ORIGINS OF exo-STEREOSELECTIVITY OF NORBORNENE IN HETERO DIELS-ALDER REACTIONS

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Figure S1 (¹H-NMR of 4b) ................................................................................................. Error! Bookmark not defined.
Figure S2 (STRUCTURES of TS(P,R,S,S) & TS(M,R,S,S)) ................................................. Error! Bookmark not defined.
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Figure S1. Partial $^1$H NMR spectrum of 4b in CDCl$_3$. ($M,S,R,R$)-x and its enantiomer is the major and ($P,S,R,R$)-x and its enantiomer is the minor product. ($^1$H and $^{13}$C NMR spectra of all compounds were recorded on a Varian-Mercury VX-400 MHz-BB in CDCl$_3$ at room temperature.)
Figure S2. Transition structures for the reaction between 3b and norbornene and their Gibbs free energies of activation in CH₂Cl₂ (ΔG‡ = G(TS) - G(3) – G(norbornene)) (M06-2X/6-31+G(d)//B3LYP/6-31+G(d)).

TS(P,R,S,S)-x and TS(M,S,R,R)-x as well as TS(P,S,R,R)-x and TS(M,R,S,S)-x are enantiomers and isoenergetic as expected.

**CARTESIAN COORDINATES (Å) AND ABSOLUTE ENERGIES (au)**

**REACTANTS**

**1b**

B3LYP/6-31+G*

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B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)

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Zero-point correction= 0.307695 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.329157
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Sum of electronic and zero-point Energies= -1390.086225
Sum of electronic and thermal Energies= -1390.065707
Sum of electronic and thermal Enthalpies= -1390.064763
Sum of electronic and thermal Free Energies= -1390.137794

M062X/6-311G(d,p) optimized with IEFPCM (toluene; $\varepsilon=2.37$)

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Sum of electronic and zero-point Energies= -1390.343178  
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59
Zero-point correction=          0.300772 (Hartree/Particle)
Thermal correction to Energy=       0.322123
Thermal correction to Enthalpy=      0.323067
Thermal correction to Gibbs Free Energy= 0.247008

Sum of electronic and zero-point Energies=   -1713.476429
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Sum of electronic and thermal Enthalpies=   -1713.454133
Sum of electronic and thermal Free Energies= -1713.530192

B3LYP/6-31+G* optimized with IEFPCM (toluene; \( \varepsilon =2.37 \))

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Sum of electronic and thermal Enthalpies= -1713.461326
Sum of electronic and thermal Free Energies= -1713.537572

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
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M062X/6-31+G(d) optimized with IEFPCM (toluene; \( \varepsilon=2.37 \))

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Sum of electronic and zero-point Energies= -1713.031160
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Sum of electronic and thermal Enthalpies= -1713.009219
Sum of electronic and thermal Free Energies= -1713.084183

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)
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Zero-point correction= 0.303101 (Hartree/Particle)
Thermal correction to Energy= 0.324154
Thermal correction to Enthalpy= 0.325098
Thermal correction to Gibbs Free Energy= 0.249766
Sum of electronic and zero-point Energies= -1713.297410
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Sum of electronic and thermal Enthalpies= -1713.275413
Sum of electronic and thermal Free Energies= -1713.350746

3b
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)
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C  -4.27256600  -0.35659000  -0.21180100
C  -0.64763700  -1.77199100  -0.45306400
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Zero-point correction=                           0.386765 (Hartree/Particle)
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Thermal correction to Enthalpy=                  0.414564
Thermal correction to Gibbs Free Energy=         0.325281
Sum of electronic and zero-point Energies=       -1982.563116
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Sum of electronic and thermal Enthalpies=         -1982.535317
Sum of electronic and thermal Free Energies=      -1982.624600

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -272.6050298

Norbornene
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)
C                  1.28079800    0.67217800    -0.50529500
C                  0.08784300    1.12988000    0.32368400
C                  1.28079400    -0.67218100    -0.50530000
C                  0.08783700    -1.12988200    0.32367800
C                 -1.19012700    0.78120400    -0.51911700
C                 -1.19013400    -0.78119500    -0.51911700
H                  1.92266500    -1.33027200    -1.08473000
H                  1.92267300    1.33026800    -1.08472100
H                 -2.08719400    1.17854200    -0.02961000
H                 -1.14337000    1.20812400    -1.52604800
H                 -2.08720000    -1.17852300    -0.02960100
H                 -1.14339100    -1.20811700    -1.52604800
C                  0.03656800    -0.00000400    1.38108500
H                 -0.88684600    -0.00000400    1.97422700
H                  0.90411400    -0.00000800    2.04998200
H                  0.11854500    2.15944600    0.68942800
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Zero-point correction=                           0.152929 (Hartree/Particle)
Thermal correction to Energy=                    0.158158

516
Thermal correction to Enthalpy = 0.159103
Thermal correction to Gibbs Free Energy = 0.124399
Sum of electronic and zero-point Energies = -272.584021
Sum of electronic and thermal Energies = -272.578792
Sum of electronic and thermal Enthalpies = -272.577848
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M06-2X/6-31+G(d)/B3LYP/6-31+G(d) (IEFPCM)
HF = -1982.3767844

TRANSITION STATES

**TS-rot-1b-O**

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H | -5.51731000 | 1.32639200 | 1.46769500
C | 3.45270500 | -0.79193800 | 3.15726000
H | 2.76375800 | -0.81221800 | 4.00346700
H | 3.98816700 | -1.74888600 | 3.09851800
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Thermal correction to Enthalpy= 0.323652
Thermal correction to Gibbs Free Energy= 0.252121
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Sum of electronic and thermal Enthalpies= -1390.466236
Sum of electronic and thermal Free Energies= -1390.537766

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)
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C | 2.34082200 | -0.40404500 | -0.28973000
C | 2.89100200 | -0.47792800 | -1.57513200
C | 4.27213000 | -0.59989400 | -1.76382100
C | 5.11413700 | -0.65322100 | -0.65489500
C | 4.58378300 | -0.58807100 | 0.64058100
C | 3.20389700 | -0.46880800 | 0.83304400
H | 2.22098100 | -0.45804100 | -2.43056400
H | 4.67747200 | -0.65763300 | -2.77009600
H | 6.18898500 | -0.74828700 | -0.78417400
H | 5.25354000 | -0.63021800 | 1.49213000
C | -1.99915300 | -0.55120500 | -0.32549500
C | -3.37294000 | -0.62945100 | 0.02382600
C | -4.05739400 | -1.84909900 | -0.99629000
C | -3.44945500 | -2.99949800 | -0.58130400
C | -2.11636500 | -2.91848600 | -0.98309700
C  -1.41862100  -1.72142800  -0.86106000
H  -5.10964400  -1.84904500  0.17386900
H  -4.00993200  -3.92599800  -0.66940400
H  -1.60605900  -3.78301400  -1.39843900
H  -0.38833700  -1.70466300  -1.17708000
C  -1.59072400  1.99430900  -0.05939600
S  0.88107500  2.14454700  -1.10761800
C  0.23524900  0.60067200  -0.43588400
N  -1.17836400  0.64922400  -0.28117500
O  -2.47616400  2.37443400  0.66997200
C  -0.72132800  2.96668900  -0.83819100
H  -0.60157000  3.88821700  -0.26694500
H  -1.20863100  3.19292900  -1.79265600
O  -4.13474000  0.45601800  0.37656400
O  2.59652600  -0.39100500  2.05149600
C  -4.46846100  0.55914900  1.76581900
H  -5.02749900  -0.32435000  2.09973600
H  -3.56478700  0.68072700  2.37275000
H  -5.09258200  1.44900300  1.86253100
C  3.40430800  -0.48099400  3.22135400
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H  3.94276300  -1.43626400  3.26022700
H  4.12033600  0.34893100  3.27466900

Zero-point correction= 0.302337 (Hartree/Particle)
Thermal correction to Energy= 0.322412
Thermal correction to Enthalpy= 0.323356
Thermal correction to Gibbs Free Energy= 0.252162
Sum of electronic and zero-point Energies= -1390.493691
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Sum of electronic and thermal Free Energies= -1390.543866

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-1390.3543234

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)
N  -0.94760800  0.53815300  -0.00119300
C  -2.33715400  0.58060100  -0.22958900
Zero-point correction= 0.306809 (Hartree/Particle)
Thermal correction to Energy= 0.326536
Thermal correction to Enthalpy= 0.327480
Thermal correction to Gibbs Free Energy= 0.255686
Sum of electronic and zero-point Energies= -1390.048083
Sum of electronic and thermal Energies= -1390.028355
Sum of electronic and thermal Enthalpies= -1390.027411
Sum of electronic and thermal Free Energies= -1390.099206

M062X/6-311G(d,p) optimized with IEPPCM (toluene; ε=2.37)

N  -0.92364000  0.69551000  0.11397800
C  -2.32137600  0.78893000  -0.05180100
C  -2.87466800  1.58690600  -1.04403900
C  -4.25671700  1.71416800  -1.16842700
C  -5.08537900  1.04011900  -0.28628600
C  -4.54669500  0.23410600  0.71705100
C  -3.16714600  0.10066400  0.84037200
H  -2.20431800  2.11003900  -1.71668000
H  -4.67381200  2.39528000  -1.94751000
H  -6.16159800  1.13271200  -0.36808100
H  -5.20962600  -0.28738300  1.39399600
C  2.00483900  0.59986900  -0.09011300
C  3.36213300  0.40779500  0.26669300
C  4.17310600  1.51460000  0.52672100
C  3.70058700  2.81134600  0.39158800
C  2.39956700  3.00968900  -0.03316300
C  1.57672500  1.91739700  -0.27367600
H  5.19960200  1.35355000  0.82287500
H  4.35525800  3.64783700  0.60252700
H  2.00509400  4.00746100  -0.17663300
H  0.56487700  2.10441800  -0.58603400
C  1.32678600  -1.87364900  -0.56366600
S  -1.13273300  -1.47396400  -1.47055500
C  -0.31012100  -0.23978800  -0.46470500
N  1.07683300  -0.47363200  -0.37676700
O  2.07961800  -2.56614300  0.04373700
C  0.40073100  -2.41543400  -1.63347600
H  0.23239600  -3.47364300  -1.45568100
H  0.85071400  -2.25848600  -2.61474300
O  3.84660500  -0.84667900  0.30322700
O  -2.54239800  -0.66706000  1.76487400
C  5.16537800  -1.06946000  0.75722900
H 5.90095200 -0.61944300  0.08332300
H 5.30751800 -0.67990500  1.76949000
H 5.29009400 -2.14955250  0.76261400
C -3.35413500 -1.41373700  2.65074900
H -2.67009800 -1.96830300  3.28822000
H -3.97545600 -0.75685600  3.26676600
H -3.99251100 -2.11376000  2.10294300

Zero-point correction=                           0.305223 (Hartree/Particle)
Thermal correction to Energy=                    0.324921
Thermal correction to Enthalpy=                  0.325866
Thermal correction to Gibbs Free Energy=         0.254736

Sum of electronic and zero-point Energies=       -1390.306449
Sum of electronic and thermal Energies=          -1390.286751
Sum of electronic and thermal Enthalpies=        -1390.285807
Sum of electronic and thermal Free Energies=     -1390.356936

**TS-rot-1b-N**
B3LYP/6-31+G*

N  0.74165300 -0.11835500  0.09341800
C  2.06326700 -0.24090900  -0.34211900
C  2.39528800 -0.33530000  -1.69945400
C  3.71577500 -0.55279000  -2.10704200
C  4.71822800 -0.67855900  -1.14852400
C  4.40737200 -0.59338500  0.21580800
C  3.08897700 -0.38218500  0.62746000
H  1.59751200 -0.26685200  -2.43439700
H  3.94984500 -0.62672700  -3.16537200
H  5.74903800 -0.84677200  -1.44887300
H  5.20061600 -0.69115900  0.94860100
C -2.44555900 -0.05574600  0.04846600
C -2.25678200 -1.46299800  -0.07233800
C -3.37585700 -2.31260600  -0.09083200
C -4.67673900 -1.82126500  -0.04289400
C -4.87366900 -0.44581600  0.00686600
C -3.77404900  0.40867200  0.04721600
H -3.21831800 -3.38176100  -0.16441100
H -5.51675700 -2.51041000  -0.06036600
H -5.87344100 -0.02190900  0.02175300
S -3.96532300  1.46821800  0.10693300
C -1.67624400  2.27845800  0.47452600
S  0.55322500  2.35375800 -0.10693300
C -0.00845300  0.83017500 -0.25735100
N -1.39254400  0.95118800  0.10263000
O -2.59417100  2.65206300  1.18018600
C -0.69734600  3.27846800 -0.12592000
H -0.23594800  3.86189100  0.67606300
H -1.26439700  3.95806000 -0.76802100
O -1.00368400 -1.95807500 -0.21464700
O  2.68992100 -0.27499500  1.92710400
C -0.77735200 -3.35855200 -0.18047400
H -1.16005500 -3.80349700  0.74715400
H -1.22790500 -3.86283200 -1.04587100
H  0.30739900 -3.47287900 -0.21848200
C  3.66257500 -0.42990600  2.95083500
H  3.11854200 -0.32880300  3.89155400
H  4.13618200 -1.41977100  2.90682200
H  4.43452900  0.34874800  2.88982300

Zero-point correction=         0.302730 (Hartree/Particle)
Thermal correction to Energy=   0.322716
Thermal correction to Enthalpy=  0.323661
Thermal correction to Gibbs Free Energy=  0.252602
Sum of electronic and zero-point Energies=  -1390.486146
Sum of electronic and thermal Energies=    -1390.466159
Sum of electronic and thermal Enthalpies=   -1390.465215
Sum of electronic and thermal Free Energies= -1390.536274

B3LYP/6-31+G* optimized with IEFPCM (toluene; \( \varepsilon=2.37 \))
N  0.70674900 -0.14729100  0.01564200
C  2.03668900 -0.21140400 -0.41793500
C  2.37920000 -0.16502800 -1.77498100
C  3.70678900 -0.31870300 -2.18874900
C  4.70364300 -0.52219700 -1.23684800
C  4.38117800 -0.57943900  0.12621800
C  3.05519400 -0.43355300  0.54342000
H  1.58624100 -0.03949900 -2.50732200
H  3.95059300 -0.28495500 -3.24684600
H  5.73963700 -0.64200800 -1.54237900
H         5.17025400  -0.73653100  0.85290100  
C         -2.44156200  -0.11785000  -0.01206000  
C         -2.22473500  -1.49253900  -0.29048300  
C         -3.32282100  -2.35717400  -0.43167500  
C         -4.63592400  -1.91920300  -0.33051500  
C         -4.86057500  -0.56093900  -0.10591500  
C         -3.78767300  0.31136600  0.03964100  
H         -3.10115800  -3.39580200  -0.66059000  
H         -5.46148300  -2.61511400  -0.45097000  
H         -5.87055900  -0.16475200  -0.04921500  
H         -4.00847600  1.35257700  0.21239800  
C         -1.72785600  2.18998400  0.62821100  
S         0.51964000  2.44029600  -0.87284700  
C         -0.03756500  0.83942400  -0.22911700  
N         -1.42117500  0.90935500  0.13546600  
O         -2.65133300  2.47467500  1.37002700  
O         -0.77046900  3.25796300  0.12319800  
C         -0.33562000  3.79081100  0.97312200  
H         -1.34399900  3.96826300  -0.47857600  
O         -0.99417000  -2.04394500  -0.54479000  
O         2.64414800  -0.46593500  1.84441100  
C         -0.45069200  -2.86138200  0.49942400  
H         -0.23861500  -2.25789200  1.38792100  
H         -1.13701100  -3.67979600  0.75143800  
H         0.48210000  -3.27152100  0.10854200  
C         3.61703200  -0.70026400  2.85853200  
H         3.06580400  -0.70245700  3.80008700  
H         4.11044500  -1.67059700  2.72030600  
H         4.37030600  0.09734600  2.87756500  

Zero-point correction=       0.302496 (Hartree/Particle)  
Thermal correction to Energy=         0.322473  
Thermal correction to Enthalpy=       0.323418  
Thermal correction to Gibbs Free Energy= -0.252783  
Sum of electronic and zero-point Energies= -1390.492909  
Sum of electronic and thermal Energies= -1390.472931  
Sum of electronic and thermal Enthalpies= -1390.471987  
Sum of electronic and thermal Free Energies= -1390.542622  

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-1390.3543793

M062X/6-31+G(d) optimized with IEFPCM (toluene; $\varepsilon=2.37$)

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### M062X/6-311G(d,p) optimized with IEFPCM (toluene; $\varepsilon=2.37$)

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Zero-point correction= 0.306755 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.327362
Thermal correction to Gibbs Free Energy= 0.256849
Sum of electronic and zero-point Energies= -1390.046929
Sum of electronic and thermal Energies= -1390.027267
Sum of electronic and thermal Enthalpies= -1390.026323
Sum of electronic and thermal Free Energies= -1390.096836
H   0.0431660  3.72621700  0.48427300
H  -0.97723100  3.89065800  -0.96205400
O  -1.12418000  -1.95447200  -0.03638500
O   2.71439300  -0.02473400  1.89660500
C  -0.98576100  -3.35488600   0.08212200
H  -1.39712700  -3.71626500  1.02918500
H  -1.46693200  -3.87624600  -0.75102100
H   0.08566300  -3.54095200   0.05687400
C   3.72977000  -0.00878600  2.88135600
H   3.22998600   0.24157000  3.81828800
H   4.23000400  -0.96084900  2.96517900
H   4.46951200   0.78420100  2.65995300

Zero-point correction= 0.305283 (Hartree/Particle)
Thermal correction to Energy= 0.324934
Thermal correction to Enthalpy= 0.325879
Thermal correction to Gibbs Free Energy= 0.255406
Sum of electronic and zero-point Energies= -1390.304443
Sum of electronic and thermal Energies= -1390.284792
Sum of electronic and thermal Enthalpies= -1390.283848
Sum of electronic and thermal Free Energies= -1390.354320

**TS-rot-2b-S**
B3LYP/6-31+G*

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Zero-point correction= 0.300246 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.321574
Thermal correction to Gibbs Free Energy= 0.249288

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Sum of electronic and thermal Energies= -1713.409878
Sum of electronic and thermal Enthalpies= -1713.408934
Sum of electronic and thermal Free Energies= -1713.481220

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)
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Zero-point correction=     0.300212  (Hartree/Particle)
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Thermal correction to Enthalpy=     0.321528
Thermal correction to Gibbs Free Energy=     0.249404
Sum of electronic and zero-point Energies=  -1713.436268
Sum of electronic and thermal Energies: -1713.415897
Sum of electronic and thermal Enthalpies: -1713.414953
Sum of electronic and thermal Free Energies: -1713.487077

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-1713.2864719

M062X/6-31+G(d) optimized with IEFPCM (toluene; \( \varepsilon = 2.37 \))

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### M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)

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Zero-point correction= 0.303952 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.325084
Thermal correction to Gibbs Free Energy= 0.252340

Sum of electronic and zero-point Energies= -1712.983707
Sum of electronic and thermal Energies= -1712.963519
Sum of electronic and thermal Enthalpies= -1712.962575
Sum of electronic and thermal Free Energies= -1713.035319
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C   0.40880900  0.03970800  0.45204900
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C  -0.40095900 -1.95686600  1.94091000
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O  -3.74386600 -0.58092400 -0.37405800
O   2.59413600 -1.04405100 -1.45554300
C  -5.05545800 -0.77860100 -0.86116600
H  -5.79696300 -0.31520700 -0.20357200
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H   4.03528100 -1.66410500 -2.81820800
H   3.97550200 -2.58351300 -1.28550700
S  -2.04474700 -2.76965300 -0.08166900

Zero-point correction=       0.302405 (Hartree/Particle)
Thermal correction to Energy=      0.322534
Thermal correction to Enthalpy=    0.323478
Thermal correction to Gibbs Free Energy= 0.251568
Sum of electronic and zero-point Energies=  -1713.250220
Sum of electronic and thermal Energies=    -1713.230091
Sum of electronic and thermal Enthalpies=   -1713.229147
Sum of electronic and thermal Free Energies= -1713.301057

**TS-rot-2b-N**

B3LYP/6-31+G*

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C   4.88150600 -0.54939900 -0.99401100
C   4.51682400 -0.31224200  0.33836000
C   3.17189400 -0.15405500  0.68340800
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Zero-point correction=  0.300037 (Hartree/Particle)
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Thermal correction to Gibbs Free Energy=  0.249437
Sum of electronic and zero-point Energies=  -1713.431963
Sum of electronic and thermal Energies=  -1713.411544
Sum of electronic and thermal Enthalpies=  -1713.410600
Sum of electronic and thermal Free Energies=  -1713.482563
B3LYP/6-31+G* optimized with IEFPCM (toluene; \( \varepsilon = 2.37 \))

N 0.83458000 -0.11626600  0.05517000
C 2.17904800 -0.19878400 -0.32373000
C 2.57311000 -0.40879100 -1.65123900
C 3.92192700 -0.56817400 -1.98596800
C 4.88831600 -0.51585400 -0.98347700
C 4.51530500 -0.31399500  0.35253800
N 0.83458000 -0.11626600  0.05517000
C 2.17904800 -0.19878400 -0.32373000
C 2.57311000 -0.40879100 -1.65123900
C 3.92192700 -0.56817400 -1.98596800
C 4.88831600 -0.51585400 -0.98347700
C 4.51530500 -0.31399500  0.35253800
N 1.38364900  0.69814700 -0.12664100
C 0.92840400  2.99260900 -0.66762200
H 0.16304900 -2.34648300  0.58701500
H -0.52676100 -3.87271700  0.83106300
H 1.01580200 -3.23807400  0.19020600
C 3.65005600  0.07380900  3.02865200
H 3.06148700  0.22988100  3.93382300
H 4.19560700 -0.87521500  3.10427500
H 4.36127100  0.90031000  2.90720800
S -2.83485300  2.58858400  1.25584300
Zero-point correction=                           0.299932 (Hartree/Particle)
Thermal correction to Energy=                    0.320363
Thermal correction to Enthalpy=                 0.321307
Thermal correction to Gibbs Free Energy=        0.249607

Sum of electronic and zero-point Energies=      -1713.437600
Sum of electronic and thermal Energies=         -1713.417169
Sum of electronic and thermal Enthalpies=       -1713.416225
Sum of electronic and thermal Free Energies=    -1713.487925

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-1713.2892488

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)

N   0.81527900  -0.10195300   0.06921800
C   2.15382900   -0.15490900  -0.33277600
C   2.52494900   -0.22801600  -1.67449400
C   3.86767500   -0.33935100  -2.03918200
C   4.84167600   -0.38016200  -1.04976400
C   4.48725100   -0.32434700   0.30219800
C   3.14678800    0.22328500   0.66950700
H   1.74391800    0.23571900  -2.43139000
H   4.14102200    0.39981000  -3.08767600
H   5.89080900   -0.46374000  -1.31721500
H   5.26337500   -0.36207500   1.05807200
C  -2.25728800   -0.45344600  -0.12142100
C  -1.84294000  -1.79786900  -0.26866200
C  -2.79981900  -2.81953400  -0.28649800
C  -4.15889600  -2.56513200  -0.21054400
C  -4.57804600  -1.23877200  -0.15640500
C  -3.64368300  -0.21549700  -0.12663600
H  -2.42828900  -3.83330500  -0.40598400
H  -4.87454700  -3.38100300  -0.23342900
H  -5.63392600  -0.98753500  -0.15004900
H  -4.00681200   0.80005500  -0.11322900
C  -1.76958400   1.97861600   0.24730200
S   0.36181300   2.14832900  -1.43889300
C   0.00401000   0.70197400  -0.44896000
N  -1.39178800   0.70113700  -0.09626700
C  -0.91728200  3.01319000  -0.47144500
H  -0.45937100  3.68725300  0.25428700
H  -1.56676600  3.59330900  -1.13055200
O  -0.55256200  -2.17910600  -0.50638300
O   2.70034900  -0.16201100  1.94760800
C   0.09641900  -2.81158800  0.59460600
H   0.10040300  -2.15163400  1.46674700
H   -0.39542300  -3.76112500  0.83606000
H    1.12377700  -2.99805200  0.27758700
C   3.66396100  -0.21518000  2.98326200
H   3.10287700  -0.16210700  3.91557500
H   4.22986600  -1.15339400  2.94800800
H   4.35394400  -0.63423300  2.92100200
S  -2.90217100  2.48599200  1.32584300

Zero-point correction=        0.303961 (Hartree/Particle)
Thermal correction to Energy=    0.324022
Thermal correction to Enthalpy=    0.324966
Thermal correction to Gibbs Free Energy= 0.254113
Sum of electronic and zero-point Energies=    -1712.987187
Sum of electronic and thermal Energies=   -1712.967127
Sum of electronic and thermal Enthalpies=   -1712.966182
Sum of electronic and thermal Free Energies= -1713.037036

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)
N   0.81116400  -0.07558600  0.04198700
C   2.15279900  -0.11062800  -0.34479800
C   2.54296200  -0.11372300  -1.67970200
C   3.88824100  -0.21184600  -2.02712300
C   4.84318100  -0.31228000  -1.02854600
C   4.46890600  -0.32875000  0.31608100
C   3.12625000  -0.24060400  0.66790100
H   1.77569700  -0.07836700  -2.44550400
H   4.17835300  -0.21807100  -3.07007500
H   5.89320500  -0.38765600  -1.28354500
H   5.23120900  -0.41476200  1.07827500
C  -2.24037000  -0.46472800  -0.14650500
C  -1.80212300  -1.79673400  -0.31984900
C  -2.74252700  -2.82988700  -0.35049500
C  -4.10205700  -2.60003200  -0.27125400
Zero-point correction=       0.302557 (Hartree/Particle)
Thermal correction to Energy=    0.322555
Thermal correction to Enthalpy=   0.323499
Thermal correction to Gibbs Free Energy=   0.252433

Sum of electronic and zero-point Energies=    -1715.253812
Sum of electronic and thermal Energies=    -1713.238314
Sum of electronic and thermal Enthalpies=    -1713.232869
Sum of electronic and thermal Free Energies=  -1713.303935

**TS(M,S,R,R)-x**

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; \( \varepsilon = 8.93 \))

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M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9665803

**TS(P.S.R.R)-x**
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; \( \varepsilon = 8.93 \))
N           2.83905000  0.28826400  0.10429900
C           3.42270600  1.56871900  0.10990100
C           3.59857500  2.30057300 -1.07240600
C           4.26651400  3.53018300 -0.10429900
C           4.77544800  4.03711600  0.10990100
C           4.61954600  3.32025000  1.31842100
C           3.95074100  2.09090000  1.31522400
H           3.21603000  1.88272700 -1.99994000
H           4.39061300  4.07749100 -2.00444100
H           5.29985700  4.98894100  0.13759500
H           5.02165100  3.72812500  2.23584200
O           3.74877000 -2.43493900  3.67600600
C           4.28346900  1.78600000  3.67600600
H           4.02203000  1.02120100  4.40882000
H           3.83781000  2.74375000  3.97165700
H           2.96765900  4.55247700  2.12692300
H           1.60035600  2.46264600  1.99451100
O           1.97623300 -2.20205900 -2.47141300
C           2.46324200 -2.72576700 -3.70961300
H           2.10142800 -2.04226900 -4.47840500
H           2.06630500 -3.73071400 -3.89402400
H           3.55905400 -2.74843800 -3.72326700
C           -3.20976300 -0.18664700  1.13760100
C           -4.72224100 -0.18852300  0.90677100
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Zero-point correction= 0.541043 (Hartree/Particle)
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Thermal correction to Gibbs Free Energy= 0.472983
Sum of electronic and zero-point Energies= -2255.114030
Sum of electronic and thermal Energies= -2255.081392
Sum of electronic and thermal Enthalpies= -2255.080448
Sum of electronic and thermal Free Energies= -2255.182090

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9655992
**TS(M,S,S,S)-x**
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

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Thermal correction to Gibbs Free Energy=   0.474713
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Sum of electronic and thermal Free Energies=  -2255.176699
M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)  
HF= -2254.9643165

**TS(P,S,S,S)-x**  
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; \( \varepsilon = 8.93 \))

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Sum of electronic and thermal Energies= -2255.078013
Sum of electronic and thermal Enthalpies = -2255.077069
Sum of electronic and thermal Free Energies = -2255.177692

M06-2X/6-31+G(d) // B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9644569

**TS(M,S,R,R)-n**
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

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M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF= -2254.9523948

**TS(P,S,R,R)-n**

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; \( \varepsilon = 8.93 \))

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M06-2X/6-31+G(d)/B3LYP/6-31+G* (IEFPCM)
HF = -2254.9515176

**TS(M.S.S.S)-n**
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; \( \varepsilon = 8.93 \))

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Thermal correction to Gibbs Free Energy= 0.474269
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Sum of electronic and thermal Energies= -2255.062433
Sum of electronic and thermal Enthalpies= -2255.061489
Sum of electronic and thermal Free Energies= -2255.161973

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9491486

TS(P,S,S,S)-n
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; \( \epsilon = 8.93 \))
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Zero-point correction=                           0.541206 (Hartree/Particle)
Thermal correction to Energy=                    0.573790
Thermal correction to Enthalpy=                  0.574734
Thermal correction to Gibbs Free Energy=         0.473690
Sum of electronic and zero-point Energies=       -2255.095991
Sum of electronic and thermal Energies=          -2255.063408
Sum of electronic and thermal Enthalpies=        -2255.062463
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M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9505211

TS-rot-4b-S
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)
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C                  3.75525400   -3.13132200    -2.95689600
C                  4.45530900   -3.75951800    -1.92633100
C                  4.53232600   -3.16534200    -0.66082000
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### Thermal correction to Energy=
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### Thermal correction to Enthalpy=
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### Thermal correction to Gibbs Free Energy=
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### Sum of electronic and zero-point Energies=
-2255.131046

### Sum of electronic and thermal Energies=
-2255.099992

### Sum of electronic and thermal Enthalpies=
-2255.099048

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**M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)**

HF= -2255.0133823

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**TS-rot-4b-N**

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

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HF= -2255.0059644

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Zero-point correction=  0.545462 (Hartree/Particle)
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Thermal correction to Gibbs Free Energy=  0.478388
Sum of electronic and zero-point Energies=  -2255.164151
Sum of electronic and thermal Energies=  -2255.132008
Sum of electronic and thermal Enthalpies=  -2255.131064
Sum of electronic and thermal Free Energies=  -2255.231226

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=  -2255.0349223

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Thermal correction to Gibbs Free Energy= 0.477761
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Sum of electronic and thermal Energies= -2255.131855
Sum of electronic and thermal Enthalpies= -2255.130911
Sum of electronic and thermal Free Energies= -2255.231572

M06-2X/6-31+G(d)/ B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0345436

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B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)
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Zero-point correction=        0.545569 (Hartree/Particle)
Thermal correction to Energy=        0.577636
Thermal correction to Enthalpy=       0.578580
Thermal correction to Gibbs Free Energy=   0.478323
Sum of electronic and zero-point Energies= -2255.157302
Sum of electronic and thermal Energies=  -2255.125235
Sum of electronic and thermal Enthalpies=  -2255.124291
Sum of electronic and thermal Free Energies=  -2255.224548

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0293027

(P.S.S.S)-x
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)
C  1.91518600  2.17852500  0.02183700
C  2.41485600  2.81523300  1.13393800
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H   3.35556600  4.61732200  2.14520600
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Zero-point correction=  0.545525 (Hartree/Particle)
Thermal correction to Energy=  0.577555
Thermal correction to Enthalpy=  0.578499
Thermal correction to Gibbs Free Energy=  0.478733
Sum of electronic and zero-point Energies=  -2255.157258
Sum of electronic and thermal Energies=  -2255.125229
Sum of electronic and thermal Enthalpies=  -2255.124284
Sum of electronic and thermal Free Energies=  -2255.224050

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=2255.0289276
(M,S,R,R)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; $\varepsilon=8.93$)

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Thermal correction to Gibbs Free Energy= 0.478940
Sum of electronic and zero-point Energies= -2255.160527
Sum of electronic and thermal Energies= -2255.128473
Sum of electronic and thermal Enthalpies= -2255.127529
Sum of electronic and thermal Free Energies= -2255.227229
M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0321409

**\((P,S,R,R)-n\)**

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; \(\varepsilon=8.93\))

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Thermal correction to Gibbs Free Energy = 0.477389
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Sum of electronic and thermal Free Energies = -2255.228394

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2255.031383

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B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

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C  -3.07536700  -2.04111200  -0.77169500
C  -3.37677900  -2.80186600  0.54707000
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C  -1.08351300  0.24321400  -0.52999600
C  -0.50939200  -0.95011200  -0.78484900
S  -1.38037000  -2.31330200  -1.49022700
S  0.11709300  1.38479800  0.10661200
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C  4.05247500  3.74597900  0.27000800
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H  4.63486000  3.49456300 -2.47827600
H  2.98991800  4.18890400 -2.31309800

Zero-point correction= 0.545862 (Hartree/Particle)
Thermal correction to Energy= 0.577785
Thermal correction to Enthalpy= 0.578729
Thermal correction to Gibbs Free Energy = 0.479574
Sum of electronic and zero-point Energies = -2255.155086
Sum of electronic and thermal Energies = -2255.123163
Sum of electronic and thermal Enthalpies = -2255.122219
Sum of electronic and thermal Free Energies = -2255.221374

M06-2X/6-31+G(d)/B3LYP/6-31+G(d) (IEFPCM)
HF = -2255.0307723

(P,S,S,S)-n
B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C  2.01603100  -2.04163800  0.05077300
C  2.56482000  -2.64241800 -1.10218900
C  3.51847900  -3.65897600  -0.95279700
C  3.92051800  -4.05580000  0.32680000
C  3.38430100  -3.45401500  1.46683900
C  2.42954400  -2.44443100  1.31881200
H  3.95209700  -4.13954500  -1.82220100
H  4.66253200  -4.84392600  0.42445200
H  3.70213400  -3.76401500  2.45776500
H  1.99674400  -1.95512000  2.18652600
O  2.11072900  -2.17770800  -2.29676600
C  2.63003400  -2.75196800  -3.49935900
H  2.12670700  -2.22908400  -4.31316300
H  2.40366700  -3.82309900  -3.55390900
H  3.71219100  -2.59470500  -3.57389400
C  -3.34323400  -1.16536700  -0.03211100
C  -3.76217800  -0.76269600  1.41002900
C  -2.69586800  -2.58572400  0.20029600
C  -2.88199800  -2.83273300  1.72118700
C  -2.55194400  -0.50285500  2.34213700
C  -4.24569000  -2.13514500  1.93955600
C  -1.94981900  -1.92877700  2.55579000
C  -2.52761000  -0.18289800  -0.93473100
C  -1.06834400  -0.12364100  -0.55117400
C  -0.32383600  -1.23084600  -0.35765100
S  -0.97940800  -2.86532300  -0.46007900
S  -0.05998900  1.33174000  -0.43258100
C  1.40739000  0.33528100  -0.14095900

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Zero-point correction= 0.545941 (Hartree/Particle)
Thermal correction to Energy= 0.577833
Thermal correction to Enthalpy= 0.578778
Thermal correction to Gibbs Free Energy= 0.479604
Sum of electronic and zero-point Energies= -2255.155153
Sum of electronic and thermal Energies= -2255.123261
Sum of electronic and thermal Enthalpies= -2255.122317
Sum of electronic and thermal Free Energies= -2255.221490

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.030698