S1 NBO analysis of the lone-electron orbitals in products P1-P1’

In Table 1, we provide the NBO characteristics of the C-H bond involved in the formation of products P1 to P1’: number of electrons on the bonding $\sigma$(C-H) orbital, energy of this orbital, contribution of C atomic orbitals, and decomposition into s and p carbon AOs.

In Table 2, we provide the characteristic of the lone-electron NBO on the radical carbon: population, energy, s-p contributions and the two principal second-order stabilisation (with neighbouring antibonding C-H and C-O orbitals).
Table S1: NBO characteristics of the C-H bonds involved in the formation of products $\text{P1}$ to $\text{P1'}$.

| End product | Population | Energy (u.a.) | C contrib. | s-p contrib. |
|--------------|------------|---------------|------------|--------------|
| $\text{P1}$  | 1.9835     | -0.55820      | 61.12%     | 27.5% s - 72.5% p |
| $\text{P2}$  | 1.9769     | -0.52660      | 62.24%     | 25.1% s - 74.8% p |
| $\text{P3}$  | 1.9784     | -0.53875      | 61.90%     | 24.7% s - 75.3% p |
| $\text{P4}$  | 1.9792     | -0.52948      | 61.96%     | 24.8% s - 74.2% p |
| $\text{P5}$  | 1.9806     | -0.53394      | 62.18%     | 25.3% s - 74.6% p |
| $\text{P1'}$ | 1.9787     | -0.54302      | 62.08%     | 25.2% s - 74.7% p |

Table S2: Characteristics of the lone-electron (spin-up) NBO on radical carbon in $\text{P1}$ to $\text{P1'}$. Nature of the acceptor NBO are indicated along with the second-order stabilisation.

| Product | Population | Energy (u.a.) | s-p contrib. | 2nd order stab. (kcal/mol) |
|---------|------------|---------------|--------------|---------------------------|
| $\text{P1}$  | 0.9525     | -0.29777      | 19.2% s - 80.8% p | 3.84, $\sigma^*(\text{C-H})$ 1.76, $\sigma^*(\text{C-O})$ |
| $\text{P2}$  | 0.9075     | -0.24294      | 8.6% s - 91.4% p | 5.01, $\sigma^*(\text{C-H})$ 4.68, $\sigma^*(\text{C-H})$ |
| $\text{P3}$  | 0.9165     | -0.25280      | 9.6% s - 90.4% p | 5.03, $\sigma^*(\text{C-H})$ 4.99, $\sigma^*(\text{C-H})$ |
| $\text{P4}$  | 0.9230     | -0.24848      | 11.4% s - 88.6% p | 4.70, $\sigma^*(\text{C-H})$ 4.49, $\sigma^*(\text{C-H})$ |
| $\text{P5}$  | 0.8974     | -0.21492      | 0.3% s - 99.7% p | 11.45, $\sigma^*(\text{C-H})$ 4.36, $\sigma^*(\text{C-H})$ |
| $\text{P1'}$ | 0.9281     | -0.26574      | 10.5% s - 89.5% p | 4.12, $\sigma^*(\text{C-H})$ 4.00, $\sigma^*(\text{C-H})$ |
In Figure 1 we provide a rudimentary illustration of the hyperconjugation interaction beneath the planarity of radical P5.

Figure S1: Schematic illustration of the hyperconjugation interaction between the lone-electron orbital and neighbouring anti-bonding $\sigma^*(C-O)$ orbital in product P5.
Figure S2: Reaction profiles for the hydrolysis of radicals P1 (black), P5 (green) and P1’ (red), in free enthalpy and relative to the pre-reacting complex formed by one H₂O molecule and target radicals (cf. Scheme 1 in main manuscript).
Figure S3: Reaction profiles for the hydrolysis of radical P1, involving one (black) and two (blue) explicit water molecules.
S3  Reaction profiles for the fragmentation reactions

Figure S4: Top: studied fragmentation reactions for carboradical P1. Bottom: associated reaction profiles in free enthalpy (relative to P1).
Figure S5: Top: studied fragmentation reactions for carboradical P2. Bottom: associated reaction profiles in free enthalpy (relative to P2). Transition state for the glycosidic bond cleavage (leading to \( F_{2_{gly}} \)) could not be isolated.
Figure S6: Top: studied fragmentation reactions for carboradical P3. Bottom: associated reaction profiles in free enthalpy (relative to P3).
Figure S7: Top: studied fragmentation reactions for carboradical $\textbf{P}4$. Bottom: associated reaction profiles in free enthalpy (relative to $\textbf{P}4$).
Figure S8: Top: studied fragmentation reactions for carboradical \( \text{P5} \). Bottom: associated reaction profiles in free enthalpy (relative to \( \text{P5} \)).
Figure S9: Top: studied fragmentation reactions for carboradical P1'. Bottom: associated reaction profiles in free enthalpy (relative to P1').
S4 Geometries

In the following we provide the Cartesian coordinates for the optimised geometries of the reagents, transition states and products, along with their free enthalpy (300K, 1 atm) and first vibration frequency.

**OH radical, \( G = -47531.87 \) kcal/mol, 3701.83 cm \(^{-1}\)**

\[
\begin{array}{ccc}
O & 0.00000000 & 0.00000000 & 0.10889000 \\
H & 0.00000000 & 0.00000000 & -0.87112200 \\
\end{array}
\]

**IB Network I, \( G = -814316.11 \) kcal/mol, 26.48 cm \(^{-1}\)**

\[
\begin{array}{cccc}
C & 0.90601100 & 0.40277800 & -0.12063600 \\
H & 0.80172800 & 0.39851500 & -1.21867800 \\
C & 1.84797400 & 1.52530300 & 0.32449300 \\
H & 1.84798600 & 1.54382700 & 1.42433400 \\
C & 3.26071000 & 1.24624300 & -0.17795200 \\
H & 3.26200400 & 1.30016300 & -1.27809100 \\
C & 3.70375400 & -0.14936100 & 0.24666200 \\
H & 3.74185500 & -0.18853900 & 1.34586000 \\
C & 2.69526700 & -1.20108500 & -0.24160100 \\
H & 2.65084600 & -1.18691000 & -1.34143200 \\
C & 3.04151800 & -2.62409500 & 0.21159800 \\
H & 3.22721800 & -2.62676100 & 1.29679700 \\
H & 2.18545100 & -3.27595500 & 0.01462700 \\
O & 1.43694500 & 2.77189700 & -0.20772700 \\
H & 0.50682900 & 2.93813700 & 0.04829500 \\
O & 4.21127600 & 2.16929000 & 0.34722500 \\
O & 4.98566300 & -0.47159100 & -0.29308700 \\
O & 1.40317800 & -0.87547800 & 0.30568200 \\
O & 4.13596200 & -3.16259100 & -0.50971500 \\
H & 4.86858500 & -2.52831400 & -0.45908300 \\
O & -0.31873000 & 0.63094300 & 0.49400900 \\
C & -4.31111000 & -0.39364000 & 0.20370900 \\
H & -4.35106300 & -0.27928800 & 1.30294100 \\
C & -3.34141300 & -1.51628700 & -0.16754700 \\
H & -3.31805000 & -1.59251000 & -1.26468200 \\
C & -1.94445400 & -1.17984000 & 0.34339300 \\
H & -1.96584300 & -1.14993700 & 1.44428100 \\
C & -1.52009000 & 0.20672800 & -0.16075300 \\
H & -1.35635000 & 0.16251100 & -1.24692200 \\
C & -2.60419000 & 1.25894500 & 0.15001100 \\
H & -2.66502000 & 1.39411600 & 1.24143400
\end{array}
\]
|  | C       | H       | O       | H       | O       | H       | O       | H       | H       | O       | H       | O       | H       | H       |  
|---|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|  
| C | -2.37621400 | 2.62900700 | -0.49548300 |  
| H | -2.09990900 | 2.51025300 | -1.55156700 |  
| H | -3.32849800 | 3.16681100 | -0.44456000 |  
| O | -3.84692300 | -2.71921300 | 0.40106200 |  
| H | -3.18866200 | -3.41579000 | 0.25728300 |  
| O | -1.08083100 | -2.16420000 | -0.10131600 |  
| H | -0.16938800 | -2.00497400 | 0.17419300 |  
| O | -3.85756100 | 0.81702000 | -0.37298100 |  
| O | -1.35607100 | 3.53366000 | 0.21229500 |  
| H | -1.47685400 | 4.29601600 | 0.04168000 |  
| O | -5.59085300 | -0.60716900 | -0.31437300 |  
| H | 3.90952600 | 3.06308200 | 0.13042700 |  
| H | 5.58373800 | 0.26271100 | -0.08943700 |  
| H | -5.78914400 | -1.55038000 | -0.21165400 |  

\( \text{R-C1, } G = -861845.64 \text{ kcal/mol, 25.57 cm } -1 \)

|  | C       | H       | O       | H       | O       | H       | O       | H       | H       | O       | H       | O       | H       | H       |  
|---|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|  
| C | 0.87454000 | -0.27426000 | -0.03696400 |  
| H | 0.76860000 | -0.34913400 | 1.06232000 |  
| C | 1.81762200 | -1.37197500 | -0.54788000 |  
| H | 1.80276500 | -1.34756100 | -1.64580600 |  
| C | 3.23928100 | -1.12542600 | -0.05244800 |  
| H | 3.26567300 | -1.25427000 | 1.04048900 |  
| C | 3.67057300 | 0.29987400 | -0.38564700 |  
| H | 3.69027100 | 0.41495700 | -1.48025500 |  
| C | 2.66762900 | 1.31143500 | 0.19002300 |  
| H | 2.62976100 | 1.21491000 | 1.28521200 |  
| C | 3.00782900 | 2.76459700 | -0.16035700 |  
| H | 3.18530700 | 2.84798600 | -1.24389100 |  
| H | 2.15093100 | 3.96629000 | 0.09010900 |  
| O | 1.40260600 | -2.65086800 | -0.07383000 |  
| H | 0.50042400 | -2.85194700 | -0.40834800 |  
| O | 4.18335100 | -2.00018000 | -0.66603500 |  
| O | 4.95909100 | 0.58626800 | 0.15435900 |  
| O | 1.37164600 | 1.02487300 | -0.37259400 |  
| O | 4.10512100 | 3.25282300 | 0.59058400 |  
| H | 4.84151800 | 2.62984600 | 0.48624600 |  
| O | -0.34804200 | -0.45702500 | -0.66834500 |  
| C | -4.35955700 | 0.43153000 | -0.24113100 |  
| H | -4.41547100 | 0.40023800 | -1.34556800 |  
| C | -3.41217100 | 1.55034700 | 0.19767400 |  
| H | -3.36665200 | 1.54305700 | 1.29655300 |  
| C | -2.01795800 | 1.29398600 | -0.36563000 |  
| H | -2.06368100 | 1.34424200 | -1.46526200 |  
| C | -1.55192400 | -0.11163900 | 0.03175500 |  
| H | -1.37290200 | -0.14682500 | 1.11451200 |  

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C    -2.61044900  -1.16882400  -0.34098500
H    -2.69373000  -1.20735400  -1.44191200
C    -2.30240400  -2.58002500   0.18535400
H    -1.91690400  -2.53434100   1.20648800
H    -3.23815000  -3.14925000   0.19330700
O    -3.96420500   2.77702600  -0.26745400
H    -3.32940600   3.48143100  -0.07195600
O    -1.17086400   2.31919100   0.13453100
H    -0.25951000   2.14966400  -0.16502700
O    -3.86579900  -0.81078700   0.23117400
O    -1.30220500  -3.27302100  -0.57823200
H    -1.66153500  -3.50948300  -1.44332800
O    -5.63462000   0.57152200   0.31008900
H    3.93404600  -2.91194700  -0.46057100
H    5.55739400  -0.12707900   0.29481600
H    -5.85339000   1.51572700  -0.26745400
O    0.60419700  -1.97843700   2.52461500
H    0.98435600  -2.55959800   1.82170700

TS-Abs-C1, G=-861844.60 kcal/mol, i 106.51cm -1
C    0.92105200   0.34357300  -0.17849500
H    0.80481200   0.33534000  -1.31529400
C    1.85830100   1.51004600   0.17643200
H    1.82695900   1.64449200   1.26726600
C    3.29821000   1.20438000  -0.25646400
H    3.33706700   1.20767000  -1.35544200
C    3.71456100  -0.17139500   0.24496800
H    3.69805200  -0.17097600   1.34590800
C    2.73302000  -1.24166100  -0.25541400
H    2.71236100  -1.24749600  -1.35401500
C    3.09229000  -2.65285300   0.24021600
H    3.22315200  -2.63137700   1.33038000
H    2.20232000  -3.31024700   0.03142100
O    1.45077700   2.69342500  -0.49336800
H    0.53514600   2.93020500  -0.22988500
O    4.21997300   2.14738200   0.27147000
O    5.02002000  -0.50757400  -0.21891000
O    1.42114900  -0.91054300   0.25199100
O    4.18457500  -3.20242800  -0.43708900
H    4.91705300  -2.56952900  -0.37214200
O    -0.29836200   0.57836400   0.42837700
C    -4.31152800  -0.39127800   0.17752100
H    -4.36628000  -0.16642900   1.25937300
C    -3.35877900  -1.56409200  -0.06086900
H    -3.31516200  -1.74951900  -1.14396000
C  -1.96270000  -1.20837200   0.44260400
H   -2.00354500  -1.06457200   1.53431500
C   -1.50496900   0.10609300  -0.20022500
H   -1.32274500  -0.04575700  -1.27079600
C   -2.56825700  1.20748800  -0.01232900
H   -2.64722600  1.43739100   1.06532500
C   -2.27335200  2.50646500  -0.77967900
H   -1.88870400  2.28218300  -1.77713100
H   -3.21519400  3.05503700  -0.88777400
O   -3.90275700  -2.69284900   0.61435900
H   -3.26856000  -3.42020600   0.53636600
O   -1.11943400  -2.30702300  -0.88777400
H   -0.20000200  -2.07503100   0.34511600
O   -3.82390200   0.75066300  -0.50709000
O   -1.28161100   3.33941000  -0.15265300
H   -1.64901500   3.72757700   0.64948300
O   -5.58653800  -0.63155000  -0.33767100
H   3.98109200   3.02598300  -0.05586500
H   5.60398200   0.24094400  -0.02546500
H   -5.79916300  -1.56056600  -0.16062600
O   0.65571700   1.91786000  -2.77205300
H   0.96208300   1.90187500  -2.47425000

P-C1, G = -861867.44 kcal/mol, 19.32 cm^-1
C    0.90457700  -0.22911200  -0.29646600
H    0.33104700  -2.76995500   3.21364400
C    1.84049400   1.37932600  -0.59273000
H    1.96152900  -1.47636900  -1.68743900
C    3.21339900  -1.12536600   0.02405200
H    3.12790000  -1.20940100  -1.11747400
C    3.69199500   0.27876700  -0.32410000
H    3.77949800   0.36351200  -1.41887400
C    2.67850200   1.32003500   0.16838900
H    2.55700400   1.24016600   1.25595800
C    3.06603800   2.75952600  -0.18833300
H    3.32405200   2.81734100  -1.25723400
H    2.20410100   3.41021900  -0.01461500
O    1.35372300  -2.60911200  -0.59273000
H    0.48275000  -2.82743600  -0.46252200
O    4.19800300  -0.03475900   0.45980200
O    4.94979600   0.56238700   0.28364900
O    1.40532500   1.05379400  -0.47018500
O    4.11291500   3.24561000   0.63199500
H    4.84750200   2.61353600   0.58731100
O   -0.32523400  -0.37886800  -0.85090100
|    | X     | Y     | Z     |
|----|-------|-------|-------|
| C  | -4.31969500 | 0.47664000 | -0.20123400 |
| H  | -4.41102800 | 0.49921200 | -1.30361600 |
| C  | -3.35817100 | 1.57120600 | 0.26228400  |
| H  | -3.27332400 | 1.50593000 | 1.35670200  |
| C  | -1.98560200 | 1.34593500 | -0.36367700 |
| H  | -2.07371700 | 1.44910500 | -1.45731400 |
| C  | -1.49951500 | -0.07483400 | -0.05461300 |
| H  | -1.24335300 | -0.17012900 | 1.00612000  |
| C  | -2.57358800 | -1.11608300 | -0.43342700 |
| H  | -2.69514000 | -1.10411300 | -1.53216100 |
| C  | -2.26505400 | -2.55051300 | 0.02380800  |
| H  | -1.87206200 | -2.55336200 | 1.04267400  |
| H  | -3.20240500 | -3.11706100 | 0.00203800  |
| O  | -3.92250400 | 2.82154500 | -0.11845300 |
| H  | -3.27686000 | 3.51290200 | 0.08785100  |
| O  | -1.12947600 | 2.35731200 | 0.15127600  |
| H  | -0.22621800 | 2.19924900 | -0.17174300 |
| O  | -3.80901900 | -0.78350000 | 0.19527600  |
| O  | -1.26958700 | -3.20853000 | -0.77876000 |
| H  | -1.60340700 | -3.33164500 | -1.67618100 |
| O  | -5.57737100 | 0.58793200 | 0.39577600  |
| H  | 3.90309000  | -2.93487900 | -0.26216900 |
| H  | 5.54153500  | -0.18152300 | 0.09582900  |
| H  | -5.79204300 | 1.53204300 | 0.44137400  |
| O  | 0.08515800  | -2.20063100 | 2.47500300  |
| H  | 0.67552500  | -2.43882500 | 1.73317600  |

R-C2, G = -861846.73 kcal/mol, 22.98 cm^-1

|    | X     | Y     | Z     |
|----|-------|-------|-------|
| C  | 0.60430700 | -0.27366500 | 0.16365100 |
| H  | 0.46856200 | -0.23102100 | 1.25716400 |
| C  | 1.61582000 | -1.35541000 | -0.21493900 |
| H  | 1.64480100 | -1.40482000 | -1.31390600 |
| C  | 3.00392300 | -0.99665600 | 0.30729700 |
| H  | 2.99586300 | -1.02255600 | 1.40638800 |
| C  | 3.40794100 | 0.40752400 | -0.14697200 |
| H  | 3.49749000 | 0.41633500 | -1.24396400 |
| C  | 2.31030700 | 1.41174300 | 0.26069800 |
| H  | 2.23324400 | 1.43433700 | 1.35873700 |
| C  | 2.59536500 | 2.83757900 | -0.22886200 |
| H  | 2.84984900 | 2.81271400 | -1.30013800 |
| H  | 1.68623800 | 3.43521000 | -0.11351300 |
| O  | 1.28067200 | -2.61278300 | 0.34497400 |
| H  | 0.37940500 | -2.87678600 | 0.06763400 |
| O  | 3.95209300 | -1.96571500 | -0.17088200 |
| O  | 4.61776700 | 0.85486800 | 0.45504900 |
O  1.05153600  1.00416100 -0.30657300
O  3.60296400  3.47343100  0.53503000
H  4.36048000  2.86652100  0.57538300
O  -0.59041000 -0.58649200 -0.47470700
C  -4.64454500  0.18885600 -0.23698700
H  -4.66949200  0.06897100 -1.33633300
C  -3.74848500  1.37212600  0.13520700
H  -3.73717400  1.45466500  1.23205300
C  -2.32949100  1.12186600 -0.36501600
H  -2.34096700  1.08494400 -1.46596800
C  -1.82742900 -0.23228200  0.15362000
H  -1.68698900 -0.17219100  1.24204200
C  -2.83906800 -3.27628400 -0.29192900
O  -5.93778400  0.32402700  0.27130100
H  3.57706400 -2.84259900  0.00682900
H  5.37645900  0.35730100  0.09030800
H  -6.19427600  1.25274200  0.16490200
O  6.50975800 -1.06375500 -0.51855500
H  5.68849600 -1.62019200 -0.44308500
TH-Abs-C2, G= -861843.21 kcal/mol, i 86.62cm -1
C  0.88168800  0.37506600 -0.11503500
H  0.78350900  0.34324100 -1.21424900
C  1.81539700  1.52698300  0.28421100
H  1.78405400  1.59864300  1.41910700
C  3.25783200  1.23651400 -0.11843100
H  3.33983100  1.28376100 -1.21464600
C  3.68061300 -0.15201000  0.34942800
H  3.67014300 -0.17639100  1.44824700
C  2.68976000 -1.20828300 -0.16506500
H  2.67706500 -1.20137900 -1.26609200
C  3.02659300 -2.62839700  0.30563900
H  3.19178400 -2.62356500  1.39370600
H  2.17296700 -3.27965800  0.09687200
| Element | X          | Y         | Z          |
|---------|------------|-----------|------------|
| O       | 1.42986200 | 2.73866500| -0.29985700|
| H       | 0.49110000 | 2.93619400| -0.08787500|
| O       | 4.16287700 | 2.18153600| 0.46482900 |
| O       | 4.98111800 | -0.48507300| -0.13849200|
| O       | 1.38262200 | -0.88386500| 0.34378200 |
| H       | 4.87050200 | -2.54844000| -0.31609400|
| O       | -0.34607100| 0.61229600 | 0.48659200 |
| C       | -4.33816800| -0.39775600| 0.14718200 |
| H       | -4.38698900| -0.31314100| 1.24886500 |
| C       | -3.36710800| -1.51329900| -0.24500400|
| H       | -3.33507000| -1.56200900| -1.34356300|
| C       | -1.97387000| -1.19281700| 0.28668500 |
| H       | -2.00503600| -1.18724300| 1.38754100 |
| C       | -1.54341200| 0.20291600 | -0.18424500|
| H       | -1.37427200| 0.18340400 | -1.27032500|
| C       | -2.62642300| 1.24968700 | 0.14483500 |
| H       | -2.69506100| 1.34217900 | 1.24324500 |
| C       | -2.38204100| 2.64118900 | -0.46021800|
| H       | -2.13087800| 2.55432400 | -1.52062700|
| H       | -3.31560800| 3.20938200 | -0.38052500|
| O       | -3.88120500| -2.72756300| 0.28955600 |
| H       | -3.22477400| -3.42225100| 0.13459900 |
| O       | -1.10592900| -2.21987300| -0.17235900|
| H       | -0.20425900| -2.03287800| 0.14732000 |
| O       | -3.87808600| 0.83025400 | -0.39216100|
| O       | -1.30157200| 3.36321500 | 0.14092900 |
| H       | -1.51933900| 3.57135500 | 1.05962500 |
| O       | -5.61316800| -0.59422900| -0.38711700|
| H       | 3.95591000 | 3.05507000 | 0.10147200 |
| H       | 5.58754300 | 0.22449000 | 0.11878600 |
| H       | -5.81740900| -1.53834000| -0.30630100|
| O       | 2.41720300 | 1.94676500 | 2.89459700 |
| H       | 3.27257000 | 2.26564600 | 2.53644200|

P-C2, \( G = -861871.45 \) kcal/mol, 21.66 cm⁻¹

| Element | X          | Y         | Z          |
|---------|------------|-----------|------------|
| C       | -0.56317100| -0.27232900| -0.37524700|
| H       | -0.31937100| -0.17152500| -1.45419900|
| C       | -1.58424400| -1.33860500| -0.12952800|
| H       | -7.10200700| -1.22956200| 0.80754100 |
| C       | -3.03566000| -1.05263000| -0.33585500|
| H       | -3.30679900| -1.14054500| -1.40478000|
| C       | -3.37211700| 0.37565000 | 0.11670500 |
| H       | -3.33305700| 0.40618700 | 1.21489600 |
| C       | -2.32104700| 1.35943100 | -0.42831700|
H       -2.30373200  1.31678600  -1.52880000  
C       -2.58977900  2.81174600  -0.01282400  
H       -2.76664900  2.85349800  1.07329800  
H       -1.69995100  3.40919500  -0.23329800  
O       -1.23316500 -2.62961500  -0.37778900  
H       -0.26925900 -2.78246200  -0.23415700  
O       -3.84601600  0.80442100  0.39720300  
O       -4.64404200  0.80442100 -0.35224100  
O       -1.02842400  0.99530900  0.09305100  
O       -3.66032200  3.38325900 -0.74122100  
O       -1.23316500 -2.62961500  -0.37778900  
O       -0.26925900 -2.78246200  -0.23415700  
O       -3.84601600  0.80442100  0.39720300  
O       -4.64404200  0.80442100 -0.35224100  
C       -1.56435800  1.55732600 -0.58176300  
H       -1.49475300  1.56643900 -1.67977000  
C       -3.00756200  1.29557500 -0.16428400  

R-C3, G = -861844.27 kcal/mol, 22.13 cm⁻¹
TS-Abs-C3, G= -861842.89 kcal/mol, i 70.51cm -1

C 0.88719200  0.44545300 -0.13145900
P-C3, \( G = -861867.46 \text{ kcal/mol}, 22.04 \text{ cm}^{-1} \)

| Atom | X         | Y         | Z         | Energy (kcal/mol) |
|------|-----------|-----------|-----------|-------------------|
| C    | -0.7115070 | 0.3945960 | -0.17754200 | -0.71143300 0.41588900 0.92323200 |
| H    | -1.6028280 | 1.5046290 | -0.73706200 | -3.02915800 1.19073800 -0.43088100 |
| C    | -3.0291580 | 1.1907380 | -0.43088100 | -3.88597300 1.07471600 2.95816500 |
| H    | -3.5243880 | -0.2036060 | -0.61884600 | -3.71169500 -0.41011900 -1.69003000 |
| C    | -2.4867110 | -1.2216300 | -0.90582500 | -2.46684400 -1.17013000 1.00147600 |
| H    | -2.9054300 | -2.6925150 | -1.62530000 | -2.79040300 -2.65933500 -0.53018000 |
| O    | -0.3488550 | 2.9688980 | -0.33793600 | -3.96062100 2.16581700 -0.66950300 |
| O    | -4.7557760 | -0.4364340 | 0.10030200 | -1.29515400 2.77310700 -0.17659200 |
| H    | -0.4588580 | 2.5546700 | 0.08765700 | -3.92276500 -3.19871800 0.13048900 |
| O    | 0.56136800 | 0.5994960 | -0.69176700 | 4.51910900 -0.35021800 0.00174800 |
| C    | 4.67326500 | -0.2129420 | -1.08469400 | 3.53832100 -1.49870900 0.24661800 |
| H    | 3.39946600 | -1.5983260 | 1.33320700 | 3.39946600 -1.59832600 1.33320700 |
| C    | 2.19046000 | -1.1761860 | -0.40514700 | 2.33677900 -1.12260700 -1.49670600 |
| H    | 1.69795700 | 0.1907890 | 0.07800800 | 1.69795700 0.19078900 0.07800800 |
| C    | 1.42404100 | 0.1222320 | 1.13955500 | 1.42404100 0.12223200 1.13955500 |
| H    | 2.78496600 | 1.2697090 | -0.09944400 | 2.78496600 1.26970900 -0.09944400 |
| C    | 2.45186700 | 2.6229710 | 0.53648100 | 2.45186700 2.62297100 0.53648100 |
| C    | 2.03286600 | 2.4811530 | 1.54108800 | 3.39369200 3.17320800 0.62723900 |
| O    | 4.12731300 | -2.6792550 | 0.28734400 | 4.12731300 -2.67925500 -0.28734400 |
| H    | 3.47742200 | -3.3934590 | -0.21736600 | 3.47742200 -3.39345900 -0.21736600 |
| O    | 1.30808000 | -2.2336910 | -0.07705500 | 1.30808000 -2.23369100 -0.07705500 |
| H    | 0.42263100 | -2.0195710 | -0.42337900 | 0.42263100 -2.01957100 -0.42337900 |
| O    | 3.98396600 | 0.8431630 | 0.54794900 | 3.98396600 0.84316300 0.54794900 |
| O    | 1.52665300 | 3.3523370 | -0.29048000 | 1.52665300 3.35233700 -0.29048000 |
| H    | 1.64593800 | 4.2953820 | -0.12151800 | 1.64593800 4.29538200 -0.12151800 |
| O    | 5.74059600 | -0.5512820 | 0.64884700 | 5.74059600 -0.55128200 0.64884700 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -3.521562 | 3.026322 | -0.562068 |
| H    | -5.405710  | 0.217556 | -0.196885 |
| H    | 5.966820   | -1.488826 | 0.551953 |
| O    | -3.955011  | 0.113027 | 2.917043 |
| H    | -4.359157  | -0.077216 | 2.053516 |

R-C4, G = -861846.64 kcal/mol, 22.03 cm⁻¹
0  -4.12440000  -0.97540100   0.35258900
0  -1.46652200  -3.36781600  -0.14649400
H  -1.54072400  -4.31422800   0.02980000
O  -5.93704900   0.34332800  0.23439700
H   3.58767100  -2.84221700  -0.08638800
H   5.37597500   0.36073600  0.08337900
H  -6.19031800   1.27002000  0.10534200
O   6.51367400  -1.03713000  -0.56771100
H   5.69401600  -1.59756000  -0.50773800

TS-Abs-C4, G= -861843.25 kcal/mol, i 123.97cm -1
C   0.91377100   0.35995300  -0.07369100
H   0.82879400   0.37167800  -1.17372400
C   1.85540000   1.46471900   0.41154400
H   1.84724500   1.44457500  1.51036500
C   3.26936700   1.19973800  -0.09258100
H   3.28531800   1.31762600  -1.18729700
C   3.71296700  -0.21774900  -0.13258100
H   3.79848500  -0.26674500   1.39521400
C   2.68257300  -1.26576100  -0.19765800
H   2.63745300  -1.26870100  -1.29898400
C   3.02242800  -2.67351300   1.35299400
H   3.15114300  -3.32557500   0.10580000
O   1.46114300  -0.17119800  -0.08600800
H   0.52732500   2.89630500   0.15914100
O   4.21976900   2.09490100   0.49225000
O   4.96543200  -0.53955400  -0.31232100
O   1.39767000  -0.92546800   0.34485200
O   4.08792900  -3.25479200  -0.46759100
H   4.85298000  -2.66378600  -0.39840000
O  -0.31778600   0.58923700   0.52347500
C  -4.31432700  -0.39422900   0.15844500
H  -4.37070400  -0.29777800  1.25859700
C  -3.34921800  -1.52000000  -0.21603200
H  -3.31039000  -1.57946400  -1.31380400
C  -1.95693800  -1.20422100   0.32067500
H  -1.99356500  -1.19225900  1.42132000
C  -1.51358500   0.18613900  -0.15497800
H  -1.33521800   0.15908200  -1.23942300
C  -2.59232600   1.24257100   0.15980100
H  -2.66858600   1.35698200  1.25258800
C  -2.34076600   2.62287900  -0.45414500
H  -2.04447600   2.52328400  -1.50675300
H  -3.28920200   3.16781500  -0.41082700
| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -3.87403500| -2.72630100| 0.32653400 |
| H     | -3.21973900| -3.42558900| 0.18370000 |
| O     | -1.09547900| -2.24081000| -0.12888400|
| H     | -0.19020700| -2.05047300| 0.17870500 |
| O     | -3.84094800| 0.82332300 | -0.39076300|
| O     | -1.32849800| 3.32440700 | 0.28783200 |
| H     | -1.44532900| 4.27175900 | 0.14114700 |
| O     | -5.58733500| -0.58700100| -0.38372100|
| H     | 3.92214200 | 2.99913700 | 0.31319000 |
| H     | 5.59543800 | 0.15638400 | -0.07218800|
| H     | -5.79908400| -1.52853200| -0.29303500|
| O     | 4.20786700 | 0.23676100 | 2.83074400 |
| H     | 4.40569200 | 1.15599200 | 2.55409300 |

P-C4, G = -861870.89 kcal/mol, 20.19 cm⁻¹

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| C     | 0.59677200 | -0.27819400| 0.13678100 |
| H     | 0.48634300 | -0.26215700| 1.23499900 |
| C     | 1.60721700 | -1.33593900| -0.30003900|
| H     | 1.65485300 | -1.30675500| -1.39764100|
| C     | 2.99430200 | -1.02866000| 0.26004700 |
| H     | 2.98188000 | -1.24583900| 1.34596100 |
| C     | 3.34949000 | 0.41319100 | 0.03325800 |
| H     | 7.03938400 | -0.88269200| -0.88448400|
| C     | 2.26465300 | 1.43899400 | 0.27296100 |
| H     | 2.10823500 | 1.58739500 | 1.35985900 |
| C     | 2.59308700 | 2.81636300 | -0.33153500|
| H     | 2.93582000 | 2.68883300 | -1.38111300|
| H     | 1.68679000 | 3.42810300 | -0.30468000|
| O     | 1.24915000 | -2.62514100| 0.16763300 |
| H     | 0.32938600 | -2.82441400| -0.10326300|
| O     | 3.95413400 | -1.91991100| -0.34851100|
| O     | 4.57927000 | 0.87799700 | 0.39887500 |
| O     | 1.02051800 | 1.00995000 | -0.31535400|
| O     | 3.57331800 | 3.51129800 | 0.41808600 |
| H     | 4.35783500 | 2.94344000 | 0.46608100 |
| O     | -0.60913700| -0.59668000| -0.47868700|
| C     | -4.65583400| 0.19707500 | -0.21363000|
| H     | -4.68590700| 0.07756000 | -1.31261000|
| C     | -3.75403200| 1.37540000 | 0.15705400 |
| H     | -3.73823100| 1.45528900 | 1.25408200 |
| C     | -2.33838300| 1.12004100 | -0.34880300|
| H     | -2.35379600| 1.08503700 | -1.44969400|
| C     | -1.83762600| -0.23794600| 0.16300500 |
| H     | -1.68645500| -0.18115500| 1.25044700 |
| C     | -2.85661300| -1.35191800| -0.15225500|
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -2.907  | 0.489   | -1.243  |
| C    | -2.544  | -2.706  | 0.489   |
| H    | -2.252  | -2.573  | 1.539   |
| H    | -3.467  | 0.489   | 0.457   |
| O    | -4.327  | 2.546   | -0.416  |
| H    | -3.709  | 3.277   | 0.275   |
| O    | -1.537  | 2.206   | 0.094   |
| H    | 0.615   | 2.049   | -0.181  |
| O    | -4.135  | -0.985  | 0.367   |
| O    | -1.506  | -3.374  | -0.240  |
| H    | -1.554  | -4.319  | 0.053   |
| O    | -5.947  | 0.338   | 0.300   |
| H    | 3.607   | -2.816  | -0.221  |
| H    | 5.316   | 0.237   | 0.225   |
| H    | -6.199  | 1.268   | 0.194   |
| O    | 6.485   | -1.595  | -0.313  |
| H    | 5.765   | -1.595  | -0.313  |

R-C5, G = -861847.00 kcal/mol, 10.13 cm^-1

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.627   | -0.707  | 0.056   |
| H    | 0.583   | -0.550  | 1.147   |
| C    | 1.376   | -2.003  | -0.271  |
| H    | 1.313   | -2.157  | -1.358  |
| C    | 2.839   | -1.879  | 0.140   |
| H    | 2.892   | -1.796  | 1.237   |
| C    | 3.453   | -0.629  | -0.478  |
| H    | 3.493   | -0.733  | -1.573  |
| C    | 2.632   | 0.611   | -0.094  |
| H    | 2.649   | 0.738   | 0.998   |
| C    | 3.153   | 1.897   | -0.744  |
| H    | 3.243   | 1.756   | -1.830  |
| H    | 2.444   | 2.708   | -0.561  |
| O    | 0.823   | -3.098  | 0.434   |
| H    | -0.134  | -3.162  | 0.233   |
| O    | 3.619   | -2.989  | -0.295  |
| O    | 4.795   | -0.433  | -0.028  |
| O    | 1.282   | 0.424   | -0.548  |
| O    | 4.378   | 2.308   | -0.183  |
| H    | 4.991   | 1.538   | -0.152  |
| O    | -0.644  | -0.824  | -0.483  |
| C    | -4.444  | 0.770   | -0.188  |
| H    | -4.555  | 0.519   | -1.259  |
| C    | -3.316  | 1.788   | -0.006  |
| H    | -3.225  | 2.000   | 1.069   |
| C    | -2.005  | 1.199   | -0.516  |
TS-Abs-C5, G=-861844.58 kcal/mol, i 140.37 cm⁻¹

H  -2.08842200  1.03352800  -1.60207100
C  -1.74291200  -0.15770500   0.15330300
H  -1.51440500   0.00239600  1.21648700
C  -2.97192500  -1.08126000  0.02783000
H  -3.11114500  -1.34625700 -1.03220500
C  -2.88770200  -2.37593800  0.84176700
H  -2.52303300  -2.16610700  1.85585100
H  -3.90489000  -2.77382300  0.91392500
O  -3.68907000   2.96451900 -0.71366400
H  -2.94524200   3.58310100 -0.67543000
O  -0.98846100   2.15238300 -0.24273600
H  -0.13064600   1.78537500 -0.52329000
O  -4.12408000  -0.40708300  0.53312000
O  -2.02689400  -3.32280800  0.18587800
H  -2.71454000  -4.21078300  0.47572100
O  -5.65529800   1.22313800  0.33846400
H  -3.05373000  -3.79616300  0.36452400
H  -5.37681900  -1.26396200 -0.15194600
H  -5.73242600  -2.16360600  0.11709600
O  -4.38228400   4.24899800  1.84848500
H  -4.44888000   3.58044700  1.11958400

C   0.89501400   0.43746900 -0.13528100
H   0.78340700   0.44274600 -1.0328100
C   1.82374600   1.56649400  0.32529200
H   1.82576300   1.57004900  1.32529200
C   3.24316300   1.32249400 -0.18186600
H   3.24759200   1.38804900 -1.28000900
C   3.70571900  -0.06864800   0.23250300
H   3.72043000  -0.12336400  1.33312900
C   2.71178800  -1.12260600 -0.27496600
H   2.66397300  -1.05366700 -1.42445000
C   3.10735100  -2.56708000  0.30806800
H   3.38593000  -2.60656400  1.09846200
H   2.25210000  -3.22069800 -0.15150900
O   1.39185500   2.81197000 -0.18869400
H   0.45872100   2.96246200  0.06742200
O   4.17538000   2.25270400  0.36324200
O   4.99960700  -0.37475300 -0.27819800
O   1.42512600  -0.85327100  0.25603500
O   4.15750200  -3.00977100 -0.81248900
H   4.90754500  -2.40451400 -0.68971800
O  -0.32275800   0.61868100  0.50076400
C  -4.31787500  -0.40992600  0.21695700
|   |   |   |   |
|---|---|---|---|
| H | -4.36297500 | -0.27415100 | 1.31359400 |
| C | -3.34541400 | -1.53825800 | -0.12827200 |
| H | -3.31723500 | -1.63656900 | -1.22335900 |
| C | -1.94979500 | -1.19081900 | 0.38043500 |
| H | -1.97469000 | -1.13783200 | 1.48053500 |
| C | -2.61180300 | 1.24118200 | -0.15119300 |
| H | -2.67744500 | 1.39116100 | 1.23001000 |
| C | -2.38180400 | 2.60373000 | -0.51972900 |
| H | -2.07105500 | 2.47555500 | -1.56491900 |
| H | -3.34154600 | 3.12997900 | -0.50447000 |
| O | -3.85194800 | -2.72992400 | 0.46290500 |
| H | -3.19981400 | -3.43153200 | 0.32210000 |
| O | -1.08753400 | -2.23831000 | -0.03985000 |
| H | -0.17140200 | -2.01080200 | 0.19879400 |
| O | -3.86214600 | 0.79153400 | -0.38062300 |
| O | -1.39299200 | 3.35020000 | 0.21017600 |
| H | -1.51611400 | 4.28868100 | 0.01899000 |
| O | -5.59491500 | -0.63446700 | -0.30258000 |
| H | 3.87603600 | 3.14398100 | 0.13336000 |
| H | 5.57326600 | 0.38460000 | -0.10472700 |
| H | 5.79082200 | -1.57678700 | -0.18772800 |
| O | 2.74528400 | -1.38078800 | -2.91685300 |
| H | 3.33919100 | -2.14984700 | -2.78427500 |

P-C5, $G = -861869.32$ kcal/mol, 21.73 cm$^{-1}$

|   |   |   |   |
|---|---|---|---|
| C | -0.87988300 | 0.40498200 | -0.16624300 |
| H | -0.85817100 | 0.26003300 | 0.92060600 |
| C | -1.83117900 | 1.52705100 | -0.57457900 |
| H | -1.78269100 | 1.64276700 | -1.66848800 |
| C | -3.24907900 | 1.16294100 | -0.15140600 |
| H | -3.26616500 | 1.03895800 | 0.94141900 |
| C | -3.67704700 | -0.15626500 | -0.79986100 |
| H | -3.84019700 | 0.04595500 | -1.87464400 |
| C | -2.63489900 | -1.22128100 | -0.61493000 |
| H | -2.12102500 | -1.71939000 | 2.30888800 |
| C | -2.95053800 | -2.59678500 | -0.15510800 |
| H | -3.75950400 | -3.04916000 | -0.74717700 |
| H | -2.06507200 | -3.23059700 | -0.23012400 |
| O | -1.49329100 | 2.73648500 | 0.07964600 |
| H | -0.54146200 | 2.92564500 | -0.05022900 |
| O | -4.19824900 | 2.14896500 | -0.54527800 |
| O | -4.89898300 | -0.63886500 | -0.22878800 |
| O | -1.31556800 | -0.86713300 | -0.75569700 |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | 0.53394600 | 3.00866200 | 0.02508400 |
| O    | -4.24102300 | 2.24721200 | -0.25977300 |
| O    | -4.99314900 | -0.44091500 | 0.17801300 |
| O    | -4.14682200 | -0.77632300 | -0.49991900 |
| O    | -4.13931000 | -3.13460500 | 0.13854600 |
| H    | -4.86881900 | -2.49494900 | 0.16163900 |
| O    | 0.29659800 | 0.75211200 | -0.57601000 |
| C    | 4.27574000 | -0.31597000 | -0.39410700 |
| H    | 4.28521000 | -0.17355500 | -1.49109300 |
| C    | 3.30682700 | -1.44532200 | -0.02947300 |
| H    | 3.31592300 | -1.55487800 | 1.06473600 |
| C    | 1.90544800 | -1.07390800 | -0.49845800 |
| H    | 1.89669000 | -1.02935100 | -1.59694100 |
| C    | 1.50270700 | 0.30427900 | 0.04685300 |
| H    | 1.35967900 | 0.23407200 | 1.13583900 |
| C    | 2.59148400 | 1.35505000 | -0.24970400 |
| H    | 2.62933200 | 1.53322600 | -1.33603000 |
| C    | 2.39087000 | 2.69745200 | 0.46025700 |
| H    | 2.16262400 | 2.53138600 | 1.52114200 |
| H    | 3.33941400 | 3.23966300 | 0.38931400 |
| O    | 3.79259900 | -2.62833500 | -0.65526500 |
| H    | 3.15964600 | -3.34242800 | -0.49506900 |
| O    | 1.01222500 | -2.10568700 | -0.06394200 |
| H    | 0.11400900 | -1.88790900 | -0.39059400 |
| O    | 3.85034900 | 0.88168800 | 0.22796300 |
| O    | 1.33902000 | 3.44534500 | -0.17122900 |
| H    | 1.45405700 | 4.37827900 | 0.04980100 |
| O    | 5.56597800 | -0.55537100 | 0.08215900 |
| H    | -3.94275300 | 3.12269000 | 0.02565400 |
| H    | -5.59652500 | 0.30573300 | 0.04788300 |
| H    | 5.76275200 | -1.49179600 | -0.07240700 |
| O    | 0.40766700 | -1.46850100 | 2.60900700 |
| H    | 0.64814200 | -2.01434900 | 1.81980200 |

**TS-Abs-C1', G= -861843.16 kcal/mol, i 276.13 cm⁻¹**

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 0.93503800 | 0.46344000 | -0.16131500 |
| H    | 0.85498100 | 0.51891200 | -1.25601300 |
| C    | 1.86756300 | 1.54575800 | 0.38720500 |
| H    | 1.82655200 | 1.50110900 | 1.48588700 |
| C    | 3.29495700 | 1.27472800 | -0.07658600 |
| H    | 3.33903700 | 1.38549400 | -1.17125600 |
| C    | 3.70207800 | -0.14679600 | 0.29449300 |
| H    | 3.69250900 | -0.24101000 | 1.39102600 |
| C    | 2.70465000 | -1.15921500 | -0.28947700 |
| H    | 2.70762300 | -1.08793700 | -1.38739700 |
|    |          |          |          |
|----|----------|----------|----------|
| C  | 3.01741900 | -2.60712000 | 0.10619800 |
| H  | 3.16225200 | -2.66579700 | 1.19605600 |
| H  | 2.16250700 | -3.23902900 | -0.15309600 |
| O  | 1.49121200 | 2.82598800  | -0.08568700 |
| H  | 0.54272300 | 2.97204900  | 0.10381800  |
| O  | 4.23540000 | 2.15443600  | 0.53343400  |
| O  | 5.00116100 | -0.46163100 | -0.20601100 |
| O  | 1.39022000 | -0.84625800 | 0.21795400  |
| H  | 4.86833400 | -2.50295500 | -0.49295000 |
| O  | -0.31256300 | 0.69148700  | 0.42877200  |
| C  | -4.25053300 | -0.39929200 | 0.26677200  |
| H  | -4.17957800 | -0.33908900 | 1.36927600  |
| C  | -3.31016000 | -1.48519700 | -0.26042700 |
| H  | -3.37992000 | -1.48281000 | -1.35716900 |
| C  | -1.87839300 | -1.73336000 | 0.16284800  |
| H  | -1.80315900 | -1.27063200 | 1.25740400  |
| C  | -1.50345200 | 0.27190900  | -0.20190400 |
| H  | -1.35314300 | 0.27527000  | -1.37105000 |
| C  | -2.59603500 | 1.29786100  | 0.15047200  |
| H  | -2.59087000 | 1.43531000  | 1.24537800  |
| C  | -2.41191200 | 2.66922500  | -0.50979600 |
| H  | -2.18948200 | 2.54694700  | -1.57670400 |
| H  | -3.36440800 | 3.19914800  | -0.40565700 |
| O  | -3.76123700 | -2.72827600 | 0.26753800  |
| H  | -3.14894900 | -3.42015500 | -0.02055100 |
| O  | -1.03088200 | -2.12788200 | -0.46792000 |
| H  | -0.11634200 | -1.96856700 | -0.16126300 |
| O  | -3.86927900 | 0.84475900  | -0.29214100 |
| O  | -1.36156000 | 3.39631400  | 0.14970100  |
| H  | -1.44570700 | 4.32890300  | -0.08680900 |
| O  | -5.57194100 | -0.60916000 | -0.12890200 |
| H  | 3.95994000  | 3.06310200  | 0.34541700  |
| H  | 5.59793300  | 0.25686000  | 0.05132800  |
| H  | -5.74272600 | -1.56184300 | -0.07450000 |
| O  | -1.01471600 | -0.08319100 | -2.72440300 |
| H  | -0.94731400 | -1.04826700 | -2.57182700 |

P-C1’, G = -861864.67 kcal/mol, 27.29 cm⁻¹
C -3.66184800 -0.02205600 -0.36736100
H -3.75982300 0.08845200 -1.45808500
C -2.63543500 -1.12765000 -0.07736900
H -2.52064900 -1.26319300 1.00673700
C -3.01004700 -2.47255700 -0.71021800
H -3.24405600 -2.32463500 -1.77605400
H -2.15071500 -3.14717500 -0.64642400
O -1.36971600 2.82629800 0.33449300
H -0.45468800 3.03335600 0.05510500
O -4.16238800 2.28841400 -0.13199600
O -4.91514900 -0.41882900 0.19090800
O -1.36767700 -0.72473600 -0.64781100
H -4.79619400 -2.46586000 0.06707200
O 0.35473800 0.80619700 -0.71910300
C 4.27433900 -0.35269700 -0.37077100
H 4.28358000 -0.24218700 -1.47200400
C 3.28248800 -1.44336300 0.04017000
H 3.24347300 -1.46052500 1.13823800
C 1.89968300 -1.10934400 -0.50951600
H 1.92018500 -1.26843600 -1.60398600
C 1.55685100 0.33458300 -0.24179000
H -0.21282000 -2.08236800 3.30671500
C 2.64779300 1.37971500 -0.30452700
H 2.79228500 1.70517700 -1.35363000
C 2.36562400 2.63719800 0.53320000
H 2.00880200 2.35240000 1.52985600
H 3.31761400 3.16818100 0.63363500
O 3.77595200 -2.67960100 -0.46533400
H 3.13349900 -3.37290200 -0.25838400
O 0.97553400 -2.04856900 0.05805000
H 0.09446100 -1.87323000 -0.33202000
O 3.87335700 0.86833500 0.21854700
O 1.39676100 3.46500100 -0.13190000
H 1.52345700 4.37773100 0.15614700
O 5.56124400 -0.60670200 0.10697600
H -3.84317500 3.14512400 0.18605600
H -5.51808900 0.33660200 0.12647200
H 5.71473600 -1.56082800 0.02971000
O -0.22567900 -1.44837500 2.58008600
H 0.35440200 -1.80632200 1.88273500

R-C1-Hydro-1H2O, G=-861868.07 kcal/mol, 20.77cm -1
C -0.94051500 -0.26172000 0.00012600
C -1.80917800 -1.50133600 0.05377100

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TS Hydro -Cl -1H2O, G= -861805.35 kcal/mol, i 227.93 cm -1
C  -1.14241100  0.01742500  0.03750200  
C  -1.74210900  -1.36255300  0.26358400  
H  -1.59933200  -1.61151500  1.32148300  
C  -3.24138200  -1.38924100  -0.05204700  
H  -3.37320000  -1.48111900  -1.13968400  
C  -3.87269200  -0.08993200  0.43064400  
H  -3.62821200  0.05284000  1.49402400  
C  -3.32156400  1.07852600  -0.38271000  
H  -3.61717700  0.98900900  -1.43168000  
H  -3.08158700  3.21534000  -0.34833900  
O  -1.10968300  -2.28399100  -0.59651100  
H  -0.15074300  -2.33074100  -0.38706700  
O  -3.91789200  -2.45132000  0.61249800  
O  -5.28516100  -0.07705000  0.24869600  
O  -5.04853200  2.77072500  -0.17707700  
O  -5.61404200  2.04511500  0.13153900  
O  0.89480700  -0.67949800  0.75916200  
C  4.84045100  0.41957200  0.14265500  
H  5.03884700  0.05454700  1.16849400  
C  3.84924900  1.58572700  0.19849400  
H  3.67144500  1.91428000  -0.83812500  
C  2.54072600  1.11280600  0.82600300  
H  2.72315800  0.85525500  1.87629300  
C  1.98414600  -0.12869700  0.10051500  
H  1.70842900  0.17968200  -0.92806400  
C  3.10682500  -1.19010900  -0.05120200  
H  3.33830400  -1.58857400  0.95329800  
C  2.74186800  -2.35109400  -0.98635400  
H  2.42539000  -1.95735800  -1.95615000  
H  3.64401200  -2.95535300  -1.14517700  
O  3.78525900  3.29216700  1.14939100  
O  1.59085900  2.19381500  0.88241400  
H  1.21724600  2.31478000  -0.00331700  
O  4.28646800  -0.62232500  -0.62902600  
O  1.66274500  -3.16532200  -0.52425700  
H  1.87046400  -3.48878900  0.36273100  
O  6.03764700  0.77310300  -0.49042300  
H  -3.58265500  -3.29195800  0.27109000  
H  -5.62405000  -0.92887700  0.56545000  

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P-C1Hydro-1H2O, G=-861865.65 kcal/mol, 9.82 cm⁻¹
R-C1-Hydro-2H2O, G= -909820.46 kcal/mol, 17.06cm -1

| Element | x          | y          | z          |
|---------|------------|------------|------------|
| H       | 1.20273800 | -2.10870400 | 1.29503700 |
| O       | 5.99236300 | -0.27297400 | -1.70952300 |
| H       | -2.55363600 | -2.36476600 | -1.88372400 |
| H       | -5.53906100 | -1.13847300 | -1.62368800 |
| H       | 6.50386600  | 0.55005100  | -1.69901900 |
| O       | -0.90047100 | 0.85300300  | 1.56906100  |
| H       | -1.09704400 | 1.64891400  | 2.08712200  |
| H       | 0.86825900  | 0.21139100  | 1.66178200  |

R-C1-Hydro-2H2O, G= -909820.46 kcal/mol, 17.06cm -1
| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | 2.44109100 | -1.09876800 | -0.50739300 |
| H       | 3.00213000  | -1.78399600  | 0.14756500   |
| C       | 1.46629500  | -1.90777800  | -1.35447000  |
| H       | 0.78286900  | -2.45514800  | -0.70288800  |
| H       | 0.88182600  | -1.21504200  | -1.98253600  |
| O       | 4.94098100  | 2.04007800   | 0.57760500   |
| H       | 4.58998600  | 2.67190000   | 1.22161100   |
| O       | 2.30273600  | 1.96802400   | 1.75791900   |
| H       | 1.64892800  | 2.41446900   | 1.19980100   |
| O       | 0.90269600  | -0.05973800  | 2.80887900   |
| P-C1-Hydro-2H2O, G=-909823.00 kcal/mol, 10.65 cm^{-1} |

| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | -2.31375900 | 0.41959600 | 1.57703900 |
| C       | -2.52498300 | -1.02736100 | 1.16891900 |
| H       | -3.40272700 | -1.41553000 | 1.71167800 |
| C       | -2.82864800 | -1.07987800 | -0.33601100 |
| H       | -1.91779800 | -0.80277800 | -0.89193700 |
| C       | -3.93473200 | -0.09714100 | -0.67495540 |
| H       | -4.84797100 | -0.37846300 | -0.14819800 |
| C       | -3.52808100 | 1.32060600  | -0.27689900 |
| H       | -2.61572200 | 1.61764100  | -0.81073400 |
| C       | -4.61314200 | 2.37136300  | -0.53263800 |
| H       | -5.57616100 | 2.01419200  | -0.13664200 |
| H       | -4.34755700 | 3.28713100  | 0.00288400   |
| O       | -1.46717900 | -1.89931500 | 1.50373100   |
| H       | -0.60372400 | -1.54005300 | 1.20524000   |
| O       | -3.26150400 | -2.37391600 | -0.73292100  |
| O       | -4.19616600 | -0.08315100 | -2.09810800  |
| O       | -3.26384900 | 1.31901200  | 1.14450900   |
| O       | -4.70226800 | 2.70944700  | -1.90542300  |
| H       | -4.82398100 | 1.88870600  | -2.40849300  |
| O       | 1.15460500  | -0.99715300 | 1.11979000   |
| C       | 4.55319600  | 0.10692600  | -1.03646000  |
H  5.16160700  -0.41542100  -0.27511900
C  3.80319600  1.27329500  -0.38196400
H  3.23875000  1.78130200  -1.18058800
C  2.83313900  0.75737100  0.68363600
H  3.40936400  0.35678400  1.52573100
C  1.92567700  -0.34532200  0.12104400
H  1.24991200  0.10795400  -0.62600700
C  2.78636300  -1.40609200  -0.59664800
H  3.41837400  -1.91446800  0.14802800
C  1.95315800  -2.44798800  -1.33530200
H  1.31835800  -2.97653100  -0.62151600
H  1.31124800  -1.93573700  -2.06958800
O  4.78188000  2.14590800  0.16840400
H  4.33344000  2.82217300  0.69590400
O  2.09786500  1.86287300  1.24929400
H  1.48300300  2.20139600  0.58092500
O  3.61258100  -0.78486800  -1.58937600
O  2.76875000  -3.42220700  -1.96430300
H  3.39317800  -2.95350300  -2.53714200
O  5.35134900  0.53125400  -2.10357700
H  -2.64480900  -3.02089000  -0.35763000
H  -4.31199200  -1.00089300  -2.38640500
H  -0.13086100  0.46295000  3.42742000
O  0.84195000  0.42400900  3.40107700
H  1.14296500  1.26930600  3.03007100
H  1.14875700  -0.50273700  1.97925100

R-C1’-Hydro-1H2O, G= 861863.24 kcal/mol, 24.48cm -1
C  0.88765000  0.22701000  -0.22163400
H  0.68843000  -0.04994500  -1.26659000
C  1.81135100  1.44654500  -0.13846600
H  1.88174300  1.74765400  0.91703700
C  3.19662200  1.07561400  -0.65077000
H  3.13071500  0.84602400  -1.72585600
C  3.71523400  -0.15601900  0.08503100
H  3.82017500  0.08966600  1.15275900
C  2.71741500  -1.31550400  -0.05186800
H  2.60604400  -1.58418300  -1.11310200
C  3.13869300  -2.56806000  0.72612100
H  3.39977600  -2.28748700  1.75809100
H  2.29209200  -3.25953400  0.77007000
O  1.33037300  2.51042600  -0.94080400

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|atom| x         | y         | z         |
|----|-----------|-----------|-----------|
|H   | 0.459794  | 2.797865  | -0.604258 |
|O   | 4.144627  | 2.119080  | -0.440859 |
|O   | 4.970804  | -0.585717 | -0.438540 |
|O   | 1.443709  | -0.887346 | 0.478304  |
|O   | 4.194947  | -3.260275 | 0.085623  |
|H   | 4.912810  | -2.627927 | -0.076372 |
|O   | -0.319426 | 0.588721  | 0.414844  |
|C   | -4.229279 | -0.668212 | 0.033641  |
|H   | -4.286161 | -0.548300 | 1.132042  |
|C   | -3.195892 | -1.735788 | -0.329582 |
|H   | -3.111834 | -1.764239 | -1.424752 |
|C   | -1.837745 | -1.366751 | 0.262716  |
|H   | -1.903356 | -1.485649 | 1.362304  |
|C   | -1.520917 | 0.077580  | -0.037824 |
|C   | -2.637400 | 1.096865  | 0.015913  |
|H   | -2.821239 | 1.400358  | 1.065601  |
|C   | -2.373451 | 2.370717  | -0.802394 |
|H   | -2.029975 | 2.107859  | -1.808424 |
|H   | -3.324338 | 2.905488  | -0.876793 |
|O   | -3.674157 | -2.979041 | 0.169712  |
|O   | -3.006599 | -3.654607 | -0.017335 |
|O   | -0.892979 | -2.301741 | -0.249505 |
|O   | -0.028102 | -2.121382 | 0.160633  |
|O   | -3.832813 | 0.562133  | -0.547811 |
|O   | -1.384972 | 3.199229  | -0.150917 |
|O   | -1.591253 | 4.127048  | -0.322644 |
|O   | -5.488776 | -0.952938 | -0.494454 |
|H   | 3.799322  | 2.923847  | -0.853460 |
|H   | 5.558000  | 0.184306  | -0.467609 |
|H   | 5.617870  | -1.911857 | -0.432230 |
|O   | -0.695821 | 2.792494  | 2.714036  |
|H   | -0.918169 | 2.919152  | 1.777445  |
|H   | -3.325807 | 1.901660  | 2.751105  |

**TS Hydro -Cl' -1H2O, G= -861801.64 kcal/mol, i 590.02 cm-1**

|atom| x         | y         | z         |
|----|-----------|-----------|-----------|
|C   | -0.913049 | 0.763484  | -0.497558 |
|H   | -0.503760 | 0.725060  | 0.529628  |
|C   | -2.137993 | 1.693967  | -0.543148 |
|H   | -2.536583 | 1.677514  | -1.567328 |
|C   | -3.207354 | 1.206924  | 0.427281  |
|H   | -2.814188 | 1.276266  | 1.453420  |
|C   | -3.556916 | -0.247880 | 0.128695  |
|H   | -4.006487 | -0.299380 | -0.874480 |
|C   | -2.292151 | -1.120708 | 0.136220  |
|H   | -1.842552 | -1.102260 | 1.141346  |
P-C1’-Hydro-1H2O, G= -861868.33 kcal/mol,  15.04 cm -1

C  1.85942900 -1.11447900 -0.49361800
H  1.57273400 -1.48746400  0.50514400
C  3.37926300 -1.17019000 -0.67032400
H  3.64880500  3.03345000 -1.15690600
H  2.38313500  4.21780100 -1.00118300
H  2.38313500 -2.43238500  1.88693400
O  2.01340200  1.19261100 -2.72386400
H  2.18100800  2.12714700 -2.45805800
H  1.05674200  1.15730700 -2.92955500

C  -2.57302200 -2.58031900 -0.24018300
H  -3.16514100 -2.61358500 -1.16778900
H  -1.62214100 -3.08525300 -0.43249800
O  -1.79094500  3.02470000 -0.16596800
H  -1.08298900  3.30592300 -0.76297400
O  -4.41804800  1.95602800  0.32560000
O  -4.47218000  0.77717000  1.09448600
O  -1.37113500 -0.58406400 -0.82478400
O  -3.20706900 -3.29270100  0.80997700
H  -3.80309300 -2.78157800  1.08926000
O  0.01568700  1.17461300 -1.39729000
C  3.51686500 -0.94345300  0.69886800
H  4.40902300 -0.93009800  0.04583400
C  2.38319600 -1.71041300  0.01357800
H  1.50969800 -1.69151400  0.68076900
C  1.99939700 -1.04251000 -1.33728400
H  2.85415800 -1.15992600 -2.02294000
C  1.76115300  0.39091400 -1.00427400
C  2.88381800  1.10333400 -0.28756300
H  3.81430900  1.08654800 -0.88963700
C  2.59309200  2.55610800  0.07523500
H  1.60593800  2.64158300  0.53955300
H  3.36577600  2.90409600  0.76859500
O  2.82933700 -3.04100800 -0.18937400
H  2.16429400 -3.49540200 -0.72895700
O  0.92775200 -1.73824500 -1.94061800
H  0.08052300 -1.40290400 -1.57590500
O  3.09579000  0.39689500  0.93253200
O  2.64880500  3.03345000 -1.15690600
H  2.38313500  4.21780100 -1.00118300
O  3.83162700 -1.46697300  1.95338400
H  -4.20536900  2.88946200  0.46572000
H  -5.21396700 -0.14843800  1.16058500
H  3.77528700 -2.43238500  1.88835400
O  2.01340200  1.19261100 -2.72386400
H  2.18100800  2.12714700 -2.45805800
H  1.05674200  1.15730700 -2.92955500
|  | X      | Y      | Z       |
|---|--------|--------|---------|
| C | 3.48325500 | 1.14269400 | 0.26234900 |
| H | 3.71915000 | 1.55824900 | -0.72883600 |
| C | 1.95486600 | 1.10782400 | 0.42134300 |
| H | 1.69921900 | 0.71221800 | 1.41677700 |
| C | 1.30929800 | 2.49033100 | 0.27096700 |
| H | 0.22636600 | 2.36652600 | 0.18281500 |
| O | 3.87983400 | -2.48757100 | -0.46772300 |
| H | 3.45882200 | -3.06925000 | -1.11894100 |
| O | 4.02422000 | 1.98509000 | 1.28099900 |
| C | 1.30929800 | 2.49033100 | 0.27096700 |
| H | 1.69921900 | 0.71221800 | 1.41677700 |
| H | 0.22636600 | 2.36652600 | 0.18281500 |
| O | 0.84941500 | 0.44153700 | 0.26234900 |

R-C5-Hydro-1H2O, G= -861865.93 kcal/mol, 21.33cm -1

C | 0.84941500 | 0.44153700 | -0.20256900 |
H | 0.77646400 | 0.44670600 | -1.29856700 |
|   |        |        |        |        |
|---|--------|--------|--------|--------|
| C | 1.75847200 | 1.56712500 | 0.29176300 |        |
| H | 1.76190000 | 1.55227100 | 1.39141700 |        |
| C | 3.17488700 | 1.34730200 | -0.22791900 |        |
| H | 3.15980000 | 1.37831500 | -1.32797500 |        |
| C | 3.68407900 | -0.02302100 | 0.21607900 |        |
| H | 3.84180000 | 0.01374800 | 1.31044100 |        |
| C | 2.70001100 | -1.11140900 | -0.11174000 |        |
| H | 3.10884000 | -2.55117600 | -0.10702900 |        |
| H | 2.18657000 | -3.18458900 | -0.06991200 |        |
| O | 1.30316200 | 2.81326700 | -0.20403800 |        |
| H | 0.38575800 | 2.96666400 | 0.10135500 |        |
| O | 4.08295700 | 2.32085500 | 0.27321900 |        |
| O | 4.91819200 | -0.35849200 | -0.42372100 |        |
| O | 1.36986000 | -0.86085700 | 0.19909800 |        |
| O | 3.82189800 | -2.92122400 | -1.29029000 |        |
| H | 4.57641300 | -2.31671200 | -1.36256100 |        |
| O | -0.39209800 | 0.59720600 | 0.39370400 |        |
| C | -4.31062000 | -0.42819000 | -0.09481600 |        |
| H | -4.41139400 | -0.43577400 | 1.01000300 |        |
| C | -3.37597800 | -1.49242500 | -0.57953500 |        |
| H | -3.33879000 | -1.44153700 | -1.67760100 |        |
| C | -1.98814000 | -1.20418700 | -0.01568300 |        |
| H | -2.02284200 | -1.31234400 | 1.08003400 |        |
| C | -1.57233900 | 0.23739200 | -0.34072400 |        |
| H | -1.37670900 | 0.32224000 | -1.41844000 |        |
| C | -2.67566600 | 1.23911400 | 0.05978100 |        |
| H | -2.75710700 | 1.25799000 | 1.15820800 |        |
| C | -2.45264600 | 2.67199000 | -0.43430800 |        |
| H | -2.15098000 | 2.66723400 | -1.48990000 |        |
| H | -3.41305200 | 3.19024500 | -0.34970300 |        |
| O | -3.87423400 | -2.75638100 | -0.15769900 |        |
| H | -3.22034300 | -3.42931000 | -0.39652200 |        |
| O | -1.11209500 | -2.17245200 | -0.57792300 |        |
| H | -0.21211000 | -2.03131100 | -0.23764800 |        |
| O | -3.91362600 | 0.84382200 | -0.52968100 |        |
| O | -1.45778900 | 3.32907600 | 0.36847200 |        |
| H | -1.59669000 | 4.28276300 | 0.30869600 |        |
| O | -5.63314000 | -0.59494300 | -0.64557600 |        |
| H | 3.73011600 | 3.19510100 | 0.05366400 |        |
| H | 5.56846200 | 0.31387200 | -0.17596200 |        |
| H | -5.82102600 | -1.54585900 | -0.65578300 |        |
| O | 1.81304100 | -0.96962700 | 3.10629300 |        |
| H | 1.31094800 | -0.98150400 | 2.27677800 |        |
| H | 1.16032000 | -0.93811800 | 3.81596900 |        |
TS Hydro -C5 -1H2O, G=-861797.89 kcal/mol, i 843.16 cm -1

|  |  |  |  |
|---|---|---|---|
| C | 0.78897800 | 0.38619000 | 0.02789000 |
| H | 0.74991200 | 0.37273400 | -1.07295800 |
| C | 1.72771200 | 1.50219000 | 0.48704200 |
| H | 1.67259200 | 1.58343900 | 1.58414400 |
| C | 3.15921500 | 1.19960400 | 0.04928800 |
| H | 3.15158600 | 0.88827400 | -1.00534900 |
| C | 3.83952100 | 0.10367700 | 0.89069200 |
| H | 3.90100100 | 0.46920100 | 1.92505800 |
| C | 3.21704200 | -1.25353000 | 0.88509500 |
| C | 3.32692800 | -2.31832500 | -0.13251600 |
| H | 4.29217600 | -2.81988200 | 0.04638300 |
| H | 2.53677600 | -3.05877800 | 0.00984100 |
| O | 1.37339900 | 2.73654500 | -0.12028900 |
| H | 0.42317900 | 2.91089400 | 0.04147800 |
| O | 3.99795800 | 2.34229600 | 0.20581000 |
| O | 5.15680300 | -0.13471500 | 0.36863400 |
| O | 1.18765000 | -0.86793000 | 0.49186200 |
| O | 3.25140700 | -1.87253400 | -1.48552100 |
| O | 4.06729700 | -1.38568600 | -1.67229900 |
| O | -0.48929000 | 0.74346500 | 0.53330300 |
| C | -4.45202000 | -0.25920300 | -1.11712700 |
| C | -3.47491700 | -1.38335900 | -0.32288200 |
| H | -3.39827000 | -1.44079100 | -1.41859200 |
| C | -2.10366500 | -1.06739100 | 0.26253700 |
| C | -2.18459600 | -1.04859900 | 1.36171000 |
| C | -1.63977000 | 0.32373400 | -0.19792000 |
| H | -1.40633000 | 0.28279600 | -1.12737600 |
| C | -2.73418400 | 1.38428600 | 0.04162000 |
| H | -2.84559700 | 1.53916100 | 1.12643100 |
| C | -2.46297100 | 2.73739200 | -0.62226100 |
| H | -2.18413800 | 2.58788900 | -1.67377700 |
| H | -3.39894000 | 3.30497600 | -0.58850400 |
| O | -4.01552400 | -2.59533600 | 0.19661400 |
| H | -3.34900400 | -3.28697100 | 0.07461800 |
| O | -1.22768200 | -2.10846000 | -0.14636500 |
| H | -0.30741900 | -1.86318900 | 0.09256500 |
| O | -3.96935500 | 0.95239300 | -0.53256000 |
| O | -1.42597800 | 3.44533600 | 0.07736300 |
| H | -1.49119900 | 4.38146600 | -0.15008000 |
| O | -5.71422300 | -0.46325200 | -0.54621200 |
| H | 3.47256200 | 3.11549700 | -0.55496000 |
| H | 5.55367000 | 0.74207300 | 0.24040500 |
|     |     |     |     |
|-----|-----|-----|-----|
| H   | -5.90733900 | -1.41078400 | -0.48064300 |
| O   | 2.17971800  | -1.39112800 | 2.51261700  |
| H   | 1.41364500  | -1.12766500 | 1.80013600  |
| H   | 2.13583600  | -2.33250000 | 2.73891000  |

P-C5-Hydro-1H2O, G= -861863.80 kcal/mol, 7.05 cm -1

|     |     |     |     |
|-----|-----|-----|-----|
| C   | 0.44852000  | 0.03674500  | -0.49188300 |
| H   | 0.28292800  | 0.17237200  | -1.56764400 |
| C   | 1.55592900  | 0.97672400  | 0.00661500  |
| H   | 1.63448200  | 0.84259800  | 1.09578300  |
| C   | 2.94304200  | 0.71036400  | -0.66175100 |
| H   | 2.83336400  | 0.00403100  | -1.49437700 |
| C   | 3.98141600  | 0.13031000  | 0.34386100  |
| H   | 3.91384600  | 0.74038100  | 1.26367200  |
| C   | 3.78489200  | -1.31458600 | 0.70825600  |
| C   | 4.85009200  | -2.33974800 | 0.54265900  |
| H   | 4.43619200  | -3.34450100 | 0.68642700  |
| H   | 5.25829900  | -2.28041600 | -0.47112300 |
| O   | 1.91845000  | 2.31727500  | -0.28405300 |
| O   | 0.30200300  | 2.51466100  | 0.07908800  |
| O   | 3.51146500  | 1.91276400  | -1.17230200 |
| O   | 5.28821600  | 0.24142500  | -0.21117000 |
| O   | 0.75212600  | -1.33143200 | -0.31226300 |
| O   | 5.90972800  | -2.22103100 | 1.51719500  |
| H   | 6.37641800  | -1.39536400 | 1.31782800  |
| O   | -0.70572100 | 0.41907600  | 0.22894900  |
| C   | -4.80659300 | -0.06229800 | 0.12313000  |
| H   | -4.75026700 | -0.13724100 | 1.22511800  |
| C   | -4.02560800 | -1.20830400 | -0.51908200 |
| H   | -4.08699600 | -1.08641500 | -1.61055200 |
| C   | -2.56385600 | -1.14590500 | -0.08922800 |
| H   | -2.50658800 | -1.31430100 | 0.99826900  |
| C   | -1.98653800 | 0.24856000  | -0.38367800 |
| H   | -1.89761900 | 0.37557700  | -1.47269400 |
| C   | -2.90214300 | 1.35432200  | 0.18274100  |
| H   | -2.87027800 | 1.31152100  | 1.28305800  |
| C   | -2.53334700 | 2.77327900  | -0.25795800 |
| H   | -2.34388200 | 2.79694200  | -1.33917200 |
| H   | -3.39546700 | 3.41210000  | -0.04049700 |
| O   | -4.64908200 | -2.42544100 | -0.12238300 |
| H   | -4.09704900 | -3.15477100 | -0.44029000 |
| O   | -1.89269100 | -2.18761400 | -0.78405800 |
| H   | -0.94150200 | -2.15748400 | -0.56403900 |
| O   | -4.23677500 | 1.16795600  | -0.28755700 |
| O   | -1.37856200 | 3.23277400  | 0.46437400  |
R-C1'-Hydro-2H2O, G= -909823.95 kcal/mol, 24.76 cm -1

H  -1.34458900  4.19625800  0.40823700
O  -6.13836400 -0.02734000 -0.29818000
H   2.85967800  2.62242200 -1.03441600
H   5.31376800  1.09938500 -0.66654400
H  -6.44868900 -0.94431700 -0.34671000
O   2.79986300 -1.50826800  1.66942000
H   1.22196600 -1.46072900  0.53382500
H   2.96781400 -2.32887100  2.15561100

C   -0.94681500  0.25881200  0.24195500
H   -0.74435600  0.39712000  1.31327900
C   -1.83120300  1.39240200 -0.30133800
H   -1.91729500  1.26352200 -1.39053700
C   -3.22385000  1.27749300  0.32203200
H   -3.13739400  1.46785500  1.40383000
C   -3.79524300 -0.11821600  0.11298700
H   -3.91118100 -0.29545300 -0.96743000
C   -2.83258400 -1.17094000  0.67967000
H   -2.71379000 -1.01895000  1.76282600
C   -3.30179800 -2.61088600  0.43864000
H   -3.56158100 -2.73808000 -0.62382400
H   -2.48045800 -3.29629400  0.66807100
O   -1.32674900  2.66615400  0.02961400
H   -0.69465300  2.99262200 -0.65874500
O   -4.13256800  2.20455600 -0.25716000
O   -5.05667000 -0.26989100  0.76467000
O   -1.55513800 -1.01686200  0.02306400
O   -4.37649800 -2.96729100  1.28864700
H   -5.06650600 -2.29076100  1.19965300
O   0.27305400  0.27293900 -0.47190200
C   4.11970400 -0.97403100  0.05381300
H   4.06536900 -1.04752000 -1.04886600
C   3.10625300 -1.92211800  0.70208400
H   3.11929700 -1.73617600  1.78471200
C   1.70857500 -1.63518300  0.15890900
H   1.67880100 -1.98848300 -0.89041000
C   1.44349000 -0.15359000  0.15205900
C   2.56805100  0.83072100 -0.06072800
H   2.66577800  1.01392700 -1.14915100
C   2.30045500  2.18603200  0.61349400
H   1.23004500  2.38736300  0.63888000
H   2.68016200  2.14181000  1.64079400
O   3.52119100 -3.25366200  0.41705300
H   2.87772400 -3.86123300  0.80882000

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TS Hydro-C1'-2H2O, G= -909760.81 kcal/mol, i 652.48 cm -1

C  -0.89934400  0.66406400  -0.51411800
H  -0.40497900  0.57903200   0.47112600
C  -2.06178600  1.66548500  -0.42955200
H  -2.54221000  1.72090600  -1.41774400
C  -3.08472900  1.19847000   0.59860300
H  -2.61571500  1.20214900   1.59467900
C  -3.53882300  -0.22034100  -0.70149100
H  -4.05759600  -0.20278900  -1.12820600
C  -2.33205400  -1.16647000  -1.41774400
H  -1.81936500  -1.22100000   0.15500900
C  -2.72793700  -2.58744100  -0.26347500
H  -3.38048600  -2.54011500  -1.14893900
H  -1.82505100  -3.13798400  -0.54218400
O  -1.60029600  2.95167700   0.02690400
O  -4.05884400  -2.76665800  -1.14893900
O  -0.02397800  1.04654900  -1.48576200
C  3.46517500  -0.84092800   0.73977300
H  4.36904200  -0.75081200   0.10914700
C  2.40695000  -1.68070900   0.02318400
H  1.51433400  -1.71227600   0.66434900
C  2.01692100  -1.05044000  -1.34243900
H  2.87974100  -1.15710200  -2.02015800
C  1.71345300  0.37916500  -1.05507200
P-C1'-Hydro-2H2O, G= -909825.78 kcal/mol, 14.34 cm⁻¹
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 3.80216800| -1.55282300| 0.69206300|
| H    | 4.46289500| -1.89693800| -0.12614800|
| C    | 2.33619300| -1.78591600| 0.32432400|
| H    | 1.72674800| -1.34036800| 1.12486000|
| C    | 2.00524200| -1.10134900| -1.00706000|
| H    | 2.47032600| -1.69313500| -1.81423800|
| C    | 2.56089400| 0.29072100| -1.01651500|
| C    | 3.86364500| 0.58970400| -0.30567200|
| H    | 4.71248500| 0.36215600| -0.98454500|
| C    | 3.98947600| 2.05636600| 0.12041200|
| H    | 3.15783600| 2.31443200| 0.78478900|
| O    | 0.60990200| -1.16823400| -1.29533000|
| H    | 0.10655800| -0.61671800| 0.26478100|
| O    | 3.99655100| -0.16283000| 0.89263600|
| O    | 3.95057100| 2.85092600| -1.08267900|
| O    | 3.86760900| 3.78433300| -0.85143800|
| O    | 4.15293200| -2.16962000| 1.89414100|
| H    | -5.71271500| 1.73657500| -0.47975700|
| H    | -5.51946600| -1.33640800| 0.60199300|
| H    | 3.66235900| -3.00430400| 1.94476300|
| O    | 2.32229400| 0.99151200| -2.17760800|
| H    | 2.79580500| 1.84735700| -2.10613000|
| H    | 0.47867000| 1.19851900| -2.69552200|
| O    | -0.40014400| 1.62642100| -2.73507100|
| H    | -0.37782200| 2.23276000| -3.48490300|
| H    | -0.68607400| 2.07136500| -1.04929600|

TSF1gly-C1, G=-861855.70 kcal/mol, i 551.85 cm⁻¹
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 0.370999| -2.74462| -0.42592|
| O    | 4.19570 | -2.09975 | -0.24549|
| O    | 4.92618 | 0.51103 | 0.34213|
| O    | 1.44212 | 1.05309 | -0.64772|
| O    | 4.08401 | 3.19254 | 0.66889|
| H    | 4.81879 | 2.55995 | 0.68570|
| O    | -0.22468| -0.33714 | -1.25411|
| C    | -4.35953| 0.44315 | -0.14576|
| H    | -4.44635| 0.58731 | -1.23938|
| C    | -3.76845| 1.46979 | 0.42790|
| H    | -3.29329| 1.30027 | 1.51068|
| C    | -2.00734| 1.26792 | -0.22694|
| H    | -2.11784| 1.46407 | -1.30697|
| C    | -1.58477| -0.16359| -0.03961|
| H    | -1.10064| -0.39376| 0.90968|
| C    | -2.62434| -1.15351| -0.51703|
| H    | -2.73682| -1.05272| -1.61234|
| C    | -2.35780| -2.62251| -0.17048|
| H    | -2.08809| -2.71902| 0.88325|
| H    | -3.27793| -3.18953| -0.34690|
| O    | -3.91770| 2.76006| 0.16400|
| H    | -3.25501| 3.41674| 0.42279|
| O    | -1.12039| 2.21507| 0.35124|
| H    | -0.23969| 2.08269| -0.03783|
| O    | -3.88705| -0.86599| 0.11372|
| O    | -1.27116| -3.19901| -0.91076|
| H    | -1.45248| -3.12270| -1.85741|
| O    | -5.61743| 0.52200| 0.45855|
| H    | 3.92455| -2.96653| 0.08685|
| H    | 5.49270| -0.27201| 0.26884|
| H    | -5.81493| 1.46205| 0.58816|
| O    | 0.38219| -1.37436| 2.44828|
| H    | 0.71413| -1.95471| 1.73472|

F1gly-C1, G=-861882.57, 9.01 kcal/mol cm⁻¹

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 1.86596| 0.06939| -1.42228|
| H    | 0.42413| 0.52457| 3.33972|
| C    | 2.04163| -0.93440| -0.26142|
| H    | 2.29004| -1.88848| -0.75504|
| C    | 3.18839| -0.59186| 0.68191|
| H    | 2.89294| 0.25051| 1.32569|
| C    | 4.40685| -0.18979| -0.13467|
| H    | 4.66928| -1.01528| -0.81610|
| C    | 4.07506| 1.05510| -0.95693|
| H    | 3.82193| 1.88572| -0.28767|
TSF12-3-C1, G= -861838.56kcal/mol, i 432.47cm -1

C  0.84882000  -0.46437700  -1.24376000
H  2.89069300  -5.13521000  0.68671700
C  1.64547300  -1.24413600  -1.94173100
H  2.63332900  -1.59151100  -1.59143200
C  2.82685400  -0.00281100  -0.53200700
H  2.78687300  -2.02849600  1.95740100
H  5.63193700  -0.59883900  1.32836500
H  -6.89967000  0.61439100  0.04668100
O  -0.04491000  0.78671500  2.53776500
H  0.23174200  0.16114300  1.83864600

C  5.20950800  1.50429800  -1.88602500
H  5.58479800  0.63958100  -2.45494400
H  4.80675800  2.22796400  -2.59897400
O  0.86650800  -1.08133400  0.51171300
H  0.14263500  -1.46529300  -0.04403400
O  3.56474400  -1.70969100  1.47841100
O  5.51809300  0.12539500  0.69457200
O  2.92345300  0.80440400  -1.81283900
H  6.24302300  2.15839700  -1.17428300
H  6.54845800  1.56864100  -0.46794000
O  0.83492600  0.12839000  -2.06029400
C  -5.04879700  0.25033700  -0.34952900
H  -4.73447100  1.13285800  -0.93890600
C  -4.70702500  0.48500500  1.13186600
H  -2.91161900  1.58680100  0.75237600
C  -3.18490500  0.66046900  1.29169900
H  -2.53279800  -0.51238300  0.64019200
C  -2.19764600  -1.34116600  1.26003400
C  -2.93924400  -0.75089800  -0.77764600
H  -2.65672000  0.11395600  -1.40572200
C  -2.34177100  -2.01910500  -1.38401000
H  -2.62751700  -2.88990300  -2.76665600
H  -2.16094000  -2.15996200  -2.40363700
O  -5.43635200  1.63457600  1.54746600
H  -5.15352100  1.85332600  2.44711900
O  -2.90600500  0.80360600  2.67440700
H  -1.93685300  0.89449500  2.76665600
O  -4.37879200  -0.89663800  -0.84028700
O  -0.90921200  -1.97043200  -1.37524100
H  -0.58954500  -1.24413600  -1.94173100
O  -6.41386900  0.00281100  -0.53200700
H  2.78687300  -2.02849600  1.95740100
H  5.63193700  -0.59883900  1.32836500
H  -6.89967000  0.61439100  0.04668100
O  -0.04491000  0.78671500  2.53776500
H  0.23174200  0.16114300  1.83864600
C  3.24689100  0.31357300  0.30455300  
H  3.88199700  0.23109400 -0.59149800  
C  2.07257700  1.24496700 -0.02562400  
H  1.34811500  1.25250600  0.79764100  
C  2.51263600  2.69050500 -0.30469000  
H  3.36676000  2.68508600 -0.99888200  
H  1.68806200  3.22037000 -0.78790800  
O  1.11363200 -2.84599600 -1.02438000  
H  0.16990300 -2.81214200 -0.74310500  
O  4.02095600  0.97749800  1.34145300  
O  3.90135800 -2.81214200 -0.74310500  
O  2.80471400  3.40286800  0.88280000  
H  3.49537700  2.90720500  1.35097800  
O -0.51320400 -0.56922700 -0.91782200  
C -4.07374300  0.88856300  0.27205900  
H -4.54666400  0.57114200 -0.67606100  
C -3.01277000  1.95299900 -0.00660500  
H -2.56129400  2.24043200  0.95430100  
C -1.92889400  1.38184600 -0.31480600  
H -2.37962700  1.12479400 -1.89038700  
C -3.13083300  0.89290000 -0.31480600  
H -0.78893000  0.31098900  0.59397800  
C -2.51217600 -0.88124700  0.02318200  
O -2.99923000 -1.17619600 -0.92348300  
C -2.09429100 -2.15125200  0.77710600  
H -1.38218200 -1.91668900  1.57239800  
H -2.99038100 -2.57749500  1.24059100  
O -3.67668300  3.06497300 -0.59493000  
H -3.00534500  3.71731600 -0.84239600  
O -0.96100200  2.40424000 -1.08825600  
H -0.16163800  2.01938300 -1.48865400  
O -3.45232400 -0.23432300  0.87611800  
O -1.44888700 -3.12403400 -0.05368700  
H -2.08293800 -3.47730100 -0.69224500  
O -5.03963600  1.32544100  1.17986200  
H  3.58059100 -2.81388900  1.02738000  
H  4.68740800  0.34857000  1.65243400  
H -5.23616300  2.25107800  0.96959700  
O  2.54625300 -4.26220100  0.90830000  
H  1.99790300 -3.96311800  0.15236800  

F12-3-C1, G= -861855.57 kcal/mol, 11.99 cm -1
C  0.857494697102  -0.631177844256  -1.121543492710
H  2.719385149315  -5.066700665307  0.913174460383
TSF15-6-C1, G= -861853.69 kcal/mol, i596.65 cm^{-1}

C  0.80529300 -0.24778100 -1.21263700
H  2.50585800 -5.15176500  0.67295600
C  1.78791200 -1.39555400 -1.10318900
H  2.44129500 -1.40585700 -1.98314900
C  2.71414600 -1.18463100  0.14020400
H  2.12514300 -1.39463400  1.04839600
C  3.27351900  0.24354700  0.23024500
H  3.81493200  0.46020300 -0.70401100
C  2.21289000  1.29006200  0.42880300
H  1.49397900  1.08431400  1.22201800
C  2.63181000  2.72993900  0.32682800
H  3.27053900  2.87225100 -0.55701500
H  1.75847800  3.38045000  0.22720100
O  1.13805200 -2.66066900 -1.05351000
H  0.30674300 -2.57831100 -0.54260300
O  3.85563000  3.38045000  0.22720100
O  4.18881200  0.34036200  1.33292300
O  1.22387600  0.95746000 -1.11057600
O  3.01693000  3.14366000  1.52131300
H  3.98776100  2.48667400  1.72001900
H  -0.48604500 -0.60539200 -0.94423300
C  -4.20245100  0.86869800  0.10327700
H  -4.58332200  0.32584600 -0.78181900
C  -3.21748300  1.95422600 -0.32717700
H  -2.85154500  2.45161300  0.58300700
C  -2.02177700  1.35000500 -1.06816600
H  -2.37248500  0.90297500 -2.01232300
C  -1.40600400  0.23371500  0.65116800
H  -0.89219700  0.67586500  0.65116800
C  -2.49230200 -0.75156400  0.27383400
H  -2.90089200 -1.26762500 -0.61251000
C  -1.98073100 -1.81063100  1.26451400
H  -1.29095400 -1.36247800  1.98480500
H  -2.84466100 -2.19282600  1.81877800
O  -3.93258600  2.87594600 -1.14074800
H  -3.30559400  3.54095300 -1.46075200
O  -1.14552600  2.43484900 -1.33647900
H  -0.23844300  2.09991700 -1.45957700
O  -3.52608500 -0.04901000  0.94981800
O  -1.26265200 -2.88338100  0.64144700
H  -1.89238700 -3.47459200  0.20786900
O  -5.25862000  1.38144100  0.85686700
H  3.60725900 -2.96383400  0.18115000
F15-6-C1, G= -861875.07 kcal/mol, 13.52 cm⁻¹

H 4.74824000 -0.45345300 1.29267100
H -5.50735800 2.23245800 0.46484800
O 2.85559000 -4.58727700 -0.02646900
H 2.09365200 -4.15407600 -0.46282400
C 0.64662200 -0.20438400 -0.98710500
H 2.77459200 -5.07807100 0.73086100
C 1.66902200 -1.34098700 -0.92242300
H 2.11252400 -1.41548500 -1.91799000
C 2.83374300 -1.10694900 0.08520700
H 2.46317200 -1.34146600 1.09497100
C 3.40593400 0.32570800 0.08437300
H 3.55499400 0.64689100 -0.95995700
O 1.01573700 -2.58688700 -0.66405000
H 0.31057500 -2.46761600 0.00527700
C 3.91837000 -1.95336600 -0.25765600
O 0.67919400 0.68834900 -1.81360100
O 3.96555200 2.96552100 1.87787000
H 1.01573700 -2.58688700 -0.66405000

O 2.85559000 -4.58727700 -0.02646900
H 2.09365200 -4.15407600 -0.46282400
C 0.64662200 -0.20438400 -0.98710500
H 2.77459200 -5.07807100 0.73086100
C 1.66902200 -1.34098700 -0.92242300
H 2.11252400 -1.41548500 -1.91799000
C 2.83374300 -1.10694900 0.08520700
H 2.46317200 -1.34146600 1.09497100
C 3.40593400 0.32570800 0.08437300
H 3.55499400 0.64689100 -0.95995700
O 1.01573700 -2.58688700 -0.66405000
H 0.31057500 -2.46761600 0.00527700
C 3.91837000 -1.95336600 -0.25765600
O 0.67919400 0.68834900 -1.81360100
O 3.96555200 2.96552100 1.87787000
H 1.01573700 -2.58688700 -0.66405000

C -4.33904000 0.64034500 -0.20633400
H -4.45407700 0.03943200 -1.12785100
C -3.38974700 1.81097900 -0.46453500
H -3.30204300 2.38415100 0.47034600
C -1.99466900 1.31762200 -0.87118800
H -2.07429900 0.79111000 -1.83375500
C -1.51199400 0.34533300 0.21276000
H -1.35654900 0.89975100 1.14456500
C -2.55920100 -0.76883600 0.43885500
H -2.67735900 -1.33035700 -0.50457700
C -2.18083400 -1.76696200 1.54607500
H -1.64935300 -1.26536300 2.35886000
H -3.10793300 -2.18479300 1.95165100
O -3.97274600 2.60906700 -1.48348200
H -3.33705500 3.30414400 -1.71067400
O -1.19988900 2.48090000 -1.00428300
H -0.37212400 2.20094400 -1.43684100
O -3.79723700 -0.18192700 0.81582900

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| Atom | X       | Y       | Z       | Energy   |
|------|---------|---------|---------|----------|
| O    | 1.31252100 | -2.80992700 | 1.08085100 |          |
| H    | -1.84356600 | -3.50191200 | 0.66545300 |          |
| O    | -5.58229100 | 1.06322700  | 0.26423700 |          |
| H    | 3.70801900  | -2.89291600 | -0.06821900 |          |
| H    | 5.12736100  | -0.50682100 | 0.47969400 |          |
| O    | -5.83611100 | 1.84601800  | -0.24813100 |          |
| H    | 2.92562300  | -4.51892800 | -0.04029200 |          |
| H    | 2.07348500  | -4.09952100 | -0.27343600 |          |

**TSF21-6-C2, G= -861853.33 kcal/mol, i 76.45 cm -1**

| Atom | X       | Y       | Z       | Energy   |
|------|---------|---------|---------|----------|
| C    | -0.42366600 | -0.66823600 | -0.57417800 |          |
| H    | -0.36254500 | -0.07107200 | -1.47535600 |          |
| C    | -1.57839100 | -1.28996000 | -0.16172700 |          |
| H    | -7.24589500 | -1.11578000 | -0.32716000 |          |
| C    | -2.94671800 | -0.84429900 | -0.57600300 |          |
| H    | -2.96976700 | -0.61821600 | -1.64741100 |          |
| C    | -3.35024700 | 0.46545000  | 0.17829200  |          |
| H    | -3.42207500 | 0.23006000  | 1.25104400  |          |
| C    | -2.27374600 | 1.55876700  | -0.01350300 |          |
| H    | -2.20918800 | 1.80243600  | -1.09124900 |          |
| C    | -2.69171500 | 2.87721500  | 0.70516500  |          |
| H    | -2.98621400 | 2.63920400  | 1.73836200  |          |
| H    | -1.81902200 | 3.53386000  | 0.74184900  |          |
| O    | -1.55556100 | -2.19148200 | 0.84546800  |          |
| H    | -0.63175700 | -2.42393300 | 1.05201400  |          |
| O    | -3.90384500 | -1.88938200 | -0.35998000 |          |
| O    | -4.58139300 | 0.96151900  | -0.31927200 |          |
| O    | -1.05424800 | 1.14204300  | 0.51003900  |          |
| O    | -3.70832500 | 3.57721600  | 0.01431000  |          |
| H    | -4.42506500 | 2.94174700  | -0.14899900 |          |
| O    | 0.70529100  | -1.04974400 | 0.04558000  |          |
| C    | 4.63407000  | 0.30676700  | 0.21056200  |          |
| H    | 4.58334200  | 0.29332500  | 1.31531300  |          |
| C    | 3.62140900  | 1.31357900  | -0.34035800 |          |
| H    | 3.70550800  | 1.30926500  | -1.43770700 |          |
| C    | 2.19869400  | 0.90965900  | 0.49588000  |          |
| H    | 2.10499500  | 0.93847100  | 1.14672700  |          |
| C    | 1.97023200  | -0.53700300 | -0.41373300 |          |
| H    | 1.99207900  | -0.58451800 | -1.51059800 |          |
| C    | 3.05836600  | -1.46137400 | 0.16075400  |          |
| H    | 3.00368000  | -1.42796400 | 1.26244000  |          |
| C    | 2.93922800  | -2.92832200 | -0.28111200 |          |
| H    | 2.60326800  | -2.99100000 | -1.32041900 |          |
| H    | 3.93713500  | -3.37738900 | -0.22237800 |          |
| O    | 3.96707600  | 2.59129800  | 0.17574500  |          |
H  3.25269700  3.20145900  -0.06254200
O  1.31643200  1.84020200  -0.54379100
H  0.42082500  1.74692200  -0.12258500
O  4.32790100  -0.99005900  -0.28061700
O  1.98886900  -3.65913100  0.49770400
H  2.42625900  -3.99291000  1.29106900
O  5.93563800  0.57723200  -0.21784500
H  -3.57723900  -2.45123800  0.36317500
H  -5.32961800  0.39503200  -0.03466200
H  6.06017100  1.53748300  -0.17479200
O  -6.47172700  -0.99998600  0.23685800
H  -5.76564100  -1.57698600  -0.11140400

F21-6-C2, G=  -861864.74 kcal/mol, 20.98 cm -1
C  -0.400215735778  -0.861057482430  -0.586161164877
H  -0.344381616773  -0.358827195325  -1.544330232798
C  -1.580039700202  -1.153653028611  0.030457785113
H  -7.228647150836  -1.116236372350  -0.537389013853
C  -2.932577004661  -0.759757967095  -0.482654252274
C  -2.893611763371  -0.594852381927  -1.563356882551
C  -3.419086628694  0.564171176915  0.182536849219
H  -3.568546455524  0.367945710652  1.254999335729
C  -2.36152782935  1.650709123264  0.029391204396
H  -2.215977890231  1.890783259053  -1.043245193482
C  -2.785168961615  2.980074885808  0.723397007960
H  -3.11609370676  2.746101551000  1.746026821252
H  -1.919378293895  3.643608330509  0.783475379987
O  -1.619932601344  -1.830090081619  1.203028140898
H  -0.714333067184  -2.040723343775  1.485539948674
O  -3.875361151920  -1.824402362258  -0.266951982951
O  -4.613607904289  1.029070976970  -0.422414255350
O  -1.159982285701  1.221328410472  0.615326725007
O  -3.779683531033  3.65691618524  -0.01576096386
H  -4.479761146839  3.010875806777  -0.210679721641
O  0.738996929557  -1.226148581596  0.033357007517
C  4.584559600786  0.335012206075  0.242318867087
H  4.501911119016  0.283684773307  1.344181094109
C  3.531142260845  1.291941712986  -0.313913762952
H  3.637681378029  1.309172235967  -1.409122286651
C  2.127717991424  0.798867781854  0.041252081896
H  2.011782060650  0.814170597480  1.136438231701
C  1.979470308038  -0.656322105805  -0.436054921283
H  1.984634546447  -0.685714115874  -1.533792245436
C  3.124764602799  -1.532860978586  0.105163064792
H  3.059696286842  -1.559234625959  1.206635358422
| C  | 3.124955129557 | -2.979371162001 | -0.417392019759 |
| H  | 2.799505383933 | -3.007821116869 | -1.461697955298 |
| H  | 4.158521877135 | -3.342595593233 | -0.378105905525 |
| Q  | 3.787214866546 | 2.580008367378  | 0.227421623313 |
| H  | 3.0446765349168| 3.149697491970  | -0.297980384641 |
| Q  | 1.207678071918 | 1.683165693848  | -0.564907882619 |
| H  | 0.328443543165 | 1.620617321763  | -0.104336171492 |
| O  | 4.365927264592 | -0.958221659120 | -0.297980384641 |
| O  | 2.392570824022 | -3.80842657222  | 0.305464728672 |
| H  | 2.688219534023 | -4.148429484367 | 1.098986569611 |
| O  | 5.880943503026 | 0.692399638900  | -0.135702280088 |
| H  | -3.621974074672 | -2.284242984583 | 0.548794429612 |
| H  | -5.374775061117 | 0.460786515706  | -0.17741646626 |
| O  | 5.941844419557 | 1.658222831862  | -0.082044531470 |
| O  | -6.49013344122 | -0.951248280292 | 0.068290481014 |
| H  | -5.756177785948 | -1.529163958096 | -0.199892916507 |

TSF23-4-C2, G= -861842.35 kcal/mol, i 423.60 cm⁻¹

| C  | -0.61568900  | -0.28466900  | -0.37536900  |
| H  | -0.44878700  | 0.01615700   | -1.42131800  |
| C  | -1.57770800  | -1.43937000  | -0.27802000  |
| H  | -6.98825700  | -1.43741700  | -0.05551900  |
| C  | -2.84408000  | -1.34160200  | -0.79143500  |
| H  | -3.08159300  | -0.77684900  | -1.68401200  |
| C  | -3.47277400  | 0.57439100   | 0.32058100   |
| H  | -3.45500300  | 0.19628000   | 1.34557500   |
| C  | -2.32119500  | 1.44778200   | -0.10788600  |
| H  | -2.31729500  | 1.53930200   | -1.20851300  |
| C  | -2.40581600  | 2.88102400   | 0.46398400   |
| H  | -2.48753000  | 2.82809900   | 1.56000200   |
| H  | -1.48558200  | 3.42078600   | 0.21605900   |
| O  | -1.36492400  | -2.38787900  | 0.69137900   |
| H  | -0.40597200  | -2.57808500  | 0.74215400   |
| O  | -3.76425600  | -2.33934800  | -0.51802600  |
| O  | -4.68389200  | 1.04102600   | -0.13855500  |
| O  | -1.07222700  | 0.89715300   | 0.34314400   |
| O  | -3.47214700  | 3.61759000   | -0.10823200  |
| H  | -4.27626800  | 3.07639400   | -0.05918300  |
| O  | 0.56210200   | -0.68529000  | 0.24824500   |
| C  | 4.60505000   | 0.23472800   | 0.16824400   |
| H  | 4.62867100   | 0.20234300   | 1.27365900   |
| C  | 3.67512400   | 1.36443500   | -0.28980500  |
| H  | 3.68668100   | 1.38638700   | -1.38970300  |
| C  | 2.25125100   | 1.09679500   | 0.19136000   |
F23-4-C2, $G = -861851.05$ kcal/mol, 18.95 cm $^{-1}$
H 4.65504500 0.21850800 0.98142700
C 3.53567200 1.35664100 -0.48527400
H 3.41359800 1.35363700 -1.57859300
C 2.17758200 1.13318400 0.17277400
H 2.29968700 1.15887800 1.26711800
C 1.66515100 -0.25482400 -0.22234300
H 1.52236000 -0.29998100 -1.31187300
C 2.70592200 -1.31255600 0.18597400
H 2.85819000 -1.25429700 1.27769900
C 2.30280300 -2.75263500 -0.16156000
H 1.78617600 -2.78895500 -1.12459000
H 3.21641500 -3.35215200 -0.24415800
O 4.15310600 2.56663400 -0.06031900
H 3.51844400 3.28608100 -0.19090000
O 1.31131900 2.18134700 -0.23915500
H 0.45732500 2.04452800 0.21246500
O 3.93027200 -1.03217500 -0.49072300
O 1.39973900 -3.31787400 0.79714800
H 1.90511000 -3.63207900 1.55787900
O 5.70744400 0.30516200 -0.79266500
H -3.03816600 -3.35661500 0.10314400
H -4.98981100 0.08332900 -0.60241200
H 5.98211400 1.23430200 -0.76773700
H -5.79321400 -1.46861000 -0.24968300
H -5.12007800 -2.15579100 -0.42490500

TSF31-2-C3, G= -861842.77 kcal/mol, i 393.87 cm -1
C -0.61142500 0.37469000 -0.07418700
H -0.61471300 0.56785600 1.00486500
C -1.75161500 2.09430500 -1.13340000
H -1.30580400 1.70968300 -2.04564700
C -2.99040500 1.68785700 -0.73364800
H -4.42114900 -2.50118200 3.57775100
C -3.47718900 0.30221700 -1.01666900
H -3.26592300 0.03499400 -2.05789200
C -2.73140300 -0.73004100 0.94378100
H -2.85088500 -0.45524100 -0.32221400
C -3.23019600 -2.16478700 -0.32221400
H -3.19884100 -2.41825100 -1.39182200
H -2.56975500 -2.85245700 0.21198000
O -1.25347900 3.26110600 -0.61347700
H -0.27795700 3.28297800 -0.70221400
O -3.61732900 2.26294700 0.35129400
O -4.89535400 0.18283700 -0.82908000

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O  -1.33373300  -0.74732400  -0.46437100
O  -4.54188900  -2.35963500   0.20378600
H  -5.09485200  -1.64372300  -0.15934300
O   0.61188400   0.39402700  -0.68617800
C   4.60997600  -0.35387400   0.08670900
H   4.76432000  -0.39977300 -1.00779600
C   3.64236000  -1.46204900   0.51531300
H   3.50581300  -1.39148900  1.60434400
C   2.30041200  -1.25699500 -1.26406900
H   2.43787300  -1.37069900 -1.26406900
C   1.78981600   0.16073300   0.09882500
H   1.54896200   0.25567800  1.16601500
C   2.85434400   1.20831200  -0.27269600
H   3.02420700   1.17089200 -1.36323600
C   2.49712600   2.64956000   0.12558100
H   2.02739800   2.67117300  1.11228800
H   3.42801400   3.22439600  0.18094900
O   4.25001500  -2.70226700   0.17055500
H   3.61634100  -3.40910200   0.35999900
O   1.41029300  -2.54950000   0.30720300
H   0.54827100  -2.15062500 -1.27147700
O   4.06363500   0.91056000   0.42354400
O   1.56823100   3.28230700  -0.76389400
H   2.00155200   3.47567300 -1.60538100
O   5.83144600  -0.43096000   0.75828200
H  -3.14606700   3.07999400   0.57934800
H  -5.16077000   0.84548300  -0.17169100
H   6.07569900  -1.36779900   0.80641000
O  -4.07189500  -1.87351800  2.93482900
H  -4.38574800  -2.17111300  2.05816900

F3i-2-C3, G= -861854.09 kcal/mol, 21.63cm -1

C   -0.64684000  -0.96977000   0.39787500
H  -1.03080300  -1.50335100   1.27415900
C  -1.73070900   2.59906400  -1.37476600
H  -1.36721300   2.21932000  -2.32417100
C  -2.69836900   1.99168300  -0.67680300
H  -4.28301200  -2.38624000   3.41349100
C  -3.38374700   0.71322500  -1.04969500
H  -3.19454800   0.49788100 -2.10630500
C  -2.89184100  -0.50015300 -2.02327000
H  -2.94502100  -0.27227700   0.84685800
C  -3.69632700  -1.77703200  -0.51484300
H  -3.79712800  -1.92117300  -1.59964200
H  -3.15694000  -2.63450600  -0.10552300
H  -2.49663500  -0.61358300  1.10468800
C  -2.96738300  -2.36307600  -0.18076400
H  -2.91369200  -2.59284300  -1.25559600
H  -2.40858600  -3.14798800  0.34984100
O  -1.06071600  2.92550500  -0.93924700
H  -0.08221300  2.96291300  -0.99342700
O  -3.37182200  2.36927100  0.20227500
O  -5.00408000  0.28347900  -0.62043300
O  -1.20445700  -0.74239900  -0.55278300
O  -4.31445100  -2.46209900  0.29936200
H  -4.81330000  -1.69706700  -0.03884200
O  0.60252300  0.64109500  -0.85782500
C  4.48516700  -0.39092600  0.13344000
H  4.67984400  -0.43173500  -0.95439300
C  3.43432500  -1.43363100  0.51453300
H  3.25719300  -1.35357100  1.59713500
C  2.13303600  -1.15146700  -0.22947800
H  2.30676600  -1.27627600  -1.31027600
C  1.69057100  0.29889100  0.01439500
H  1.37678200  0.41203600  1.06153500
C  2.84694200  1.27641100  -0.28444500
H  3.06415200  1.24914800  -1.36404800
C  2.58116100  2.73018900  0.11489700
H  2.12328500  2.77673200  1.11179300
H  3.55198100  3.23425800  0.15338300
O  3.96929200  -2.71280300  0.19354000
H  3.27557500  -3.37109000  0.34476400
O  1.18501200  -2.10519500  0.22622400
H  0.31865500  -1.89647400  -0.16788500
O  3.99781800  0.89676900  0.46916400
O  1.73090500  3.35959000  -0.85802200
H  1.84343400  4.31664800  -0.79562200
O  5.67305400  -0.54872500  0.85094800
H  -2.73523600  3.10348400  0.24902500
H  -5.15097300  0.92616800  0.09230200
H  5.85094200  -1.49983400  0.90819400
O  -4.10041600  -1.87448500  3.05629600
H  -4.46289000  -2.51352800  3.68054100

F34-5-C3, G= -861854.85 kcal/mol, 19.67 cm -1
C  -0.70221300  0.42393500  -0.2852100
H  -0.74378700  0.69951600  0.77768400
C  -1.54657900  1.39868900  -1.14303100
H  -1.38142300  1.12349900  -2.19317500
C  -3.00682800  1.32409500  -0.81785000

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TSF42-3-C4, G= -861841.62 kcal/mol, i395.27 cm -1

C 0.60354700 -0.51363700 -0.09927900
H 0.47821500 -0.72893600 0.98070100
C 1.53865000 -1.50314600 -0.72002400
H 2.02197500 -1.24373800 -1.65903400
C 3.32807200 -0.98118700 0.64020900
H 3.39435500 0.35207300 0.33373500
H 6.94598500 -0.78706600 -1.59707200
C 2.17886800 1.17753000 0.65911200
H 1.85542300 0.96840400 1.68804600
C 2.38895200 2.68535500 0.47561200
H 2.51549100 2.89818300 -0.59251700
H 1.50366500 3.21757200 0.83252900
O 1.22170700 -2.83087300 -0.58244900
H 0.30125800 -2.93441300 -0.25826900
O 4.30661600 -1.88453000 0.23412400
O 4.24566700 0.92378300 -0.56395300
O 1.07635600 0.82375900 -0.24100000
O 3.48768200 3.15695000 1.23915100
H 4.29259400 2.81384200 0.82448100
O -0.65274000 -0.62050400 -0.72861700
C -4.63886300 0.27727400 -0.25893500
H -4.72014200 0.00217700 -1.32675400
C -3.70006400 1.47283000 -0.09645700
H -3.61912600 1.69480900 0.97778800
C -2.32450400 1.11472700 -0.64488600
H -2.41078500 0.94085300 -1.72943800
C -1.80773100 -0.17926400 -0.00254700
H -1.54198300 0.02469600 1.04459800
C -2.86725300 -1.29972000 -0.0506100
H -2.98065100 -1.63430800 -1.09364100
C -2.55704700 -2.51203000 0.83213300
H -2.32598200 -2.17701400 1.85180900
H -3.46310700 -3.12548800 0.86648800
O -4.28735200 2.57220500 -0.78562000
H -3.65125700 3.30198000 -0.77842100
O -1.46867600 2.22044700 -0.39577700
H -0.54594400 1.94289700 -0.54647600
O -4.11103100 -0.82101100 0.46448000
O -1.46251000 -3.27718500 0.29733300
H -1.51545000 -4.17355200 0.65186100
O -5.90422600 0.51879000 0.28234000
H 3.88199900 -2.74637300 0.11147900
H 5.07727800 0.40074600 -0.68923600
H -6.13517000 1.43676600 0.07342300
O 6.53265800 -0.56851900 -0.75299200
F42-3-C4, G= -861852.79 kcal/mol, 14.54 cm -1

H 6.05289600 -1.35993300 -0.44959000

C 0.65642500 -0.57562200 -0.54647200
H 0.68952800 -0.80779500 0.53776500
C 1.42307700 -1.54841700 -1.37105700
H 2.45260600 -1.36806000 -1.64779800
C 3.55255000 -0.19299400 1.58795400
H 2.84051000 -0.18544900 2.40507200
C 3.30061200 0.45692800 0.43950400
H 5.93043800 -2.20170900 -1.16741500
C 2.03562500 1.26418200 0.28679900
H 1.51041300 1.27491800 1.2512300
C 2.32973000 2.71276000 -0.14723700
H 2.73356000 2.70090200 -1.16561200
H 1.39537000 3.27943300 -0.14724800
O -0.69157600 -0.65768600 -0.97456900
O 0.07612900 -2.90831200 -1.13726100
C -4.53220200 0.28679900 0.24883100
H -4.83871500 0.18380700 -0.80854500
C -3.50978000 1.41715100 0.38372600
H -3.22336400 1.48981800 1.44339800
C -2.32792410 1.08975800 -0.45163200
H -2.56966000 1.04964800 -1.51369100
C -2.84563700 -1.34840000 -0.12697500
H -3.16066300 -1.47077700 -1.17520000
C -2.46622200 -2.72281400 0.42735200
H -1.96725200 -2.61464700 1.39990300
H -3.39773900 -3.27924500 0.57559200
O -4.14898800 2.61783000 -0.03844000
H -3.47817500 3.31511100 -0.07330800
O -1.33353500 2.12986900 -0.24874500
H -0.49450200 1.85899700 -0.66726500
O -3.94587200 -0.92734500 0.68321300
O -1.61732400 -3.41256900 -0.50355400
H -1.60536600 -4.35081200 -0.27540700
O -5.64913500 0.48430200 1.06618700

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H 4.93935400 -0.96326100 2.70956900
H 4.85289300 -0.13053000 -0.62113100
H -5.88002400 1.42416300 1.01289300
O 6.05405600 -1.43430500 -0.59507300
H 5.79976300 -1.69936400 0.30494800

TSF45-6-C4, G= -861851.16 kcal/mol, i50.31 cm -1
C 0.37830200 0.07209800 0.58330500
H 0.29613200 -0.73038300 1.34646300
C 1.61249700 -0.35403900 -0.34613000
H 1.59837000 0.38781200 -1.14735900
C 2.94189800 -0.34169900 0.45337700
H 2.70216500 -0.14816800 1.50636600
C 3.93883800 1.44121300 -1.10509100
H 5.97200300 1.99375000 -1.51574900
H 4.76344400 2.99117500 -2.33875400
O 1.38703400 -1.64175000 -0.84279500
H 0.51210100 -1.70409700 -1.29015800
O 3.58437100 -1.63189800 0.40851200
O 4.90519200 0.99796200 0.96320800
O 0.60922000 1.23328200 1.17611500
O 5.08009800 3.51664200 -0.41457000
H 5.25065100 3.08418700 0.43515500
O -0.72542100 0.02884800 -0.30539700
C -4.86315400 -0.01407800 -0.20541900
H -4.84369500 0.58522400 -1.13463400
C -4.20558300 0.77128400 0.93171400
H -2.74994400 1.06705200 0.58367600
H -2.71979000 1.72875000 -0.29589500
C -2.02516900 -0.23808200 0.22334600
H -1.94390300 -0.86618200 1.12325100
C -2.80912400 -1.00511700 -0.85983000
H -2.79891000 -0.41494500 -1.79006500
C -2.26697800 -2.40162800 -1.17376100
H -2.04509800 -2.94478400 -0.24595100
H -3.05315600 -2.93903000 -1.71318800
O -4.96614700 1.95900900 1.11887800
H -4.49943000 2.51079000 1.76341900
O -2.18537400 1.72521700 1.71030800
H -1.27049500 1.98561000 1.50497300
O -4.14799700 -1.21944000 -0.41588500

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|  | x         | y         | z         |
|---|-----------|-----------|-----------|
| O | -1.084909 | -2.301900 | -1.989700 |
| H | -0.966742 | -3.134555 | -2.464580 |
| O | -6.170200 | -0.397032 | 0.104711  |
| H | 3.040369  | -2.208221 | -0.155319 |
| H | 4.997633  | 0.284340  | 1.636472  |
| O | 5.098774  | -1.202537 | 2.614604  |
| H | 4.681160  | -1.765409 | 1.932802  |
| H | 3.173187  | 1.268364  | -1.851324 |

F45-6-C4, G= -861856.03 kcal/mol, 20.46 cm⁻¹
H  3.73531300  3.29060800  -0.40603300
O  1.58877300  2.16365000  -0.66675700
H  0.63600600  2.00782100  -0.49791700
O  4.18385800  -1.01123700  -0.16656000
O  1.53642000  -4.21736200  0.64295600
H  5.99437600  0.31834900  -0.24235900
H  -3.38827100  -2.74182200  0.50917500
H  -5.07263700  0.15613400  -0.89294900
H  6.22943000  1.25427600  -0.33371300
O  -5.82833000  -1.29588400  -1.33878100
H  -5.39939300  -1.84754100  -0.65107400
H  -2.04670500  0.95028600  1.68209000

TSF54-3-C5, G= -861838.10 kcal/mol, i 354.99cm -1
C  -1.04071600  0.45816700  -0.26693500
H  -1.09327400  0.24034200  0.80528800
C  -1.93625300  1.65437700  -0.64122500
H  -1.84986000  1.77677700  -1.73697700
C  -3.37561500  1.43317100  -0.28065200
H  -3.62339100  1.17833800  0.74710500
C  -3.73843600  -0.64528500  -1.22154700
H  -3.63752400  -0.08638400  -2.14727100
C  -2.65832100  -1.28422400  -0.67344000
H  -1.10186100  -1.30401000  2.60147100
C  -2.71686800  -2.34876900  0.36650800
H  -3.62492100  -2.94574200  0.23836300
H  -1.84614900  -3.00272600  0.27600100
O  -1.48918500  2.83535800  0.02025700
H  -0.50972200  2.87601400  -0.65832200
O  -4.31047400  2.28423000  -0.82558900
O  -5.00626100  -1.03461600  -0.87012700
O  -1.41502700  -0.74491600  -1.00946600
O  -2.66181800  -1.86266400  1.74259400
H  -3.48941300  -1.40247000  1.93807100
O  0.24701800  0.79306800  -0.65832200
C  4.19842600  -0.31224900  -0.08984300
H  4.41356900  0.20224000  -1.04499000
C  3.23650300  -1.47486400  -0.32975200
H  3.03535500  -1.95135500  0.64064400
C  1.92683100  -0.95363700  -0.91163300
H  2.12886300  -0.50741300  -1.89920800
C  1.35473300  0.14199400  -0.00117500
H  1.01715300  -0.29320500  0.94728200
C  2.42563100  1.21992500  0.27135500

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| Element | x     | y     | z     |
|---------|-------|-------|-------|
| H       | 2.66363500 | 1.73639500 | -0.67259100 |
| C       | 2.01425700 | 2.27691100 | 1.29807300 |
| H       | 1.43419400 | 1.82162300 | 2.11073100 |
| H       | 2.93458900 | 2.70375000 | 1.71139600 |
| O       | 3.88448000 | -2.39314500 | -1.20616300 |
| O       | 1.06932000 | -2.07758000 | 1.05625300 |
| C       | 0.16929300 | -1.75778500 | -1.25402600 |
| O       | 3.59888300 | 0.60369600  | 0.80646500 |
| O       | 1.24669200 | 3.29669400  | 0.63615000 |
| H       | 1.24669200 | 4.01933600  | 1.25943600 |
| O       | 3.59888300 | -3.06618200 | -1.45632100 |
| O       | 0.16929300 | -1.75778500 | -1.25402600 |
| C       | 0.16929300 | -1.75778500 | -1.25402600 |
| O       | 1.24669200 | 4.01933600  | 1.25943600 |

F54-3-C4, G= -861859.15 kcal/mol, 20.92 cm⁻¹
TSF51-6-C5, G= -861856.18 kcal/mol, i 345.22 cm^-1

C  -0.74458400  0.54816400  -0.03744100
H  -0.78063000  0.14176000  0.97250200
C  -1.80807800  1.47238700  -0.52866200
H  -1.71484700  1.58343400  -1.61823000
C  -3.21005600  0.97216600  -0.16984000
H  -3.24353700  0.75981000  0.90829300
C  -3.63233100  -0.29570800  -0.94632200
H  -3.66255500  -0.02800300  -2.01459000
C  -2.63663400  -1.41496700  -0.73943100
H  -2.44686400  -1.48042800  2.36318200
C  -3.02942300  -2.67225200  -0.00556900
H  -3.74134700  -3.25986200  -0.60018900
H  -2.13505700  -3.27292700  0.17036300
O  -1.67141300  2.76476700  0.09781400
H  -0.72862500  3.01176000  0.08716200
O  -4.19437800  1.95229900  -0.49891800
O  -4.93136800  -0.71537800  -0.51720600
O  -1.42828200  -1.13761100  -1.02573800
O  -3.61366600  -2.39983100  1.28946700
H  -4.42534500  -1.89271800  1.11452400
O  0.45394800  0.81020500  -0.57707400
C  4.43242200  -0.18408000  -0.30792200
F51-6-C5, G= -861865.34 kcal/mol, 25.24 cm$^{-1}$

|    |        |        |          |
|----|--------|--------|-----------|
| C  | -0.89483000 | 0.73506700 | -0.12931700 |
| H  | -0.93430100 | 0.54493400 | 0.93338200 |
| C  | -1.91320800 | 1.58301800 | -0.78561000 |
| H  | -1.77789700 | 1.56076600 | -1.87449300 |
| C  | -3.28953200 | 1.03797800 | -0.39947100 |
| H  | -3.33468800 | 1.01650600 | 0.69005000 |
| C  | -3.53593300 | -0.38527600 | -0.91793200 |
| H  | -3.72760900 | -0.34095500 | -1.99651300 |
| C  | -2.34973800 | -1.34937800 | -0.72036700 |
| H  | -1.60250500 | -0.23844000 | 2.83531100 |
| C  | -2.20372400 | -2.06956100 | 0.62360000 |
| H  | -2.71032600 | -3.04033600 | 0.51929600 |
| H  | -1.14539700 | -2.26834000 | 0.80196000 |
| O  | -1.88176100 | 2.96350700 | -0.34767400 |
| H  | -1.04662200 | 3.12507800 | 0.11789900 |
| O  | -4.35460100 | 1.83586100 | -0.90248600 |
| O  | -4.66134000 | -0.96339600 | -0.23349900 |
O  -1.67146200  -1.70954700  -1.68078000
O  -2.71380500  -1.36062000   1.75308700
H   -3.66312800  -1.22092700   1.59590300
O    0.29932000   0.63509200  -0.74038400
C    4.24361500  -0.20859000  -0.27540100
H    4.30383000   0.38381900  -1.20747600
C    3.37230600  -1.44614700  -0.49273300
H    3.29161600  -1.97223400   0.46981800
C    1.98962600  -1.01072200  -0.95823800
H    2.08825300  -0.54754000  -1.95144100
C    1.39017200   0.03576400   0.00853900
H    1.00255500  -0.47116000   0.88296900
C    2.39313700   1.14295000   0.39699400
H    2.50351000   1.82651300  -0.45975500
C    2.00070100   1.93045900   1.66378200
H    2.14019700   1.26346800   2.52209800
H    2.70005000   2.76517700   1.77134000
O    4.02053700  -2.26981400  -1.45546300
H    3.41952300  -2.99635900  -1.67576200
O    1.18700100  -2.18186600  -1.03748300
H    0.32380600  -1.99014200  -1.45031000
O    3.65677000   0.57492200   0.74489600
O    0.67434400   2.45600600   1.64183300
H    0.11792300   1.91637500   2.22818500
O    5.52344400  -0.53738200   0.17957100
H   -4.16604600   2.75454800  -0.65562100
H   -5.41115700  -0.36136300  -0.35472700
H    5.80515000  -1.32958700  -0.30278300
O    -0.92204800   0.38026600   3.17089900
H   -0.88942300   0.26272200   4.12793700

TSF51-6-C5-Frag2, G= -861847.53kcal/mol, i 465.05cm -1
C   -0.52017900   2.00774600  -0.95949300
H   -0.49082900   2.91508600  -0.34536100
C   -1.85231700   1.45198300  -1.40050900
H   -1.64609000   0.59877700  -2.05584600
C   -2.74004900   0.97284800  -0.21636200
H   -2.11024700   0.75041800   0.65028600
C   -3.55172600  -0.31177500  -0.58550400
H   -3.98321400  -0.18825800  -1.58749800
C   -2.62349600  -1.52344800  -0.62201800
H   -1.47234400  -0.72320300   2.59277700
C   -2.52005500  -2.44228700   0.59582500
H   -3.24063900  -3.26233000   0.45282100
H   -1.51680500  -2.87386100   0.60718000

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F51-6-C5-Frag2, G = -861871.11 kcal/mol, 17.09 cm⁻¹
| Atoms | X  | Y  | Z  |   |
|-------|----|----|----|---|
| H     | -1.64143200 | -0.64242800 | 2.85859600 |   |
| C     | -2.34032100 | -2.29429500 | 0.72746200 |   |
| H     | -2.99277700 | -3.14332100 | 0.47093800 |   |
| H     | -1.34334900 | -2.68778900 | 0.93723700 |   |
| O     | -2.47696400 | 2.01134800 | -2.53334100 |   |
| H     | -2.16677000 | 2.90037400 | -2.79490200 |   |
| O     | -3.90579100 | 1.97430600 | -0.23914000 |   |
| O     | -4.45761200 | -0.59668500 | 0.05607500 |   |
| O     | -1.37210500 | -1.56025600 | -1.33585400 |   |
| O     | -2.80579200 | -1.63154300 | 1.89826100 |   |
| H     | -3.67363400 | -1.24694100 | 1.67160700 |   |
| O     | -1.04695100 | 3.94560200 | -1.47556700 |   |
| C     | 4.19531600   | -0.29987600 | -0.26558000 |   |
| H     | 4.06099200   | 0.32913300 | -1.16707000 |   |
| C     | 3.45419500   | -1.63217100 | -0.46668000 |   |
| H     | 3.59148200   | -2.24226000 | 0.43712000 |   |
| C     | 1.95185700   | -1.35758400 | -0.66024200 |   |
| H     | 1.85476700   | -0.80136500 | -1.61044100 |   |
| C     | 1.48897800   | -0.51027000 | 0.47835890 |   |
| H     | 0.94299100   | -0.97098400 | 1.29834900 |   |
| C     | 2.28797900   | 0.73407100 | 0.71168300 |   |
| H     | 2.19925600   | 1.41395400 | -0.15493700 |   |
| C     | 1.89637900   | 1.50028700 | 1.97745100 |   |
| H     | 2.08985700   | 0.86914400 | 2.85337100 |   |
| H     | 2.51899700   | 2.39582100 | 2.06016300 |   |
| O     | 4.03963900   | -2.26932900 | -1.59686500 |   |
| H     | 3.52315400   | -3.06586900 | -1.78596400 |   |
| O     | 1.29748200   | -2.61808700 | -0.77370200 |   |
| H     | 0.38918700   | -2.45616600 | -1.08146300 |   |
| O     | 3.68651900   | 0.38144100 | 0.86064600 |   |
| O     | 0.53254900   | 1.90730900 | 1.92468000 |   |
| O     | 0.01240500   | 1.24913800 | 2.39786400 |   |
| O     | 5.55755900   | -0.50125100 | -0.01131500 |   |
| H     | -4.05632300  | 2.32275000 | -1.13711200 |   |
| H     | -4.94515300  | 0.24383900 | 0.13014000 |   |
| H     | 5.86153700   | -1.19263400 | -0.61863600 |   |
| O     | -0.94495900  | -0.07307800 | 3.24843200 |   |
| H     | -1.09202000  | -0.05426300 | 4.20123200 |   |

**TSF1’gly-C1’, G=-861845.90 kcal/mol, i 442.45 cm^-1**

| Atoms | X  | Y  | Z  |   |
|-------|----|----|----|---|
| C     | -1.09591200 | 0.39034300 | 0.24691000 |   |
| H     | -0.61021700 | 0.42297800 | 1.22175900 |   |
| C     | -1.87712500 | 1.57274900 | -0.24429700 |   |
| H     | -1.74815200 | 1.63087700 | -1.33774300 |   |
| C     | -3.36711900 | 1.36233200 | 0.04297800 |   |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -3.530023 | 1.373411  | 1.131302  |
| C    | -3.795507 | 0.012242  | -0.520703 |
| H    | -3.635606 | 0.020614  | -1.609885 |
| C    | -2.958595 | -1.118021 | 0.092068  |
| H    | -3.132089 | -1.160786 | 1.175495  |
| C    | -3.257995 | -2.493249 | -0.512002 |
| H    | -3.229000 | -2.426122 | -1.610530 |
| H    | -2.480064 | -3.193951 | -0.195200 |
| O    | -1.477051 | 2.777075  | 0.377773  |
| H    | -0.521884 | 2.920642  | 0.212414  |
| O    | -4.180186 | 2.353890  | -0.577788 |
| O    | -5.167429 | -0.263404 | -0.237390 |
| O    | -1.546733 | -0.847970 | -0.148194 |
| O    | -4.490741 | -3.016540 | -0.050069 |
| H    | -5.175103 | -2.343723 | -0.194093 |
| O    | 0.454425  | 0.602671  | -0.912040 |
| C    | 4.337497  | 0.340042  | 0.511098  |
| H    | 4.295637  | 0.117250  | -1.594329 |
| C    | 3.413931  | -1.506316 | -0.157010 |
| H    | 3.402358  | -1.577964 | 0.938622  |
| C    | 2.005425  | -1.210434 | -0.660525 |
| H    | 1.949616  | -1.516936 | -1.717910 |
| C    | 1.636105  | 0.305943  | -0.589830 |
| H    | 0.986752  | -1.216277 | 3.440245  |
| C    | 2.664830  | 1.337307  | -0.249010 |
| H    | 2.849095  | 1.936611  | -1.158909 |
| C    | 2.220836  | 2.306184  | 0.859665  |
| H    | 1.751778  | 1.757495  | 1.683620  |
| H    | 3.128851  | 2.795797  | 1.225870  |
| O    | 3.967556  | -2.690795 | -0.730630 |
| H    | 3.443095  | -3.451198 | -0.445269 |
| O    | 1.091394  | -2.026367 | 0.098857  |
| H    | 0.181079  | -1.857909 | -0.209920 |
| O    | 3.895966  | 0.785814  | 0.220878  |
| O    | 1.313644  | 3.281475  | 0.314070  |
| H    | 1.377329  | 4.087427  | 0.841977  |
| O    | 5.654786  | 0.575014  | 0.113504  |
| H    | -3.855713 | 3.221575  | -0.296570 |
| H    | -5.680952 | 0.518882  | -0.488596 |
| H    | 5.827778  | -1.520803 | -0.239975 |
| O    | 0.874534  | -0.729448 | 2.615451  |
| H    | 0.989985  | -1.371925 | 1.888185  |

**F1′gly -C1′, G = -861881.19 kcal/mol, 7.35 cm⁻¹**

C -2.486591569347 -0.288073825560 0.936746682396
TSF1’2’-3’-C1’, G= -861841.16 kcal/mol, i 401.45 cm⁻¹
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -3.71119400 | 3.37957900 | 0.30854300 |
| H    | -5.05668300 | 0.61278400 | 1.42012400 |
| H    | 3.76602800  | -1.41561900 | 2.62380200 |
| O    | 1.24631600  | -4.14601600 | -0.80085300 |
| H    | 1.09295500  | -3.41321800 | -1.43086500 |

F1'2'-3'-C1', G=-861861.56 kcal/mol, 16.57 cm⁻¹
|    | X          | Y          | Z          |
|----|------------|------------|------------|
| 0  | 2.273570   | 0.650867   | 1.058140   |
| 0  | 1.683690   | 3.201841   | -1.447679  |
| H  | 2.389072   | 3.165711   | -2.106317  |
| 0  | 3.255280   | -0.339991  | 2.856410   |
| H  | -3.578308  | 3.364829   | 0.105890   |
| H  | -4.954393  | 0.763287   | 1.553113   |
| H  | 2.608910   | -0.920849  | 3.281985   |
| 0  | 1.655719   | -3.861848  | -1.477701  |
| H  | 1.433560   | -3.180801  | -2.140415  |

TSF1’5’-6’-C1’, G=-861843.13kcal/mol, i255.26cm -1
| C  | -0.684807 | 0.718073  | -0.209121 |
| H  | -0.180822 | 0.711467  | 0.767240  |
| C  | -1.755434 | 1.808807  | -0.276839 |
| H  | -2.116087 | 1.856935  | -1.315704 |
| C  | -2.915582 | 1.444170  | 0.647284  |
| H  | -2.556251 | 1.473276  | 1.687546  |
| C  | -3.427518 | 0.041724  | 0.342876  |
| H  | -3.816048 | 0.019057  | -0.686612 |
| C  | -2.276329 | -0.968726 | 0.449381  |
| H  | -1.868254 | -0.961537 | 1.470662  |
| C  | -2.684248 | -2.403965 | 0.096043  |
| H  | -3.206076 | -2.405661 | -0.873963 |
| H  | -1.784450 | -3.018494 | 0.000610  |
| O  | -1.254277 | 3.058216  | 0.152108  |
| H  | -0.396301 | 3.226434  | -0.285699 |
| O  | -4.157360 | 2.337134  | 0.494866  |
| O  | -4.453440 | -0.343195 | 1.256177  |
| O  | -1.253791 | -0.563034 | -0.488006 |
| O  | -3.471886 | -2.993567 | 1.115635  |
| H  | -4.207779 | -2.393110 | 1.313633  |
| O  | 0.256291  | 1.003459  | -1.231861 |
| C  | 3.057047  | -0.218900 | 1.179129  |
| H  | 4.067527  | -0.299391 | 0.728130  |
| C  | 2.126452  | -1.241661 | 0.481710  |
| H  | 1.159205  | -1.213103 | 1.005200  |
| C  | 1.905701  | -0.866906 | -1.014857 |
| H  | 2.857191  | -1.038591 | -1.529369 |
| C  | 1.559527  | 0.607750  | -1.119777 |
| C  | 1.132581  | -5.068466 | -0.955641 |
| C  | 2.568546  | 1.523380  | -0.943270 |
| H  | 3.576030  | 1.133380  | -1.064573 |
| C  | 2.569739  | 3.020930  | -0.949897 |
| H  | 3.138619  | 3.336347  | -0.065762 |
| H  | 3.124259  | 3.342681  | -1.845191 |

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|   |   |   |   |   |
|---|---|---|---|---|
| H | 3.716860957338 | 1.257336035941 | -1.428253051416 |
| C | 2.602139301451 | 3.096250297128 | -1.602100532263 |
| H | 3.188200916392 | 3.578972065409 | -0.803694392619 |
| H | 3.094706685900 | 3.340524039949 | -2.556119782408 |
| O | 2.862037420156 | -2.552644141491 | 0.480741486444 |
| H | 2.316284383170 | -3.306866609620 | 0.161937089449 |
| O | 1.263767492671 | -1.610997382487 | -1.813955549061 |
| H | 0.338340631739 | -1.357975876116 | -1.631378187719 |
| O | 1.938376167563 | 0.565177646773 | 1.840231141073 |
| O | 1.26932476574 | 3.619078316141 | -1.609147405177 |
| H | 1.323494547699 | 4.565723303716 | -1.793696584937 |
| O | 3.205600333517 | -1.156299960670 | 2.644254792142 |
| H | -3.505779392654 | 3.280190704133 | 0.561861421937 |
| H | -4.863522203355 | 0.432290910208 | 1.369410226487 |
| H | 3.439802188931 | -2.040841092661 | 2.312715878807 |
| O | 1.220806467714 | -4.224090871343 | -0.918715756350 |
| H | 1.224618765250 | -3.467127963451 | -1.540334191211 |

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S5 Additional calculations

S5.1 Reaction profiles comparison

We provide below the comparison between the reaction profiles computed at the B3LYP/6-31++G(d,p) and wB97x-D/6-311++G(2d,p) levels, for the reactions initiated at carbon atoms C1 and C5.

Table S3: Relative free energies (298 K, 1 atm) for the reaction initiated at carbon atom C1, computed at the B3LYP/6-31++G(d,p) and wB97x-D/6-311++G(2d,p) levels; with respect to the pre-reacting complexes. Values in kcal/mol. For the fragmentation reaction, cleaved bond is indicated within brackets.

| Species         | B3LYP/6-31++G(d,p) | wB97x-D/6-311++G(2d,p) |
|-----------------|-------------------|------------------------|
| R               | 0.0               | 0.0                    |
| TS-Abs-C1       | 3.40              | 2.03                   |
| P1              | -19.05            | -21.09                 |
| TS F1(gly)      | -7.35             | -4.53                  |
| F1(gly)         | -34.15            | -31.43                 |
| TS F1(C2-C3)    | 9.75              | 11.41                  |
| F1(C2-C3)       | -7.15             | 3.40                   |
| TS F1(C5-O6)    | -5.35             | -3.34                  |
| F1(C5-O6)       | -26.65            | -25.93                 |

Table S4: Relative free energies (298 K, 1 atm) for the reaction initiated at carbon atom C5, computed at the B3LYP/6-31++G(d,p) and wB97x-D/6-311++G(2d,p) levels; with respect to the pre-reacting complexes. Values in kcal/mol. For the fragmentation reaction, cleaved bond is indicated within brackets.

| Species         | B3LYP/6-31++G(d,p) | wB97x-D/6-311++G(2d,p) |
|-----------------|-------------------|------------------------|
| R               | 0.0               | 0.0                    |
| TS-Abs-C5       | 3.40              | 3.41                   |
| P5              | -21.30            | -21.42                 |
| TS F5(C1-O6)    | -7.90             | -4.20                  |
| F5(C1-O6)       | -17.30            | -18.72                 |
| TS F5(C4-C3)    | 9.90              | 12.08                  |
| F5(C4-C3)       | -11.10            | 0.26                   |
S5.2  wB97xD/6-311++G(2d,p) geometries

R-C1, G = -861817.1395 kcal/mol, 22.34 cm-1

|   |   |   |
|---|---|---|
| C | 0.86734300 | -0.26739300 | -0.10149500 |
| H | 0.75850300 | -0.32066000 | 0.99647900  |
| C | 1.80954300 | -1.36571200 | -0.58121100 |
| H | 1.84251300 | -1.33250600 | -1.67649400 |
| C | 3.19911700 | -1.12435100 | -0.02272200 |
| H | 3.16142200 | -1.23748500 | 1.07054600  |
| C | 3.64785300 | 0.29003600  | -0.34295800 |
| H | 3.72169100 | 0.39690700  | -1.43419100 |
| C | 2.61812200 | 1.29803600  | 0.16587900  |
| H | 2.52857800 | 1.21083000  | 1.25738400  |
| C | 2.97039500 | 2.73992300  | -0.17902200 |
| H | 3.18430200 | 2.81268200  | -1.25441500 |
| O | 1.37468200 | -2.63215100 | -0.13189000 |
| H | 0.47908800 | -2.81569700 | -0.47738000 |
| O | 4.15941000 | -2.00324600 | -0.56897000 |
| O | 4.89359100 | 0.57646400  | 0.25870300  |
| O | 1.36753400 | 1.00858600  | -0.45152000 |
| O | 4.02939700 | 3.23311300  | 0.59975300  |
| H | 4.75705100 | 2.60395000  | 0.54355500  |
| O | 0.34556800 | -0.45705600 | -0.72221900 |
| C | -4.31139800 | 0.41317100  | -0.17159300 |
| H | -4.40617700 | 0.36732500  | -1.27145000 |
| C | -3.35981900 | 1.53913400  | 0.21051900  |
| H | -3.26489400 | 1.53886200  | 1.30453900  |
| C | -1.99662500 | 1.28563500  | -0.40426700 |
| H | -2.09189900 | 1.31871200  | -1.49952300 |
| C | -1.51916300 | -0.10546000 | -0.00720300 |
| H | -1.31791500 | -0.12408900 | 1.07080400  |
| C | -2.58301900 | -1.16040100 | -0.32285900 |
| H | -2.71259100 | -1.20837400 | -1.41752200 |
| C | -2.22941300 | -2.55506800 | 0.19324700  |
| H | -1.77098400 | -2.48873300 | 1.18075000  |
| H | -3.15772100 | -3.12568100 | 0.27988800  |
| O | -3.93352900 | 2.74616800  | -0.23923800 |
| H | -3.29810100 | 3.45054100  | -0.08364800 |
| O | -1.13873900 | 2.30848000  | 0.04336200  |
| H | -0.24075000 | 2.12225100  | -0.26631400 |
| O | -3.80074300 | -0.80946800 | 0.29355600  |
| O | -1.29267900 | -3.24491000 | -0.62616700 |
TS-Abs-C1, G = -861816.3011 kcal/mol, i300.88 cm⁻¹
|  | x       | y       | z       |
|---|---------|---------|---------|
| H | -3.24052100 | -3.38546800 | 0.57664800 |
| O | -1.09332600 | -2.28656500 | 0.24070400 |
| H | -0.18197000 | -2.03171600 | 0.43756400 |
| O | -3.76253100 | 0.73272500 | -0.56383100 |
| O | -1.27874300 | 3.31349000 | -0.12035200 |
| H | -1.68818100 | 3.64532400 | 0.68118400 |
| O | -5.51144200 | -0.64167900 | -0.42935700 |
| H | 3.95231400 | 3.01213700 | -0.08438800 |
| H | 5.54885200 | 0.23286600 | -0.12358200 |
| H | -5.71311900 | -1.56845800 | -0.26540000 |
| O | 0.64763600 | 0.93549000 | -2.64150400 |
| H | 0.92891200 | 1.82832300 | -2.37155700 |

P-C1, $G = -861839.4271$ kcal/mol, 17.37 cm$^{-1}$

|  | x       | y       | z       |
|---|---------|---------|---------|
| C | 0.89268900 | -0.24717000 | -0.36424700 |
| H | 0.30732700 | -2.43845200 | 3.13397600 |
| C | 1.82708100 | -1.39734200 | -0.61824500 |
| H | 1.98954200 | -1.50219500 | -1.70421100 |
| C | 3.16840000 | -1.14007800 | 0.04465700 |
| H | 3.03405500 | -1.20895600 | 1.13267600 |
| C | 3.65419200 | 0.25547000 | -0.29282900 |
| H | 3.78190800 | 0.33472600 | -1.38214200 |
| C | 2.61718700 | 1.28487300 | 0.14648400 |
| H | 2.44853400 | 1.20409800 | 1.22566500 |
| C | 3.01141700 | 2.71754500 | -0.19235700 |
| H | 3.30588600 | 2.77318100 | -1.24971000 |
| H | 2.13797200 | 3.35827600 | -0.05573200 |
| O | 1.32005800 | -2.60674200 | -0.09428500 |
| H | 0.45631200 | -2.81014200 | -0.50477500 |
| O | 4.16091400 | -2.04744000 | -0.38508200 |
| O | 4.87210800 | 0.54562200 | 0.36024800 |
| O | 1.93249000 | 1.01796200 | -0.54620500 |
| O | 4.01511200 | 3.20716800 | 0.65767900 |
| H | 4.74193500 | 2.57464900 | 0.65231200 |
| O | -0.32797800 | -0.40313600 | -0.91077800 |
| C | -4.26407600 | 0.45425200 | -0.14711600 |
| H | -4.37834300 | 0.49264800 | -1.24545000 |
| C | -3.29297600 | 1.53506500 | 0.30231600 |
| H | -3.16979000 | 1.44192300 | 1.38925000 |
| C | -1.95066000 | 1.31928000 | -0.36919900 |
| H | -2.08023000 | 1.43145200 | -1.45601400 |
| C | -1.46578800 | -0.09836900 | -0.90948000 |
| H | -1.18732100 | -0.20525600 | 0.96176600 |
| C | -2.55221600 | -1.12166600 | -0.44225800 |

86
TSF1gly-C1, G = -861822.8592 kcal/mol, i724.30 cm⁻¹

C       0.96451700  -0.27779300  -0.90261800
H       0.66768500  -1.03558200   3.24359700
C      1.80375700  -1.51000100  -0.63184000
H      2.00530300  -1.97626600  -1.60560600
C      3.15273900  -1.22265400   0.01636300
H      3.02480400  -1.24777800   1.10401600
C      3.63884500   0.15960700  -0.35557300
H      3.73842000   0.24215600  -1.44824200
C      2.60685200   1.17154700   0.12265700
H      2.39965000   1.01693700   1.18645000
C      3.02394000   2.61995900  -0.10801600
H      3.37487200   2.73862800  -1.14254500
H      2.14545600   3.25516000   0.02022000
O      1.12842900  -2.44642000   0.19510900
H      0.30613300  -2.73768500  -0.25094200
O      4.14752900  -2.14748600  -0.38093200
O      4.87237700   0.44686400   0.26493700
O      1.39283700   0.97971000  -0.61525200
O      3.98146400   3.05173100   0.82260700
H      4.71917700   2.43340900   0.79244500
O     -0.22058900  -0.37873900  -1.31366000
C     -4.33056900   0.40637100  -0.14806000
H     -4.42871900   0.56694100  -1.23348200
C     -3.34498500   1.41920400   0.42642300
H     -3.24454700   1.22716800   1.50239800
|    |     |     |     |     |
|----|-----|-----|-----|-----|
| C  | -1.98955100 | 1.23133100 | -0.24067100 |
| H  | -2.11236200 | 1.43886600  | -1.31530000 |
| C  | -1.57560100 | -0.19831400 | -0.08075600 |
| H  | -1.08491500 | -0.43473800 | 0.86121400  |
| C  | -2.62611300 | -1.16140600 | -0.56175700 |
| H  | -2.75192200 | -1.02282600 | -1.65036800 |
| C  | -2.34851900 | -2.63100500 | -0.28171600 |
| H  | -2.14005800 | -2.77470100 | 0.77949900  |
| H  | -3.24499800 | -3.20264100 | -0.53512400 |
| O  | -3.88385500 | 2.70197800  | 0.19541300  |
| H  | -3.21594600 | 3.34849200  | 0.44100000  |
| O  | -1.10838500 | 2.16134300  | 0.33981200  |
| H  | -0.22268300 | 1.99604200  | -0.00784800 |
| O  | -3.86296600 | -0.89647500 | 0.08640800  |
| O  | -1.22484700 | -3.13751400 | -0.99231700 |
| H  | -1.21791300 | -2.75491700 | -1.87401600 |
| O  | -5.57084500 | 0.48248000  | 0.46996600  |
| H  | 3.95209800  | -3.00026100 | 0.01352900  |
| H  | 5.44092900  | -0.32051100 | 0.14736300  |
| H  | -5.74909500 | 1.41320100  | 0.63821600  |
| O  | 0.72908900  | -0.73725800 | 2.33522100  |
| H  | 0.81408400  | -1.53260900 | 1.78374800  |

FIGL-\text{C1}, G = -861849.7665 \text{kcal/mol}, 12.51\text{cm}^{-1}

|    |     |     |     |     |
|----|-----|-----|-----|-----|
| C  | 1.54160100 | -0.07190000 | -1.23757900 |
| H  | 0.59011800  | 0.19739200  | 3.22366600  |
| C  | 1.92411900 | -1.17940400 | -0.24115400 |
| H  | 2.24399200 | -2.01787100 | -0.87734500 |
| C  | 3.08778900 | -0.82596500 | 0.66435900  |
| H  | 2.73901900 | -0.14153700 | 1.44844700  |
| C  | 4.15449900 | -0.12637700 | -0.14629300 |
| H  | 4.46427200 | -0.77783600 | -0.97746900 |
| C  | 3.57157500 | 1.15806500  | -0.71368200 |
| H  | 3.24421200 | 1.80702200  | 0.10403400  |
| C  | 4.54725500 | 1.93365000  | -1.59323600 |
| H  | 4.99840400 | 1.24937100  | -2.32526200 |
| H  | 3.98450800 | 2.68814600  | -2.14390500 |
| O  | 0.84517500 | -1.56501700 | 0.56800800  |
| H  | 0.12428000 | -1.94124100 | 0.01408100  |
| O  | 3.67113500 | -1.97681000 | 1.23498800  |
| O  | 5.26954400 | 0.21420800  | 0.64415100  |
| O  | 2.42988600 | 0.86927700  | -1.54269500 |
| O  | 5.51586700 | 2.60895900  | -0.83638100 |
| H  | 5.95118600 | 1.96923700  | -0.26337300 |

88
O  0.49176600  -0.10087100  -1.82488900
C  -4.70279900   0.40468000  -0.47035700
H  -4.28223200   1.14089700  -1.17948900
C  -4.30291600   0.79967100   0.95163000
H  -4.71738300  -0.05362400   1.64170400
C  -2.77771100   0.78782300   1.08130300
H  -2.39466000  1.57579400   0.40934000
C  -2.30347300  -0.53622400   0.60338600
H  -2.05686000  -1.30439700  -1.32950500
C  -2.78307200  -0.90974600  -0.75620800
H  -2.40020800    0.18420000  -1.49443200
C  -2.37294200  -2.30572600  -1.19184200
H  -2.70967000  -3.04172500  -0.46082900
H  -2.83757100  -2.53734700  -2.15365000
O  -4.85626300   2.07339000   1.19732500
H  -4.52055600   2.37945900   2.04445000
O  -2.46181400   1.08895600   2.41742100
H  -1.49574600   1.04702800   2.50338800
O  -4.21172800  -0.86980600  -0.78601100
O  -0.95921500  -2.42077000  -1.27837100
H  -0.62199800  -1.67901300  -1.80442600
O  -6.08168400   0.32894500  -0.61190300
H  3.00459100   0.22410800  -0.48626800
H  5.52083800   1.06102900  -0.11351400
O  0.32296400   0.53819100   2.36759300
H  0.35802800  -0.22281600   1.76025900

TSF12-3-C1, G = -861806.9262 kcal/mol, i540.34 cm⁻¹

C  0.89358800  -0.46289500  -1.38996300
H  2.38425900  -4.95868400   1.16208800
C  1.68190900  -1.55958900  -1.20742600
H  2.70522500  -1.55194900  -1.55834700
C  2.59834600  -0.97454000   0.74040900
H  1.73660400  -1.00246400   1.41083800
C  3.10015300   0.36332200   0.32114600
H  3.83413000   0.22410800  -0.48626800
C  2.00155700   1.28959300  -0.19228800
H  1.20792600   1.38427300   0.55586900
C  2.51628000   2.69170800  -0.51446200
H  3.43500900   2.61164200  -1.11151600
H  1.76765300   3.20290200  -1.12119000
O  1.17155500  -2.81890100  -1.09093600
H  0.20070100  -2.79941000  -0.96173800
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 2.09927300 | 2.52926100 | 0.03985300 |
| H       | 2.92194900 | 2.81715000 | -0.62716600|
| H       | 1.16541500 | 2.88381200 | -0.39414000|
| O       | 0.91033400 | -3.04481300| -1.22060100|
| H       | -0.03179700| -2.97243600| -0.96766400|
| O       | 4.10517100 | -1.95797400| 0.68409700 |
| O       | 4.16984700 | 1.25746000 | 1.22731700 |
| O       | 1.49668200 | 0.54935800 | -1.12490600|
| O       | 2.21259600 | 3.13454900 | 1.30240000 |
| H       | 3.03581900 | 2.80754700 | 1.68260000 |
| O       | -0.49204000| -0.61045200| -1.35343200|
| O       | -0.88941100| 0.97237200 | 0.36477000 |
| H       | -4.46517500| 0.59626200 | -0.49986200|
| C       | -2.86191900| 1.98795100 | -0.11924800|
| H       | -2.30129500| 2.34220200 | 0.75609000 |
| C       | -1.89828200| 1.32129800 | -1.08446800|
| H       | -2.45750300| 0.97909900 | -1.96791000|
| C       | -1.29033600| 0.09854300 | -0.41172800|
| H       | -0.69067400| 0.41247500 | 0.44721800 |
| C       | -2.41136300| -0.81948300| 0.08307000 |
| H       | -2.99893400| -1.14687600| -0.79130200|
| C       | -1.91996500| -2.06333700| 0.81885900 |
| H       | -1.01876900| -1.84777800| 1.39505200 |
| H       | -2.70165500| -2.37751600| 1.51478800 |
| O       | -3.57639800| 3.04687000 | -0.71512000|
| H       | -2.94128600| 3.67433600 | -1.07086800|
| O       | -0.94423900| 2.28225500 | -1.46380500|
| H       | -0.18258200| 1.83096400 | -1.84668600|
| O       | -3.23518200| -0.10929500| 0.97959600 |
| O       | -1.57296000| -3.12436400| -0.06052600|
| H       | -2.35664300| -3.41759400| -0.53059600|
| O       | -4.73795400| 1.50134100 | 1.32191000 |
| H       | 3.69148700 | -2.82333600| 0.87621100 |
| H       | 4.68508500 | 0.72675000 | 1.83891500 |
| H       | -4.92140400| 2.41252500 | 1.07173200 |
| O       | 2.44124800 | -4.10739900| 0.88641000 |
| H       | 1.84872500 | -3.91417800| 0.13713200 |

TS-F1(5-6), \( G = -861821.6713 \) kcal/mol, \( i777.05 \) cm\(^{-1}\)
H   1.92636100  -1.40080100   0.96236700
C   3.15780700   0.22851500   0.28062400
H   3.77589800   0.45510000  -0.60020400
C   2.08850200   1.26800200   0.39361500
H   1.31703800   1.05748500   1.13181700
C   2.50502900   2.70243100   0.32364000
H   3.20950200   2.84051800  -0.50644200
H   1.63748400   3.33933700   0.14185400
O   1.17819000  -2.63447300  -1.24673000
H   0.34549700  -2.57879200  -0.74565600
O   3.72857200  -2.02851900   0.16609400
O   3.95958400   0.30393000  -1.45122000
O   1.17819000   0.94818400   1.45122000
H   0.34549700  -2.57879200  -0.74565600
O   3.72857200  -2.02851900   0.16609400
O   3.95958400   0.30393000 -1.1.45122000
O   1.17819000   0.94818400  1.45122000

P-F1(5-6), G = -861844.2658 kcal/mol, 28.38cm-1
|     | X         | Y         | Z         |        |        |
|-----|-----------|-----------|-----------|--------|--------|
| O   | 2.98124700| -4.50432300| 0.21980400| 0.21980400|
| H   | 2.16745700| -4.10922200| -0.13658500| -0.13658500|

R-C5, G = -861815.5914 kcal/mol, 27.55 cm⁻¹

|     | X         | Y         | Z         |        |        |
|-----|-----------|-----------|-----------|--------|--------|
| C   | 0.64824900| -0.65568000| 0.01322700| 0.01322700|
| H   | 0.61757600| -0.44512400| 1.09389900| 1.09389900|
| C   | 1.39698600| -1.95658600| -0.24733800| -0.24733800|
| H   | 1.34079600| -2.15993100| -1.32506600| -1.32506600|
| C   | 2.85025500| -1.80087200| 0.15763100| 0.15763100|
| H   | 2.89798300| -1.65179100| 1.24606800| 1.24606800|
| C   | 3.44610100| -0.58430700| -0.52210000| -0.52210000|
| H   | 3.42272500| -0.74030900| -1.60923000| -1.60923000|
| C   | 2.60891800| 0.65126300| -0.19592900| -0.19592900|
| H   | 2.61327200| 0.82406400| 0.88936800| 0.88936800|
| C   | 3.11871200| 1.91105800| -0.88275300| -0.88275300|
| H   | 3.24136400| 1.72828500| 1.95650400| 1.95650400|
| H   | 2.38238400| 2.70580700| -0.75381900| -0.75381900|
| O   | 0.84911300| -3.00756000| 0.50223500| 0.50223500|
| H   | -0.09936600| -3.08128600| 0.29732900| 0.29732900|
| O   | 3.63317200| -2.91639600| -0.20992700| -0.20992700|
| O   | 4.77503300| -0.35121600| -0.09431600| -0.09431600|
| O   | 1.28168200| 0.42986700| -0.65167900| -0.65167900|
| O   | 4.32684300| 2.37231200| -0.30808000| -0.30808000|
| H   | 4.94483700| 1.62953400| -0.29088500| -0.29088500|
| O   | -0.62003800| -0.80738700| -0.49729200| -0.49729200|
| C   | -4.37604200| 0.78598600| -0.15078500| -0.15078500|
| H   | -4.51599700| 0.50022200| -1.20828300| -1.20828300|
| C   | -3.25138400| 1.80543000| -0.04197400| -0.04197400|
| H   | -3.11735800| 2.04059000| 1.02231600| 1.02231600|
| C   | -1.96725300| 1.20567900| -0.58164500| -0.58164500|
| H   | -2.09793700| 0.99813300| -1.65354900| -1.65354900|
| C   | -1.68749500| 0.11554700| 0.12686000| 0.12686000|
| H   | -1.44013800| 0.08907900| 1.17644400| 1.17644400|
| C   | -2.91373000| -1.03280400| 0.07511100| 0.07511100|
| H   | -3.08630300| -1.33211800| -0.96887000| -0.96887000|
| C   | -2.77523100| -2.29491100| 0.91709400| 0.91709400|
| H   | -2.33098200| -2.05413600| 1.88942500| 1.88942500|
| H   | -3.78452000| -2.67854100| 1.08260000| 1.08260000|
| O   | -3.64752800| 2.95250300| -0.75950200| -0.75950200|
| H   | -2.90362200| 3.56116000| -0.77586700| -0.77586700|
| O   | -0.95103700| 2.16057800| -0.38724700| -0.38724700|
| H   | -0.10487400| 1.77259700| -0.65318800| -0.65318800|
| O   | -4.03901100| -0.35557200| 0.59290600| 0.59290600|
| O   | -1.98115400| -3.26037600| 0.23355300| 0.23355300|
|          |          |          |          |
|----------|----------|----------|----------|
| H        | -2.21210500 | -4.13007100 | 0.56411500 |
| O        | -5.56267700 | 1.25832300  | 0.38663100 |
| H        | 3.22756600  | -3.70095600 | 0.16925400 |
| H        | 5.25648800  | -1.18128600 | -0.16087400 |
| H        | -5.62438400 | 2.19337100  | 0.16690300 |
| O        | 3.52994000  | 2.96472700  | 2.33104300 |
| H        | 3.91717300  | 2.88165400  | 1.42938500 |

**TS-Abs-C5, \( G = -861814.9263 \text{kcal/mol}, \text{i363.79cm}^{-1} \)**

|          |          |          |          |
|----------|----------|----------|----------|
| C        | 0.89228200 | 0.42984200 | -0.06610000 |
| H        | 0.78049400 | 0.42797800 | -1.15995700 |
| C        | 1.81702400 | 1.55908500 | 0.36948800 |
| H        | 1.85777800 | 1.55622600 | 1.46718400 |
| C        | 3.21040400 | 1.31973100 | -0.18556000 |
| H        | 3.16703600 | 1.37435500 | -1.28200100 |
| C        | 3.68734000 | -0.06456400 | 0.20811000 |
| H        | 3.75092400 | -0.12003200 | 1.30495400 |
| C        | 2.66940700 | -1.10410900 | -0.24859100 |
| H        | 2.56928900 | -1.01104000 | -1.40649400 |
| C        | 3.06598900 | -2.54744600 | 0.01361800 |
| H        | 3.38558800 | -2.66211800 | 1.05780500 |
| H        | 2.19380500 | -3.18235200 | -0.14834800 |
| O        | 1.36447000 | 2.79074300  | -0.12396000 |
| H        | 0.44163200 | 2.92844600  | 0.15220000 |
| O        | 4.15225100 | 2.24599200  | 0.31249000 |
| O        | 4.94103700 | -0.37204900 | -0.36167800 |
| O        | 1.42369100 | -0.83766100 | 0.33037100 |
| O        | 4.06393500 | -2.98032800 | -0.88236000 |
| H        | 4.81118300 | -2.37624200 | -0.79540600 |
| O        | -0.31638900 | 0.61002700  | 0.56061100 |
| C        | -4.27115600 | -0.40549500 | 0.12860900 |
| H        | -4.37870900 | -0.23525000 | 1.21440100 |
| C        | -3.29181600 | -1.54493700 | -0.11471400 |
| H        | -3.19413800 | -1.67474100 | -1.20076000 |
| C        | -1.00390000 | -1.18973300 | 0.46115600 |
| H        | -2.02576200 | -1.09106100 | 1.55266600 |
| C        | -1.48635900 | 0.15434600  | -0.10005800 |
| H        | -1.29189100 | 0.04533500  | -1.17417600 |
| C        | -2.57446100 | 1.21248900  | 0.10517700 |
| H        | -2.70164000 | 1.38703400  | 1.18337700 |
| C        | -2.26624300 | 2.54938900  | -0.55683600 |
| H        | -1.80819800 | 2.39232500  | -1.53987900 |
| H        | -3.22060700 | 3.06217900  | -0.69573400 |
| O        | -3.83733300 | -2.70336500 | 0.47620400 |
H  -3.18648500  -3.40672800  0.40073900
O  -1.06079200  -2.24481500  0.13502800
H  -0.15613700  -1.98670500  0.35913500
O  -3.78251900  0.76510600  -0.47281000
O  -1.40220000  3.31759900  0.27604000
H  -1.50996300  4.24353300  0.05190200
O  -5.50675900  -0.64581200  -0.45082200
H  3.84153300  3.12916700  0.09557600
H  5.51961600  0.38417900  -0.22599500
H  -5.69750300  -1.58276700  -0.34088200
O  2.54818900  -1.22951400  -2.84042300
H  3.13585400  -2.00301400  -2.78504000

P-C5, G = -861839.7534 kcal/mol, 31.28 cm⁻¹

C  -0.94010800  0.45576000  -0.21395200
H  -0.92293200  0.27396600  0.86646400
C  -1.87222500  1.59852500  -0.57090100
H  -1.87159100  1.72556600  -1.66241300
C  -3.26579600  1.24486600  -0.08974600
H  -3.22472300  1.10484900  1.00024100
C  -3.73171200  -0.06193700  -0.71846000
H  -3.95125200  0.15054500  -1.77894700
C  -2.68236400  -1.20499000  -0.61661600
H  -1.37487500  -2.06634800  2.01643800
C  -2.96156800  -2.51265400  -0.21097300
H  -3.88015000  -2.87632600  -0.67802700
H  -2.13683200  -3.16157200  -0.50901200
O  -1.48370100  2.77764800  0.08179500
H  -0.54969900  2.96259400  -0.11857000
O  -4.21704100  2.23228900  -0.41747800
O  -4.89860000  -0.55038600  -0.08240400
O  -1.38683200  -2.65496300  1.21832300
H  -3.83534100  -2.13408000  1.48668600
O  0.31336800  0.74306100  -0.69671000
C  4.22241400  -0.25847400  0.02859700
H  4.40453100  -0.05196900  -1.04125500
C  3.24038300  -1.41613600  0.15868300
H  3.05814000  -1.58065300  1.22913700
C  1.93800900  -1.04327300  -0.52041400
H  2.12265000  -0.90876400  -1.59466500
C  1.42499900  0.27388700  0.05090900
H  1.13462100  0.12236400  1.09673600
C  2.51302100  1.34945900  -0.01540200
TS F5(1-6), G=-861822.5379 kcal/mol, i512.3143 cm⁻¹
H 2.1439158015 -0.7328897856 -1.757016805
C 1.5964947944 0.2962162599 0.0371324058
H 1.3635314199 0.0481238007 1.0786416428
C 2.6700083068 1.3852664877 0.0001657636
H 2.7898777076 1.7285187825 -1.0376312579
C 2.3466800948 2.5867399414 0.8794719596
H 2.059155269 2.2420726746 1.879500832
H 3.2657572817 3.1719928415 0.9679462873
O 3.9603015377 -2.4517828617 -0.8790232045
H 3.2959084846 -3.1454566877 -0.9250982717
O 1.177291916 -2.0518600454 -0.4915092869
H 0.2887336802 -1.834943661 -0.819820187
O 3.8848556378 0.8712174403 0.5012896746
O 1.3082013228 3.3671240566 0.2980660464
H 1.3479376646 4.250139498 0.6808482057
O 5.6177133678 -0.5111415751 0.2808682608
H -3.8633501845 2.7631850147 0.0109314123
H -5.4592075661 0.0652464804 -0.4569305666
H 5.8146507414 -1.4236028578 0.0463634001
O -1.7206197984 -0.8465123202 2.6663084849
H -1.4044860491 -1.2815028563 3.4588194716

F5(1-6), G=-861837.0514 kcal/mol, 35.5377 cm⁻¹
C -0.9168576128 0.7334096824 -0.152426752
H -0.9619739421 0.5243944164 0.9048864533
C -1.9298929396 1.6080522506 -0.7688962492
H -1.8178042931 1.6012426405 -1.858944574
C -3.2840216751 1.043704875 -0.3688352621
H -3.3018181674 0.995246622 0.7286171896
C -3.4931341338 -0.3645967849 -0.9149720608
H -3.7050331369 -0.2975112233 -1.9861629518
C -2.2634877019 -1.2740251136 -0.7765379287
H -1.4543352958 -0.2770811704 2.7604775781
C -2.0450942369 -2.0082100685 0.5426514964
H -2.492206562 -3.0026267178 0.4219985905
H -0.9734759777 -2.1450012216 0.687287884
O -1.8723538559 2.9568531143 -0.3014483154
H -1.0272432143 3.0905862823 0.1458559541
O -4.3647972542 1.8224598102 -0.8282492742
O -4.5653594096 -1.0070723486 -0.2325674533
O -1.6198559427 -1.5951214978 -1.7593594725
O -2.5671455876 -1.3618113727 1.6875984495
H -3.515604933 -1.2497816969 1.5438785367
O 0.2732968976 0.6613226355 -0.7466275424
C 4.1611338651 -0.2459191928 -0.2232072312
TS F5(4-3), G=-861806.2510 kcal/mol, -455.9585 cm⁻¹

H 4.2368958181 0.3177680187 -1.1699032909
C 3.2747049791 -1.4671994921 -0.4175512483
H 3.1626854402 -1.9545359332 0.5602485308
C 1.9196492676 -1.0162035848 -0.9184036844
H 2.0538464278 -0.575950084 -1.9156834543
C 1.3347975332 0.0562492407 -0.007050555
H 0.9370227897 -0.4226379185 0.894018205
C 2.3504382886 1.1418213783 0.3809747059
H 2.4829857953 1.7997466334 -0.4899566759
C 1.9438635934 1.9583520542 1.6138453414
H 2.0701256089 1.3087118885 2.484813985
H 2.6428381558 2.7907869091 1.7147051951
O 3.9133503012 -2.328378269 -1.3329495105
C 3.2938715609 -1.9559522667
O 1.0956531536 -2.156452434 -0.990007932
H 0.2583566621 -1.4372468719
O 3.5853519703 0.5699185733 0.7599527263
O 0.6293511638 2.4786409587 1.5697217446
H 0.0742995305 1.9239434832 2.1315950438
O 5.4216765292 -0.5834957322 0.244935194
H -4.198328152 2.7320126011 -0.5605614033
H -5.3368969894 -0.4374331303 -0.3102551033
H 5.675530342 -1.4069202876 -0.1843762025
O -0.766378413 0.333911055 3.0782002114
H -0.6703311526 0.171357526 4.0177939659

TS F5(4-3), G=-861806.2510 kcal/mol, -455.9585 cm⁻¹

C -1.0128815216 0.4587881335 -0.353855453
H -1.0633505266 0.2628577799 0.7220766773
C -1.9107902244 1.6393038813 -0.72919331
H -1.8673247438 1.7266241332 -1.8288923612
C -3.326876026 1.4049840902 -0.308531718
H -3.5122878208 1.9253313363 0.7406923061
C -3.7077269145 -0.6656042824 -1.1402389606
H -3.6695836423 -0.1488050576 -2.093642981
C -2.5963956343 -1.2680742382 -0.6422191839
H -1.0962769866 -0.9833778215 2.6169455066
C -2.5872958074 -2.2316752673 0.4884340184
H -3.4236045733 -2.9283245024 0.3953841011
H -1.6551167518 -2.7969879747 0.4714375506
O -1.4553220259 2.8263186766 -0.1204499438
H -0.482351926 2.8262934507 -0.0895349815
O -4.29234565 2.21481524 -0.8369350235
O -4.9352199192 -1.042079924 -0.6873805386
O -1.3928852269 -0.7325197706 -1.067265385
| Atom | X   | Y   | Z    |
|------|-----|-----|------|
| O    | -2.632 | 1.616 | 1.794 |
| H    | -3.482 | -0.179 | 1.887 |
| O    | 0.266 | 0.779 | -0.742 |
| C    | 4.145 | -0.348 | -0.026 |
| H    | 4.402 | 0.242 | -0.924 |
| C    | 3.215 | -1.488 | -0.411 |
| H    | 2.956 | -2.036 | 0.507 |
| C    | 1.947 | -0.932 | -1.030 |
| H    | 2.207 | -0.420 | -1.969 |
| C    | 1.329 | 0.091 | 0.341 |
| H    | 0.949 | -0.415 | 0.808 |
| C    | 2.369 | 1.132 | 0.341 |
| H    | 2.664 | 1.726 | -0.537 |
| C    | 1.856 | 2.072 | 1.407 |
| H    | 1.168 | 1.573 | 2.086 |
| C    | 2.723 | 2.441 | 1.973 |
| O    | 3.918 | -2.329 | -1.301 |
| H    | 3.298 | -2.983 | -1.637 |
| O    | 1.104 | -2.036 | -1.295 |
| H    | 0.208 | -1.701 | -1.455 |
| O    | 3.495 | 0.483 | 0.897 |
| O    | 1.206 | 3.183 | 0.763 |
| H    | 0.922 | 3.804 | 1.437 |
| O    | 5.294 | -0.801 | 0.604 |
| H    | -3.918 | 2.756 | -1.537 |
| H    | -5.602 | -0.469 | -1.070 |
| H    | 5.561 | -1.612 | 0.160 |
| O    | -0.257 | -0.553 | 2.850 |
| H    | 0.139 | -1.098 | 3.531 |

F5(4-3), G= -861818.0694 kcal/mol, 28.8649 cm⁻¹
C  -1.044 | 0.565 | -0.363 |
H  -1.084 | 0.296 | 0.692 |
C  -1.878 | 1.821 | -0.610 |
H  -1.753 | 2.085 | -1.674 |
C  -3.354 | 1.615 | -0.281 |
H  -3.979 | 1.075 | -0.964 |
C  -3.439 | -1.719 | -1.529 |
H  -3.419 | -1.358 | -2.552 |
C  -2.509 | -1.329 | -0.662 |
H  -1.395 | 0.337 | 2.739 |
C  -2.444 | -1.801 | 0.753 |
H  -3.058 | -2.698 | 0.846 |
H  -1.401 | -2.060 | 1.002 |
O  -1.428 | 2.864 | 0.214 |
