400 | -0.98610200 | C | -5.86597900 | 0.65250300 | 0.19724800 |
| H | 4.33759800 | 3.77991200 | -2.44612400 | H | -4.76654000 | 0.02218900 | 1.94004300 |
| H | 5.92015300 | 1.24749500 | 0.64450600 | H | -6.71265500 | 1.46409100 | -1.61083500 |
| H | 6.16308900 | 2.33421500 | -1.57612200 | H | -6.71076300 | -0.00158300 | 0.39455700 |
| C | -2.29240200 | -1.63208900 | -1.22869100 | C | 1.75542300 | -1.74008900 | 0.51528100 |
| C | -2.69942100 | -1.27854000 | -2.57050500 | C | 1.21337400 | -2.38935800 | 1.68525900 |
| C | -2.82043900 | -2.89445400 | -0.74056200 | C | 3.08019700 | -2.19085100 | 0.12186100 |
| C | -3.53227800 | -2.06846300 | -3.32756200 | C | 1.83358700 | -3.46240200 | 2.28600000 |
| H | -2.35323200 | -0.34101600 | -2.99548000 | H | 0.26285300 | -2.04403600 | 2.08495700 |
| C | -3.67039500 | -3.66238200 | -1.54813500 | C | 3.66915300 | -3.29124300 | 0.75558300 |
| C | -4.04235800 | -3.28443700 | -2.83064500 | C | 3.06566800 | -3.95915700 | 1.81433300 |
| H | -3.80772200 | -1.73622100 | -4.32722400 | H | 1.35441600 | -3.93431300 | 3.14246000 |
| H | -4.06937400 | -4.59502800 | -1.15738500 | H | 4.63756600 | -3.64126700 | 0.40342900 |
| H | -4.70615900 | -3.90284500 | -3.42592800 | H | 3.53961400 | -4.81820300 | 2.27774700 |
| C | -2.81017200 | -4.58340400 | 1.13703900 | C | 5.20687900 | -1.44788200 | -1.01153700 |
| C | -2.45022700 | -4.98048200 | 2.41378300 | C | 5.88716900 | -0.62932800 | -1.90153100 |
| C | -1.68503700 | -4.13596000 | 3.22545300 | C | 5.19036700 | 0.31237200 | -2.66278400 |
| C | -1.28976200 | -2.90778900 | 2.71730100 | C | 3.81093200 | 0.40958800 | -2.51822500 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -1.64367300 | -2.49451900 | 1.42685200 | C | 3.11452400 | -0.42108400 | -1.63640400 |
| C | -2.43145800 | -3.32913200 | 0.60396000 | C | 3.80598800 | -1.38022400 | -0.86222700 |
| H | -3.39343900 | -5.27121300 | 0.53386800 | H | 5.77900800 | -2.13558700 | -0.39596500 |
| H | -2.76664700 | -5.95350500 | 2.78033700 | H | 6.96739700 | -0.71191900 | -1.98835300 |
| H | -1.40301600 | -4.43683600 | 4.23011300 | H | 5.71800900 | 0.96163000 | -3.35563200 |
| H | -0.67950600 | -2.23872500 | 3.31962900 | H | 3.24825200 | 1.13764300 | -3.09501200 |
| R-TS10 | | | | S-TS10 | | | |
| G(M062X/6-31G(d)): -1806.86974 | | | | G(M062X/6-31G(d)): -1806.86359 | | | |
| Number of Imaginary frequency: -327.01 | | | | Number of Imaginary frequency: -316.42 | | | |
| -1 I | | | | -1 I | | | |
| C | -0.66226300 | 0.50864400 | 0.44601200 | C | 0.97236600 | -0.34498400 | 0.63000100 |
| C | 0.73229500 | 0.41706300 | 1.08477200 | C | -0.04403800 | -0.12247000 | -0.50859600 |
| C | 1.41975400 | -0.86862000 | 0.68392800 | C | -1.47170200 | -0.25948600 | -0.04219000 |
| C | 1.68024200 | -0.94877500 | -0.67791500 | C | -1.67238700 | -0.44792200 | 1.32686400 |
| C | -0.73974800 | 0.27974400 | -1.09510400 | C | 0.72792000 | 0.50214900 | 1.93207400 |
| H | 0.58742500 | 0.48581800 | 2.17129700 | H | 0.18958400 | -0.84374000 | -1.30502100 |
| H | -1.06533700 | 1.50134300 | 0.69349600 | H | 1.95548900 | -0.08979500 | 0.20996000 |
| H | -1.83724700 | 0.27172100 | -1.30659200 | H | 1.04387800 | -0.19408000 | 2.74389100 |
| H | 1.88804200 | -0.03070500 | -1.22088000 | H | -1.00747800 | -1.09567700 | 1.88938000 |
| O | -0.15284200 | -0.89093600 | -1.50414100 | O | -0.54465300 | 0.99230500 | 2.10754200 |
| C | -0.21137000 | 1.47724500 | -1.93169400 | C | 1.70558100 | 1.68758300 | 2.01061400 |
| H | 0.71197300 | 1.89913900 | -1.51392600 | H | 1.64244100 | 2.30294800 | 1.10176300 |
| H | 0.01348800 | 1.05527200 | -2.91647700 | H | 1.38625100 | 2.30459500 | 2.85721700 |
| O | 1.45444800 | 1.57298600 | 0.65843900 | O | 0.25558600 | 1.13369900 | -1.15172300 |
| O | -1.42308800 | -0.47762000 | 1.14308800 | O | 1.01722500 | -1.72299000 | 1.01404900 |
| O | -1.13495900 | 2.53405500 | -2.18631900 | O | 3.06135000 | 1.33233900 | 2.26348500 |
| C | -2.81409700 | -0.26436300 | 1.18813000 | C | 1.65067400 | -2.59255500 | 0.10068600 |
| H | -3.13744400 | -0.38823100 | 2.23175800 | H | 2.45810500 | -2.07071400 | -0.43531800 |
| H | -3.05672600 | 0.76953000 | 0.90496600 | H | 2.12426100 | -3.37521500 | 0.70757300 |
| C | 2.65333400 | 1.76276000 | 1.37933700 | C | -0.39569300 | 2.29905200 | -0.68617700 |
| H | 2.43537800 | 2.03031100 | 2.42490100 | H | -1.37785100 | 2.40511200 | -1.17297400 |
| H | 3.22669100 | 0.82276200 | 1.39457300 | H | -0.57344200 | 2.23192000 | 0.39616800 |
| C | -1.36604100 | 3.42388700 | -1.11996000 | C | 3.92892200 | 1.23853400 | 1.15897400 |
| H | -0.54082600 | 3.39068100 | -0.39348800 | H | 3.45850600 | 1.64144000 | 0.25110200 |
| H | -1.38056400 | 4.43896700 | -1.54130300 | H | 4.80546000 | 1.87012900 | 1.36522300 |
| C | 3.46453800 | 2.84770000 | 0.71946000 | C | 0.44095400 | 3.51226700 | -1.01699000 |
| C | 4.11287600 | 3.81975500 | 1.48211500 | C | 1.73396000 | 3.40842300 | -1.53398500 |
| C | 3.60245200 | 2.87235400 | -0.67208200 | C | -0.08877900 | 4.78615900 | -0.78014500 |
| C | 4.89349200 | 4.79892200 | 0.86833000 | C | 2.48386500 | 4.55443100 | -1.80450300 |
| H | 4.00325200 | 3.81185100 | 2.56402400 | H | 2.14387700 | 2.42209100 | -1.72683300 |
| C | 4.37521400 | 3.85310500 | -1.28769200 | C | 0.65714800 | 5.92942300 | -1.04874100 |
| H | 3.09676800 | 2.11711000 | -1.26879500 | H | -1.09710700 | 4.87834300 | -0.38123700 |
| C | 5.02484000 | 4.81904600 | -0.51829700 | C | 1.95027700 | 5.81753400 | -1.56306200 |
| H | 5.39189400 | 5.55062700 | 1.47379100 | H | 3.48791400 | 4.45637400 | -2.20835900 |
| H | 4.47315300 | 3.86406600 | -2.36958100 | H | 0.22933100 | 6.91014600 | -0.85985400 |
| H | 5.62701900 | 5.58468200 | -0.99883500 | H | 2.53291300 | 6.70896200 | -1.77639700 |
| C | -3.60527000 | -1.22178300 | 0.32003900 | C | 0.71065900 | -3.24952100 | -0.89040100 |
| C | -2.97895300 | -2.03788500 | -0.62364800 | C | -0.62220300 | -3.49760300 | -0.55343300 |
| C | -4.99506900 | -1.28257300 | 0.46787800 | C | 1.17970600 | -3.64880700 | -2.14393600 |
| C | -3.74387800 | -2.90321100 | -1.40881600 | C | -1.47405400 | -4.12386800 | -1.46097500 |
| H | -1.89870400 | -1.96178200 | -0.76101800 | H | -0.99080600 | -3.17561000 | 0.41588300 |
| C | -5.75455700 | -2.14480600 | -0.31902300 | C | 0.33242600 | -4.28594500 | -3.04887800 |
| H | -5.48327700 | -0.64864200 | 1.20682300 | H | 2.21548000 | -3.45195400 | -2.41414200 |
| C | -5.12801900 | -2.96215000 | -1.26045600 | C | -0.99939900 | -4.52139000 | -2.71047100 |
| H | -3.25278300 | -3.53413600 | -2.14545600 | H | -2.51186400 | -4.30194100 | -1.19274600 |
| H | -6.83336700 | -2.18269700 | -0.19485800 | H | 0.70895600 | -4.58931800 | -4.02174000 |
| H | -5.71751300 | -3.63794700 | -1.87366000 | H | -1.66485400 | -5.00805500 | -3.41765000 |
| C | -2.68673700 | 3.17130200 | -0.41862100 | C | 4.40544800 | -0.17789800 | 0.90625800 |
| C | -2.88653400 | 3.62402200 | 0.88837600 | C | 5.05142100 | -0.49042300 | -0.29384100 |
| C | -3.72565700 | 2.50505800 | -1.07194400 | C | 4.24129100 | -1.17459600 | 1.86860700 |
| C | -4.10010700 | 3.40610100 | 1.53700000 | C | 5.52758300 | -1.77848900 | -0.52729000 |
| H | -2.07788200 | 4.13678700 | 1.40570000 | H | 5.17761100 | 0.28091200 | -1.05125000 |
| C | -4.94176200 | 2.28524300 | -0.42496900 | C | 4.72493100 | -2.46258300 | 1.63984600 |
| H | -3.56584300 | 2.14602200 | -2.08406600 | C | 3.72705900 | -0.93190400 | 2.79314700 |
| C | -5.13170700 | 2.73201500 | 0.88200800 | H | 5.36739000 | -2.76988700 | 0.44226700 |
| H | -4.23795800 | 3.75411100 | 2.55691900 | H | 6.02395500 | -2.00926800 | -1.46580200 |
| H | -5.73985600 | 1.75773100 | -0.94024900 | H | 4.59247900 | -3.23006600 | 2.39770900 |
| H | -6.07645400 | 2.55536700 | 1.38831900 | H | 5.73975600 | -3.77437300 | 0.26290500 |
| C | 1.46749400 | -2.03688800 | 1.49871300 | C | -2.56480100 | 0.00260200 | -0.91301700 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 1.04989600 | -2.04000500 | 2.86278100 | C | -2.36819800 | 0.16855300 | -2.31717800 |
| C | 1.97234600 | -3.27084100 | 0.96821900 | C | -3.90691200 | 0.07738300 | -0.41969000 |
| C | 1.13428500 | -3.16607300 | 3.65015700 | C | -3.42543400 | 0.36651300 | -3.17696500 |
| H | 0.63769800 | -1.13372600 | 3.29284100 | H | -1.35363600 | 0.15196500 | -2.70394400 |
| C | 2.03514800 | -4.40730700 | 1.80158500 | C | -4.96431100 | 0.28203100 | -1.32949400 |
| C | 1.63147600 | -4.37202100 | 3.12131400 | C | -4.74426100 | 0.42197900 | -2.68637600 |
| H | 0.80323300 | -3.12342200 | 4.68480800 | H | -3.23863300 | 0.48309200 | -4.24167800 |
| H | 2.40316800 | -5.34621700 | 1.39956200 | H | -5.98521300 | 0.32817600 | -0.96229700 |
| H | 1.68652200 | -5.26459700 | 3.73693400 | H | -5.57792300 | 0.57704500 | -3.36436800 |
| C | 2.97084400 | -4.46312500 | -1.02516500 | C | -5.40358600 | 0.03947600 | 1.61575000 |
| C | 3.36740600 | -4.46428400 | -2.34804300 | C | -5.57876900 | -0.14383100 | 2.97319500 |
| C | 3.21601000 | -3.31230500 | -3.13980600 | C | -4.48194800 | -0.44836700 | 3.79884800 |
| C | 2.66942200 | -2.17823300 | -2.57533200 | C | -3.22653700 | -0.55070300 | 3.23604000 |
| C | 2.26518600 | -2.15585400 | -1.22593000 | C | -3.02523700 | -0.36183100 | 1.85405800 |
| C | 2.39988700 | -3.31485700 | -0.42563100 | C | -4.12690100 | -0.06808300 | 1.01393600 |
| H | 3.11046700 | -5.36929200 | -0.44486500 | H | -6.27089200 | 0.27824400 | 1.00885600 |
| H | 3.80017800 | -5.36379200 | -2.77695600 | H | -6.57187200 | -0.05029100 | 3.40359900 |
| H | 3.52529100 | -3.31856100 | -4.18086300 | H | -4.62390200 | -0.59442500 | 4.86561500 |
| H | 2.53165800 | -1.27608600 | -3.16751900 | H | -2.35813300 | -0.76498700 | 3.85471500 |
| R-17 G(M062X/6-31G(d)): -1806.88959 Number of Imaginary frequency: 0 | | | | S-17 G(M062X/6-31G(d)): -1806.88217 Number of Imaginary frequency: 0 | | | |
| C | -0.93090000 | 0.18401100 | 0.32557800 | C | 0.94635900 | -0.60924200 | 1.18986100 |
| C | 0.50588000 | 0.12699600 | 0.90481300 | C | 0.27316900 | 0.07917600 | -0.02452100 |
| C | 1.49471800 | -0.91271000 | 0.37006300 | C | -1.16719000 | 0.53733300 | 0.12835800 |
| C | 2.55502000 | -0.50525500 | -0.37567300 | C | -1.72142800 | 0.76715300 | 1.34653500 |
| C | -1.08254700 | -0.34395700 | -1.12168700 | C | 1.50475800 | 0.24837200 | 2.36723700 |
| H | 0.38550400 | -0.04946900 | 1.98516100 | H | 0.24710500 | -0.70443500 | -0.79458300 |
| H | -1.21336700 | 1.24182300 | 0.411157800 | H | 1.80225600 | -1.13976900 | 0.75671300 |
| H | -2.18102700 | -0.18492900 | -1.35005600 | H | 1.67862400 | -0.56091900 | 3.13633600 |
| H | 2.64482100 | 0.53915700 | -0.66243100 | H | -1.06288500 | 0.76062500 | 2.22028000 |
| O | -0.66300100 | -1.61166800 | -1.23264700 | O | 0.76370300 | 1.28357700 | 2.79835300 |
| C | -0.36000300 | 0.58642900 | -2.13876500 | C | 2.94375200 | 0.73537600 | 2.04569200 |
| H | 0.62058200 | 0.91245300 | -1.75806500 | H | 2.93927500 | 1.46115700 | 1.22218300 |
| H | -0.18937000 | -0.03861000 | -3.02114800 | C | 3.28924400 | 1.26053500 | 2.94428000 |
| O | 1.03664900 | 1.43838200 | 0.72413400 | O | 1.13396200 | 1.06248600 | -0.60285200 |
| O | -1.77223800 | -0.54288100 | 1.22820300 | O | 0.08327000 | -1.61532000 | 1.72988000 |
| O | -1.07214900 | 1.72686500 | -2.62446900 | O | 3.90895100 | -0.28677000 | 1.78288000 |
| C | -3.13874900 | -0.19846900 | 1.17977900 | C | -0.04613600 | -2.78596500 | 0.94662400 |
| H | -3.46758400 | 0.03178800 | 2.20346600 | H | 0.86549000 | -2.95891900 | 0.35356600 |
| H | -3.27895700 | 0.71775400 | 0.58881400 | H | -0.13892200 | -3.61876300 | 1.65611000 |
| C | 1.99082400 | 1.80495100 | 1.69542500 | C | 0.96272700 | 2.38375100 | -0.11082300 |
| H | 1.49541900 | 1.98355500 | 2.66225800 | H | 0.03209500 | 2.80991600 | -0.51994800 |
| H | 2.71435600 | 0.99069100 | 1.84923700 | H | 0.88014600 | 2.36388800 | 0.98790200 |
| C | -1.19802000 | 2.80472300 | -1.72863800 | C | 4.14602300 | -0.58765600 | 0.42714200 |
| H | -0.40648100 | 2.77934900 | -0.96515300 | H | 3.51116100 | 0.02721500 | -0.22576100 |
| H | -1.05521900 | 3.72652000 | -2.31075200 | H | 5.19209000 | -0.34171300 | 0.18653300 |
| C | 2.72438200 | 3.04711600 | 1.25386400 | C | 2.12685000 | 3.23052500 | -0.56025800 |
| C | 3.49329400 | 3.75195400 | 2.18521500 | C | 2.93337600 | 2.86072900 | -1.63968800 |
| C | 2.68118500 | 3.49326200 | -0.06795100 | C | 2.40120300 | 4.42876200 | 0.10716600 |
| C | 4.21186100 | 4.87992900 | 1.80163800 | C | 3.99025700 | 3.67535200 | -2.04533600 |
| H | 3.52560500 | 3.41142400 | 3.21806000 | H | 2.73152300 | 1.92741600 | -2.15613700 |
| C | 3.39812800 | 4.62759300 | -0.45192000 | C | 3.45278700 | 5.24560500 | -0.29969100 |
| H | 2.08095400 | 2.95206700 | -0.79380100 | H | 1.78650900 | 4.71782400 | 0.95701400 |
| C | 4.16560000 | 5.32266600 | 0.47885100 | C | 4.25302900 | 4.87036600 | -1.37899700 |
| H | 4.80462000 | 5.41795900 | 2.53594500 | H | 4.60999200 | 3.37439900 | -2.88554700 |
| H | 3.35491500 | 4.96661900 | -1.48313900 | H | 3.65420700 | 6.17155800 | 0.23170900 |
| H | 4.72362400 | 6.20495400 | 0.17955300 | H | 5.07797100 | 5.50283400 | -1.69377600 |
| C | -4.01488200 | -1.29663300 | 0.61533900 | C | -1.25333000 | -2.77822700 | 0.03095000 |
| C | -3.48629900 | -2.28841500 | -0.21638100 | C | -2.52365200 | -2.51343800 | 0.55427800 |
| C | -5.38127100 | -1.29623700 | 0.91136500 | C | -1.12380800 | -3.02314900 | -1.33579500 |
| C | -4.33401700 | -3.26813800 | -0.73764300 | C | -3.63949600 | -2.48675300 | -0.27605400 |
| H | -2.41682800 | -2.26546400 | -0.46961100 | H | -2.62603900 | -2.30609700 | 1.61706800 |
| C | -6.22138700 | -2.27418600 | 0.38393900 | C | -2.24132500 | -3.00079900 | -2.17353300 |
| H | -5.78852900 | -0.52399100 | 1.56217300 | H | -0.13644800 | -3.22084900 | -1.74994700 |
| C | -5.69662900 | -3.26816400 | -0.44192600 | C | -3.50026900 | -2.72794600 | -1.64602500 |
| H | -3.92581800 | -4.03883500 | -1.38731100 | H | -4.61981200 | -2.27019800 | 0.14058600 |
| H | -7.28146700 | -2.26503400 | 0.62241400 | H | -2.12333800 | -3.18360600 | -3.23806000 |
| H | -6.34736500 | -4.03609000 | -0.85108300 | H | -4.37082600 | -2.69985400 | -2.29516000 |

| | | | | | | | |
|----------------------------------|-------------|-------------|-------------|----------------------------------|-------------|-------------|-------------|
| C | -2.55670400 | 2.86326300 | -1.05599500 | C | 3.89769300 | -2.05132300 | 0.11929700 |
| C | -2.71546400 | 3.53193100 | 0.16082500 | C | 3.73954600 | -2.46352600 | -1.20679600 |
| C | -3.66941700 | 2.26294900 | -1.64806000 | C | 3.79779800 | -2.99775000 | 1.14072900 |
| C | -3.96153500 | 3.58936700 | 0.78207600 | C | 3.48737800 | -3.80008700 | -1.50872500 |
| H | -1.85029300 | 3.99330000 | 0.63382200 | H | 3.80377900 | -1.72803400 | -2.00665800 |
| C | -4.91726400 | 2.31660100 | -1.02839000 | C | 3.54758600 | -4.33657300 | 0.84064800 |
| H | -3.54142700 | 1.73621200 | -2.58879100 | H | 3.89444200 | -2.66874700 | 2.17083400 |
| C | -5.06700100 | 2.97727600 | 0.19049400 | C | 3.38985800 | -4.74221500 | -0.48369000 |
| H | -4.06801400 | 4.10176100 | 1.73418400 | H | 3.35910900 | -4.10566400 | -2.54349300 |
| H | -5.77290400 | 1.83641100 | -1.49542400 | H | 3.46658500 | -5.06367500 | 1.64413900 |
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| C | 1.43309000 | -2.30091600 | 0.79827900 | C | -1.98563200 | 0.64714400 | -1.06800300 |
| C | 0.36359600 | -2.76714600 | 1.59531500 | C | -1.41947000 | 0.51633900 | -2.35960900 |
| C | 2.45822000 | -3.21007000 | 0.42882500 | C | -3.38228800 | 0.88546200 | -0.95707700 |
| C | 0.31784200 | -4.07132900 | 2.04059900 | C | -2.20089800 | 0.57323600 | -3.49501800 |
| H | -0.45066500 | -2.08955900 | 1.82702300 | H | -0.34554000 | 0.39176700 | -2.45542300 |
| C | 2.38439800 | -4.54236600 | 0.89728700 | C | -4.15912600 | 0.93310600 | -2.13637800 |
| C | 1.34191000 | -4.96821900 | 1.69242400 | C | -3.58674300 | 0.77033900 | -3.38129400 |
| H | -0.51505800 | -4.40696100 | 2.65213400 | H | -1.74386400 | 0.46818900 | -4.47471000 |
| H | 3.16269100 | -5.25075000 | 0.63452200 | H | -5.22824200 | 1.10585500 | -2.07441300 |
| H | 1.31159100 | -5.99635200 | 2.04136700 | H | -4.20716500 | 0.80896500 | -4.27174400 |
| C | 4.59440500 | -3.61015800 | -0.86600200 | C | -5.35752300 | 1.27704300 | 0.56576200 |
| C | 5.61627000 | -3.13257800 | -1.66333000 | C | -5.87203600 | 1.46035800 | 1.83357400 |
| C | 5.64645900 | -1.77942800 | -2.04472500 | C | -5.02463200 | 1.44044600 | 2.95660100 |
| C | 4.64573700 | -0.93086100 | -1.62115700 | C | -3.67381600 | 1.22894800 | 2.78447300 |
| C | 3.58863900 | -1.40195400 | -0.81161600 | C | -3.12541400 | 1.03444900 | 1.49576000 |
| C | 3.55861200 | -2.76067600 | -0.41835800 | C | -3.97469100 | 1.06648900 | 0.36243000 |
| H | 4.59781000 | -4.65960300 | -0.59133600 | H | -6.03787300 | 1.29534000 | -0.27876600 |
| H | 6.39889500 | -3.80751300 | -1.99711700 | H | -6.93842100 | 1.62034400 | 1.96322400 |
| H | 6.45235500 | -1.40798800 | -2.67090400 | H | -5.43628400 | 1.58610400 | 3.95090800 |
| H | 4.65198800 | 0.11833800 | -1.90747700 | H | -3.00421700 | 1.20188600 | 3.64054000 |
| 3b from R | | | | 3b from S | | | |
| G(M062X/6-31G(d)): -1807.40667 | | | | G(M062X/6-31G(d)): -1807.40098 | | | |
| Number of Imaginary frequency: 0 | | | | Number of Imaginary frequency: 0 | | | |
| C | 0.86383400 | 0.09271300 | -0.38944400 | C | 0.71621500 | -0.83344100 | 1.69161700 |
| C | -0.55603700 | 0.22042300 | -1.00098100 | C | 0.32739600 | -0.15588600 | 0.34928000 |
| C | -1.59518300 | -0.81011200 | -0.56141000 | C | -1.02490000 | 0.52039700 | 0.22824000 |
| C | -2.51198300 | -0.46077300 | 0.38201700 | C | -1.75898000 | 0.92149500 | 1.29507600 |
| C | 0.97099200 | -0.18453500 | 1.12105300 | C | 1.42912400 | -0.03425100 | 2.78445500 |
| H | -0.41438400 | 0.15142100 | -2.08878500 | H | 0.29271600 | -0.99604400 | -0.35633800 |
| H | 1.32731600 | 1.06572000 | -0.59255600 | H | 1.45040400 | -1.60080500 | 1.41224800 |
| H | 2.04292600 | -0.23653000 | 1.35222600 | H | 1.44413700 | -0.71803400 | 3.64486900 |
| H | -2.51193100 | 0.54778400 | 0.78842700 | H | -1.36939400 | 0.80223100 | 2.29747200 |
| O | 0.45590500 | -1.46236700 | 1.46112700 | O | 0.80775500 | 1.18916000 | 3.15138800 |
| C | 0.37240800 | 0.89158500 | 2.04815600 | C | 2.88789900 | 0.32166800 | 2.47251800 |
| H | -0.57683500 | 1.27588000 | 1.65488000 | H | 2.94314000 | 1.10981200 | 1.71722600 |
| H | 0.17356400 | 0.39463100 | 3.00233000 | H | 3.32350600 | 0.71908100 | 3.39737100 |
| O | -0.98238300 | 1.53317700 | -0.67789700 | O | 1.40981900 | 0.63838600 | -0.13701900 |
| O | 1.55576200 | -0.90022600 | -1.12588700 | O | -0.39130200 | -1.48681900 | 2.29751600 |
| O | 1.23902900 | 1.96570800 | 2.36094100 | O | 3.64178500 | -0.80961300 | 2.08341000 |
| C | 2.95603400 | -0.71537800 | -1.23515100 | C | -0.74889300 | -2.73917000 | 1.72568200 |
| H | 3.21736600 | -0.89486400 | -2.28592900 | H | 0.15058300 | -3.25172600 | 1.35436700 |
| H | 3.22701700 | 0.32664000 | -1.01036600 | H | -1.15927300 | -3.33045600 | 2.55191400 |
| C | -1.95644600 | 2.05269400 | -1.56393200 | C | 1.31662600 | 2.04714300 | 0.04852700 |
| H | -1.50556700 | 2.23092800 | -2.55088800 | H | 0.46167400 | 2.44088600 | -0.51844600 |
| H | -2.76842600 | 1.32374800 | -1.70199300 | H | 1.16621700 | 2.29956400 | 1.10541400 |
| C | 1.45210400 | 2.91657600 | 1.33511300 | C | 4.10232500 | -0.85147000 | 0.73798600 |
| H | 0.62832700 | 2.90006500 | 0.60824000 | H | 3.92599700 | 0.10492700 | 0.23317700 |
| H | 1.44386200 | 3.90430300 | 1.81411700 | H | 5.18727100 | -1.01606300 | 0.77782400 |
| C | -2.51564400 | 3.33557900 | -1.00197600 | C | 2.59588700 | 2.64775000 | -0.47501100 |
| C | -3.18814200 | 4.21884300 | -1.85151600 | C | 3.02786200 | 2.33339100 | -1.76834800 |
| C | -2.41113900 | 3.64542700 | 0.35525800 | C | 3.36657700 | 3.50752200 | 0.30797900 |
| C | -3.75369800 | 5.38834100 | -1.35207000 | C | 4.21307100 | 2.86588900 | -2.26632900 |
| H | -3.26664800 | 3.98699500 | -2.91141900 | H | 2.42556000 | 1.66818600 | -2.38283900 |
| C | -2.97289400 | 4.82049700 | 0.85490600 | C | 4.55098200 | 4.05046600 | -0.19263300 |
| H | -1.88243100 | 2.96941000 | 1.02126400 | H | 3.04100300 | 3.74916000 | 1.31741700 |
| C | -3.64674000 | 5.69368300 | 0.00504100 | C | 4.97819600 | 3.72731300 | -1.47768700 |
| H | -4.27273800 | 6.06594600 | -2.02395800 | H | 4.53980700 | 2.61278900 | -3.27085900 |
| H | -2.88161000 | 5.05195400 | 1.91235900 | H | 5.14330400 | 4.71737200 | 0.42711700 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -4.08210700 | 6.60891500 | 0.39507200 | H | 5.90374800 | 4.14242200 | -1.86562300 |
| C | 3.76315300 | -1.65263800 | -0.36169600 | C | -1.77835500 | -2.64042800 | 0.61999800 |
| C | 3.15791000 | -2.66825400 | 0.37722000 | C | -3.05440400 | -2.14019500 | 0.90087300 |
| C | 5.15466200 | -1.51380400 | -0.32346800 | C | -1.47831400 | -3.03407200 | -0.68376100 |
| C | 3.93566400 | -3.52871600 | 1.15427000 | C | -4.00681100 | -2.02412100 | -0.10634900 |
| H | 2.07634200 | -2.76000700 | 0.35696900 | H | -3.29250500 | -1.82806400 | 1.91571400 |
| C | 5.92953200 | -2.37356000 | 0.44961200 | C | -2.43251700 | -2.92477500 | -1.69835000 |
| H | 5.63069800 | -0.72411000 | -0.90192000 | H | -0.48579100 | -3.42134800 | -0.90842600 |
| C | 5.32029900 | -3.38566200 | 1.19318000 | C | -3.69623700 | -2.41656200 | -1.41151700 |
| H | 3.45429900 | -4.31429900 | 1.73036900 | H | -4.99165700 | -1.62490900 | 0.12154600 |
| H | 7.00897400 | -2.25324900 | 0.47434100 | H | -2.18246200 | -3.22765300 | -2.71133100 |
| H | 5.92366600 | -4.05521200 | 1.79928300 | H | -4.43872600 | -2.32134900 | -2.19883000 |
| C | 2.77899900 | 2.72134900 | 0.62868500 | C | 3.45625600 | -1.97149800 | -0.04694700 |
| C | 2.97875200 | 3.25881900 | -0.64646300 | C | 2.92141600 | -1.74496500 | -1.31609700 |
| C | 3.82181000 | 2.02703100 | 1.24465800 | C | 3.39144000 | -3.25790700 | 0.49906500 |
| C | 4.20023900 | 3.10197100 | -1.29740700 | C | 2.32538900 | -2.78608200 | -2.02973400 |
| H | 2.16557400 | 3.79155000 | -1.13576500 | H | 2.95534400 | -0.74217400 | -1.73450500 |
| C | 5.04519500 | 1.86828100 | 0.59427200 | C | 2.79156400 | -4.29732300 | -0.20690600 |
| H | 3.66537100 | 1.60517500 | 2.23293100 | H | 3.80154200 | -3.43592700 | 1.49027200 |
| C | 5.23806600 | 2.40394500 | -0.67839900 | C | 2.25658600 | -4.06299800 | -1.47532600 |
| H | 4.34017400 | 3.51910400 | -2.29062400 | H | 1.90529500 | -2.59708300 | -3.01410100 |
| H | 5.84776700 | 1.32181700 | 1.08196800 | H | 2.74162400 | -5.29121800 | 0.22884700 |
| H | 6.19026200 | 2.27701100 | -1.18558500 | H | 1.78593900 | -4.87251500 | -2.02609000 |
| C | -1.64244500 | -2.14298500 | -1.14217400 | C | -1.57680800 | 0.67048500 | -1.10977400 |
| C | -0.75698700 | -2.53520900 | -2.17321500 | C | -0.82011100 | 0.32254700 | -2.25579100 |
| C | -2.61732100 | -3.07418800 | -0.68551200 | C | -2.90017200 | 1.15673200 | -1.28556400 |
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| H | -0.00014200 | -1.84202000 | -2.51835200 | H | 0.20699900 | -0.00910900 | -2.13682200 |
| C | -2.65564900 | -4.35687400 | -1.27464100 | C | -3.42614500 | 1.22880400 | -2.59474500 |
| C | -1.77932500 | -4.71475500 | -2.27707200 | C | -2.67748500 | 0.85820000 | -3.69251200 |
| H | -0.13425400 | -4.07117000 | -3.52536200 | H | -0.75938300 | 0.13622500 | -4.38661100 |
| H | -3.39071300 | -5.08106200 | -0.94211100 | H | -4.43861000 | 1.58323500 | -2.75340600 |
| H | -1.83467100 | -5.70707000 | -2.71453800 | H | -3.10801800 | 0.92403200 | -4.68717700 |
| C | -4.53500400 | -3.57014000 | 0.88348400 | C | -5.01038500 | 2.02864000 | -0.20275200 |
| C | -5.41348200 | -3.15432900 | 1.86367800 | C | -5.71310900 | 2.37896700 | 0.93280400 |
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| H | -4.60653000 | -4.58946600 | 0.52090400 | H | -5.49955300 | 2.12671800 | -1.16549000 |
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