**Styrene H**

M06-2X/GCP(DFT/6-31G(d))

---------------------------------

CARTESIAN COORDINATES (ANGSTROEM)

---------------------------------

C -0.052191 -0.404117 -0.144131

C 0.255715 0.944147 -0.354792

C 0.983319 -1.279211 0.192722

H -0.533670 1.648873 -0.582973

H 0.754334 -2.323101 0.371575

C 1.559947 1.393625 -0.247656

C 2.290217 -0.830072 0.297111

H 1.781569 2.440591 -0.409151

H 3.080302 -1.522817 0.556061

C 2.582653 0.508197 0.074941

H 3.601175 0.863997 0.159622

C -1.412940 -0.923168 -0.249544

H -1.562585 -1.928156 0.131332

C -2.480072 -0.256781 -0.733743

H -2.391891 0.712261 -1.204048

H -3.444683 -0.740007 -0.803302

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VIBRATIONAL FREQUENCIES

-----------------------

Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: 50.34 cm\*\*-1

7: 212.01 cm\*\*-1

8: 239.80 cm\*\*-1

9: 415.40 cm\*\*-1

10: 441.78 cm\*\*-1

11: 459.35 cm\*\*-1

12: 555.27 cm\*\*-1

13: 629.07 cm\*\*-1

14: 665.40 cm\*\*-1

15: 726.31 cm\*\*-1

16: 792.96 cm\*\*-1

17: 818.22 cm\*\*-1

18: 876.76 cm\*\*-1

19: 956.92 cm\*\*-1

20: 960.72 cm\*\*-1

21: 1012.20 cm\*\*-1

22: 1018.62 cm\*\*-1

23: 1034.90 cm\*\*-1

24: 1036.29 cm\*\*-1

25: 1046.15 cm\*\*-1

26: 1065.08 cm\*\*-1

27: 1111.89 cm\*\*-1

28: 1164.71 cm\*\*-1

29: 1194.14 cm\*\*-1

30: 1236.02 cm\*\*-1

31: 1311.35 cm\*\*-1

32: 1341.60 cm\*\*-1

33: 1353.69 cm\*\*-1

34: 1435.82 cm\*\*-1

35: 1487.34 cm\*\*-1

36: 1540.16 cm\*\*-1

37: 1665.04 cm\*\*-1

38: 1692.27 cm\*\*-1

39: 1743.83 cm\*\*-1

40: 3158.93 cm\*\*-1

41: 3169.58 cm\*\*-1

42: 3186.20 cm\*\*-1

43: 3193.77 cm\*\*-1

44: 3203.48 cm\*\*-1

45: 3210.64 cm\*\*-1

46: 3218.09 cm\*\*-1

47: 3258.18 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -309.24594782 Eh

Zero point energy ... 0.13416187 Eh 84.19 kcal/mol

Thermal vibrational correction ... 0.00387796 Eh 2.43 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

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Total thermal energy -309.10507545 Eh

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ENTHALPY

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The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -309.10507545 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

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Total Enthalpy ... -309.10413124 Eh

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GIBBS FREE ENERGY

-------------------

The Gibbs free energy is G = H - T\*S

Total enthalpy ... -309.10413124 Eh

Total entropy correction ... -0.03842091 Eh -24.11 kcal/mol

-----------------------------------------------------------------------

Final Gibbs free energy ... -309.14255215 Eh

**Styrene-α-d1**

M06-2X/GCP(DFT/6-31G(d))

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CARTESIAN COORDINATES (ANGSTROEM)

---------------------------------

C -0.052191 -0.404117 -0.144131

C 0.255715 0.944147 -0.354792

C 0.983319 -1.279211 0.192722

H -0.533670 1.648873 -0.582973

H 0.754334 -2.323101 0.371575

C 1.559947 1.393625 -0.247656

C 2.290217 -0.830072 0.297111

H 1.781569 2.440591 -0.409151

H 3.080302 -1.522817 0.556061

C 2.582653 0.508197 0.074941

H 3.601175 0.863997 0.159622

C -1.412940 -0.923168 -0.249544

H -1.562585 -1.928156 0.131332

C -2.480072 -0.256781 -0.733743

H -2.391891 0.712261 -1.204048

H -3.444683 -0.740007 -0.803302

-----------------------

VIBRATIONAL FREQUENCIES

-----------------------

Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: 47.51 cm\*\*-1

7: 199.86 cm\*\*-1

8: 237.71 cm\*\*-1

9: 415.33 cm\*\*-1

10: 435.77 cm\*\*-1

11: 453.65 cm\*\*-1

12: 548.18 cm\*\*-1

13: 628.98 cm\*\*-1

14: 658.77 cm\*\*-1

15: 723.30 cm\*\*-1

16: 786.16 cm\*\*-1

17: 816.61 cm\*\*-1

18: 865.17 cm\*\*-1

19: 877.12 cm\*\*-1

20: 898.70 cm\*\*-1

21: 958.23 cm\*\*-1

22: 964.31 cm\*\*-1

23: 1012.20 cm\*\*-1

24: 1018.70 cm\*\*-1

25: 1042.28 cm\*\*-1

26: 1061.20 cm\*\*-1

27: 1105.88 cm\*\*-1

28: 1121.02 cm\*\*-1

29: 1164.70 cm\*\*-1

30: 1194.38 cm\*\*-1

31: 1250.51 cm\*\*-1

32: 1325.65 cm\*\*-1

33: 1353.41 cm\*\*-1

34: 1428.55 cm\*\*-1

35: 1485.18 cm\*\*-1

36: 1538.96 cm\*\*-1

37: 1664.78 cm\*\*-1

38: 1691.77 cm\*\*-1

39: 1727.47 cm\*\*-1

40: 2347.15 cm\*\*-1

41: 3164.71 cm\*\*-1

42: 3186.14 cm\*\*-1

43: 3193.77 cm\*\*-1

44: 3203.45 cm\*\*-1

45: 3210.63 cm\*\*-1

46: 3218.08 cm\*\*-1

47: 3257.60 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -309.24594782 Eh

Zero point energy ... 0.13095717 Eh 82.18 kcal/mol

Thermal vibrational correction ... 0.00399178 Eh 2.50 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

-----------------------------------------------------------------------

Total thermal energy -309.10816633 Eh

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ENTHALPY

--------

The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -309.10816633 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

-----------------------------------------------------------------------

Total Enthalpy ... -309.10722212 Eh

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GIBBS FREE ENERGY

-------------------

The Gibbs free energy is G = H - T\*S

Total enthalpy ... -309.10722212 Eh

Total entropy correction ... -0.03865556 Eh -24.26 kcal/mol

-----------------------------------------------------------------------

Final Gibbs free energy ... -309.14587768 Eh

**Styrene-β,β-d2**

M06-2X/GCP(DFT/6-31G(d))

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CARTESIAN COORDINATES (ANGSTROEM)

---------------------------------

C -0.052191 -0.404117 -0.144131

C 0.255715 0.944147 -0.354792

C 0.983319 -1.279211 0.192722

H -0.533670 1.648873 -0.582973

H 0.754334 -2.323101 0.371575

C 1.559947 1.393625 -0.247656

C 2.290217 -0.830072 0.297111

H 1.781569 2.440591 -0.409151

H 3.080302 -1.522817 0.556061

C 2.582653 0.508197 0.074941

H 3.601175 0.863997 0.159622

C -1.412940 -0.923168 -0.249544

H -1.562585 -1.928156 0.131332

C -2.480072 -0.256781 -0.733743

H -2.391891 0.712261 -1.204048

H -3.444683 -0.740007 -0.803302

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VIBRATIONAL FREQUENCIES

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Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: 46.65 cm\*\*-1

7: 199.71 cm\*\*-1

8: 222.51 cm\*\*-1

9: 409.36 cm\*\*-1

10: 418.93 cm\*\*-1

11: 434.46 cm\*\*-1

12: 514.86 cm\*\*-1

13: 593.91 cm\*\*-1

14: 628.87 cm\*\*-1

15: 722.38 cm\*\*-1

16: 750.50 cm\*\*-1

17: 764.56 cm\*\*-1

18: 805.20 cm\*\*-1

19: 876.55 cm\*\*-1

20: 920.11 cm\*\*-1

21: 953.22 cm\*\*-1

22: 994.46 cm\*\*-1

23: 1012.10 cm\*\*-1

24: 1018.53 cm\*\*-1

25: 1032.29 cm\*\*-1

26: 1042.61 cm\*\*-1

27: 1062.81 cm\*\*-1

28: 1113.24 cm\*\*-1

29: 1164.74 cm\*\*-1

30: 1194.80 cm\*\*-1

31: 1241.39 cm\*\*-1

32: 1310.80 cm\*\*-1

33: 1341.90 cm\*\*-1

34: 1355.46 cm\*\*-1

35: 1485.12 cm\*\*-1

36: 1538.55 cm\*\*-1

37: 1660.12 cm\*\*-1

38: 1690.50 cm\*\*-1

39: 1703.05 cm\*\*-1

40: 2327.15 cm\*\*-1

41: 2433.96 cm\*\*-1

42: 3164.67 cm\*\*-1

43: 3186.19 cm\*\*-1

44: 3193.75 cm\*\*-1

45: 3203.46 cm\*\*-1

46: 3210.63 cm\*\*-1

47: 3218.09 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -309.24594782 Eh

Zero point energy ... 0.12794678 Eh 80.29 kcal/mol

Thermal vibrational correction ... 0.00415680 Eh 2.61 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

-----------------------------------------------------------------------

Total thermal energy -309.11101170 Eh

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ENTHALPY

--------

The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -309.11101170 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

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Total Enthalpy ... -309.11006749 Eh

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GIBBS FREE ENERGY

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The Gibbs free energy is G = H - T\*S

Total enthalpy ... -309.11006749 Eh

Total entropy correction ... -0.03898680 Eh -24.46 kcal/mol

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Final Gibbs free energy ... -309.14905429 Eh

**Styrene-α,β,β-d3**

M06-2X/GCP(DFT/6-31G(d))

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CARTESIAN COORDINATES (ANGSTROEM)

---------------------------------

C -0.052191 -0.404117 -0.144131

C 0.255715 0.944147 -0.354792

C 0.983319 -1.279211 0.192722

H -0.533670 1.648873 -0.582973

H 0.754334 -2.323101 0.371575

C 1.559947 1.393625 -0.247656

C 2.290217 -0.830072 0.297111

H 1.781569 2.440591 -0.409151

H 3.080302 -1.522817 0.556061

C 2.582653 0.508197 0.074941

H 3.601175 0.863997 0.159622

C -1.412940 -0.923168 -0.249544

H -1.562585 -1.928156 0.131332

C -2.480072 -0.256781 -0.733743

H -2.391891 0.712261 -1.204048

H -3.444683 -0.740007 -0.803302

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VIBRATIONAL FREQUENCIES

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Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: 44.33 cm\*\*-1

7: 190.97 cm\*\*-1

8: 221.08 cm\*\*-1

9: 408.07 cm\*\*-1

10: 417.32 cm\*\*-1

11: 430.38 cm\*\*-1

12: 510.18 cm\*\*-1

13: 592.64 cm\*\*-1

14: 628.83 cm\*\*-1

15: 720.24 cm\*\*-1

16: 740.33 cm\*\*-1

17: 750.07 cm\*\*-1

18: 783.21 cm\*\*-1

19: 835.19 cm\*\*-1

20: 843.94 cm\*\*-1

21: 876.72 cm\*\*-1

22: 962.94 cm\*\*-1

23: 1004.73 cm\*\*-1

24: 1013.78 cm\*\*-1

25: 1018.52 cm\*\*-1

26: 1042.25 cm\*\*-1

27: 1054.09 cm\*\*-1

28: 1064.71 cm\*\*-1

29: 1113.98 cm\*\*-1

30: 1164.73 cm\*\*-1

31: 1195.25 cm\*\*-1

32: 1265.12 cm\*\*-1

33: 1325.14 cm\*\*-1

34: 1353.58 cm\*\*-1

35: 1483.92 cm\*\*-1

36: 1536.54 cm\*\*-1

37: 1658.71 cm\*\*-1

38: 1681.84 cm\*\*-1

39: 1695.16 cm\*\*-1

40: 2311.56 cm\*\*-1

41: 2361.33 cm\*\*-1

42: 2434.14 cm\*\*-1

43: 3186.14 cm\*\*-1

44: 3193.75 cm\*\*-1

45: 3203.45 cm\*\*-1

46: 3210.63 cm\*\*-1

47: 3218.08 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -309.24594782 Eh

Zero point energy ... 0.12472406 Eh 78.27 kcal/mol

Thermal vibrational correction ... 0.00427203 Eh 2.68 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

-----------------------------------------------------------------------

Total thermal energy -309.11411919 Eh

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ENTHALPY

--------

The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -309.11411919 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

-----------------------------------------------------------------------

Total Enthalpy ... -309.11317498 Eh

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GIBBS FREE ENERGY

-------------------

The Gibbs free energy is G = H - T\*S

Total enthalpy ... -309.11317498 Eh

Total entropy correction ... -0.03921474 Eh -24.61 kcal/mol

-----------------------------------------------------------------------

Final Gibbs free energy ... -309.15238972 Eh

**O(3P) Addition Transition State: TS H**

M06-2X/GCP(DFT/6-31G(d))

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CARTESIAN COORDINATES (ANGSTROEM)

---------------------------------

C -0.052262 -0.404272 -0.144394

C 0.255556 0.944018 -0.355006

C 0.983265 -1.279283 0.192615

H -0.533858 1.648691 -0.583281

H 0.754329 -2.323185 0.371442

C 1.559724 1.393618 -0.247626

C 2.290099 -0.830021 0.297244

H 1.781273 2.440609 -0.409039

H 3.080199 -1.522701 0.556328

C 2.582449 0.508282 0.075156

H 3.600918 0.864176 0.160056

C -1.412994 -0.923332 -0.249791

H -1.562665 -1.928310 0.131084

C -2.480161 -0.256786 -0.733737

H -2.391949 0.712219 -1.204117

H -3.444868 -0.739859 -0.803037

O -2.970818 0.617570 1.179055

-----------------------

VIBRATIONAL FREQUENCIES

-----------------------

Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: -374.26 cm\*\*-1 \*\*\*imaginary mode\*\*\*

7: 25.07 cm\*\*-1

8: 66.24 cm\*\*-1

9: 152.77 cm\*\*-1

10: 243.33 cm\*\*-1

11: 291.67 cm\*\*-1

12: 409.61 cm\*\*-1

13: 448.14 cm\*\*-1

14: 481.44 cm\*\*-1

15: 556.52 cm\*\*-1

16: 627.43 cm\*\*-1

17: 697.48 cm\*\*-1

18: 723.33 cm\*\*-1

19: 797.03 cm\*\*-1

20: 816.50 cm\*\*-1

21: 864.20 cm\*\*-1

22: 946.91 cm\*\*-1

23: 951.67 cm\*\*-1

24: 981.18 cm\*\*-1

25: 1010.39 cm\*\*-1

26: 1012.65 cm\*\*-1

27: 1033.37 cm\*\*-1

28: 1038.51 cm\*\*-1

29: 1062.60 cm\*\*-1

30: 1113.14 cm\*\*-1

31: 1165.41 cm\*\*-1

32: 1191.64 cm\*\*-1

33: 1235.26 cm\*\*-1

34: 1294.72 cm\*\*-1

35: 1333.12 cm\*\*-1

36: 1354.05 cm\*\*-1

37: 1429.58 cm\*\*-1

38: 1485.76 cm\*\*-1

39: 1535.00 cm\*\*-1

40: 1620.14 cm\*\*-1

41: 1665.40 cm\*\*-1

42: 1683.75 cm\*\*-1

43: 3171.33 cm\*\*-1

44: 3178.40 cm\*\*-1

45: 3189.06 cm\*\*-1

46: 3196.94 cm\*\*-1

47: 3206.18 cm\*\*-1

48: 3213.50 cm\*\*-1

49: 3220.29 cm\*\*-1

50: 3268.71 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -384.21940649 Eh

Zero point energy ... 0.13433064 Eh 84.29 kcal/mol

Thermal vibrational correction ... 0.00435491 Eh 2.73 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

-----------------------------------------------------------------------

Total thermal energy -384.07788840 Eh

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ENTHALPY

--------

The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -384.07788840 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

-----------------------------------------------------------------------

Total Enthalpy ... -384.07694419 Eh

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GIBBS FREE ENERGY

-------------------

The Gibbs free energy is G = H - T\*S

Total enthalpy ... -384.07694419 Eh

Total entropy correction ... -0.04104838 Eh -25.76 kcal/mol

-----------------------------------------------------------------------

Final Gibbs free energy ... -384.11799257 Eh

**O(3P) Addition Transition State: TS ad1**

M06-2X/GCP(DFT/6-31G(d))

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CARTESIAN COORDINATES (ANGSTROEM)

---------------------------------

C -0.052262 -0.404272 -0.144394

C 0.255556 0.944018 -0.355006

C 0.983265 -1.279283 0.192615

H -0.533858 1.648691 -0.583281

H 0.754329 -2.323185 0.371442

C 1.559724 1.393618 -0.247626

C 2.290099 -0.830021 0.297244

H 1.781273 2.440609 -0.409039

H 3.080199 -1.522701 0.556328

C 2.582449 0.508282 0.075156

H 3.600918 0.864176 0.160056

C -1.412994 -0.923332 -0.249791

H -1.562665 -1.928310 0.131084

C -2.480161 -0.256786 -0.733737

H -2.391949 0.712219 -1.204117

H -3.444868 -0.739859 -0.803037

O -2.970818 0.617570 1.179055

-----------------------

VIBRATIONAL FREQUENCIES

-----------------------

Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: -373.96 cm\*\*-1 \*\*\*imaginary mode\*\*\*

7: 25.30 cm\*\*-1

8: 66.11 cm\*\*-1

9: 152.04 cm\*\*-1

10: 233.69 cm\*\*-1

11: 272.71 cm\*\*-1

12: 409.49 cm\*\*-1

13: 440.15 cm\*\*-1

14: 468.86 cm\*\*-1

15: 549.67 cm\*\*-1

16: 627.32 cm\*\*-1

17: 676.70 cm\*\*-1

18: 710.22 cm\*\*-1

19: 789.91 cm\*\*-1

20: 808.23 cm\*\*-1

21: 859.61 cm\*\*-1

22: 865.44 cm\*\*-1

23: 895.89 cm\*\*-1

24: 949.18 cm\*\*-1

25: 956.95 cm\*\*-1

26: 1010.36 cm\*\*-1

27: 1012.61 cm\*\*-1

28: 1037.75 cm\*\*-1

29: 1058.99 cm\*\*-1

30: 1104.73 cm\*\*-1

31: 1119.02 cm\*\*-1

32: 1165.39 cm\*\*-1

33: 1192.26 cm\*\*-1

34: 1242.81 cm\*\*-1

35: 1325.61 cm\*\*-1

36: 1353.82 cm\*\*-1

37: 1414.91 cm\*\*-1

38: 1484.13 cm\*\*-1

39: 1533.15 cm\*\*-1

40: 1608.02 cm\*\*-1

41: 1661.83 cm\*\*-1

42: 1683.49 cm\*\*-1

43: 2352.85 cm\*\*-1

44: 3173.49 cm\*\*-1

45: 3189.00 cm\*\*-1

46: 3196.94 cm\*\*-1

47: 3206.16 cm\*\*-1

48: 3213.49 cm\*\*-1

49: 3220.28 cm\*\*-1

50: 3268.19 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -384.21940648 Eh

Zero point energy ... 0.13113460 Eh 82.29 kcal/mol

Thermal vibrational correction ... 0.00449232 Eh 2.82 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

-----------------------------------------------------------------------

Total thermal energy -384.08094703 Eh

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ENTHALPY

--------

The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -384.08094703 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

-----------------------------------------------------------------------

Total Enthalpy ... -384.08000282 Eh

-------------------

GIBBS FREE ENERGY

-------------------

The Gibbs free energy is G = H - T\*S

Total enthalpy ... -384.08000282 Eh

Total entropy correction ... -0.04130540 Eh -25.92 kcal/mol

-----------------------------------------------------------------------

Final Gibbs free energy ... -384.12130822 Eh

**O(3P) Addition Transition State: TS bd2**

M06-2X/GCP(DFT/6-31G(d))

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CARTESIAN COORDINATES (ANGSTROEM)

---------------------------------

C -0.052262 -0.404272 -0.144394

C 0.255556 0.944018 -0.355006

C 0.983265 -1.279283 0.192615

H -0.533858 1.648691 -0.583281

H 0.754329 -2.323185 0.371442

C 1.559724 1.393618 -0.247626

C 2.290099 -0.830021 0.297244

H 1.781273 2.440609 -0.409039

H 3.080199 -1.522701 0.556328

C 2.582449 0.508282 0.075156

H 3.600918 0.864176 0.160056

C -1.412994 -0.923332 -0.249791

H -1.562665 -1.928310 0.131084

C -2.480161 -0.256786 -0.733737

H -2.391949 0.712219 -1.204117

H -3.444868 -0.739859 -0.803037

O -2.970818 0.617570 1.179055

-----------------------

VIBRATIONAL FREQUENCIES

-----------------------

Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: -371.95 cm\*\*-1 \*\*\*imaginary mode\*\*\*

7: 25.81 cm\*\*-1

8: 66.11 cm\*\*-1

9: 150.42 cm\*\*-1

10: 227.37 cm\*\*-1

11: 279.96 cm\*\*-1

12: 409.10 cm\*\*-1

13: 425.20 cm\*\*-1

14: 459.76 cm\*\*-1

15: 515.83 cm\*\*-1

16: 603.66 cm\*\*-1

17: 627.24 cm\*\*-1

18: 708.48 cm\*\*-1

19: 719.13 cm\*\*-1

20: 750.07 cm\*\*-1

21: 791.73 cm\*\*-1

22: 863.77 cm\*\*-1

23: 911.04 cm\*\*-1

24: 921.08 cm\*\*-1

25: 960.02 cm\*\*-1

26: 1009.92 cm\*\*-1

27: 1012.46 cm\*\*-1

28: 1026.85 cm\*\*-1

29: 1037.83 cm\*\*-1

30: 1060.44 cm\*\*-1

31: 1115.35 cm\*\*-1

32: 1165.40 cm\*\*-1

33: 1192.24 cm\*\*-1

34: 1239.55 cm\*\*-1

35: 1305.29 cm\*\*-1

36: 1333.70 cm\*\*-1

37: 1354.99 cm\*\*-1

38: 1478.81 cm\*\*-1

39: 1531.10 cm\*\*-1

40: 1578.95 cm\*\*-1

41: 1663.93 cm\*\*-1

42: 1683.46 cm\*\*-1

43: 2323.96 cm\*\*-1

44: 2442.51 cm\*\*-1

45: 3176.93 cm\*\*-1

46: 3189.06 cm\*\*-1

47: 3196.91 cm\*\*-1

48: 3206.16 cm\*\*-1

49: 3213.49 cm\*\*-1

50: 3220.29 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -384.21940649 Eh

Zero point energy ... 0.12791803 Eh 80.27 kcal/mol

Thermal vibrational correction ... 0.00465014 Eh 2.92 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

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Total thermal energy -384.08400578 Eh

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ENTHALPY

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The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -384.08400578 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

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Total Enthalpy ... -384.08306157 Eh

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GIBBS FREE ENERGY

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The Gibbs free energy is G = H - T\*S

Total enthalpy ... -384.08306157 Eh

Total entropy correction ... -0.04157517 Eh -26.09 kcal/mol

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Final Gibbs free energy ... -384.12463674 Eh

**O(3P) Addition Transition State: TS d3**

M06-2X/GCP(DFT/6-31G(d))

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CARTESIAN COORDINATES (ANGSTROEM)

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C -0.052262 -0.404272 -0.144394

C 0.255556 0.944018 -0.355006

C 0.983265 -1.279283 0.192615

H -0.533858 1.648691 -0.583281

H 0.754329 -2.323185 0.371442

C 1.559724 1.393618 -0.247626

C 2.290099 -0.830021 0.297244

H 1.781273 2.440609 -0.409039

H 3.080199 -1.522701 0.556328

C 2.582449 0.508282 0.075156

H 3.600918 0.864176 0.160056

C -1.412994 -0.923332 -0.249791

H -1.562665 -1.928310 0.131084

C -2.480161 -0.256786 -0.733737

H -2.391949 0.712219 -1.204117

H -3.444868 -0.739859 -0.803037

O -2.970818 0.617570 1.179055

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VIBRATIONAL FREQUENCIES

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Scaling factor for frequencies = 1.000000000 (already applied!)

0: 0.00 cm\*\*-1

1: 0.00 cm\*\*-1

2: 0.00 cm\*\*-1

3: 0.00 cm\*\*-1

4: 0.00 cm\*\*-1

5: 0.00 cm\*\*-1

6: -371.71 cm\*\*-1 \*\*\*imaginary mode\*\*\*

7: 26.00 cm\*\*-1

8: 65.97 cm\*\*-1

9: 149.67 cm\*\*-1

10: 221.42 cm\*\*-1

11: 260.71 cm\*\*-1

12: 408.96 cm\*\*-1

13: 417.95 cm\*\*-1

14: 453.55 cm\*\*-1

15: 511.26 cm\*\*-1

16: 603.37 cm\*\*-1

17: 627.18 cm\*\*-1

18: 702.01 cm\*\*-1

19: 714.90 cm\*\*-1

20: 740.90 cm\*\*-1

21: 753.44 cm\*\*-1

22: 809.59 cm\*\*-1

23: 837.63 cm\*\*-1

24: 864.05 cm\*\*-1

25: 954.58 cm\*\*-1

26: 999.25 cm\*\*-1

27: 1010.05 cm\*\*-1

28: 1012.38 cm\*\*-1

29: 1037.70 cm\*\*-1

30: 1050.74 cm\*\*-1

31: 1061.63 cm\*\*-1

32: 1116.08 cm\*\*-1

33: 1165.39 cm\*\*-1

34: 1193.35 cm\*\*-1

35: 1264.54 cm\*\*-1

36: 1325.13 cm\*\*-1

37: 1353.90 cm\*\*-1

38: 1478.77 cm\*\*-1

39: 1523.48 cm\*\*-1

40: 1564.26 cm\*\*-1

41: 1661.29 cm\*\*-1

42: 1683.31 cm\*\*-1

43: 2317.49 cm\*\*-1

44: 2358.73 cm\*\*-1

45: 2442.54 cm\*\*-1

46: 3189.00 cm\*\*-1

47: 3196.91 cm\*\*-1

48: 3206.15 cm\*\*-1

49: 3213.48 cm\*\*-1

50: 3220.29 cm\*\*-1

Summary of contributions to the inner energy U:

Electronic energy ... -384.21940649 Eh

Zero point energy ... 0.12471369 Eh 78.26 kcal/mol

Thermal vibrational correction ... 0.00478667 Eh 3.00 kcal/mol

Thermal rotational correction ... 0.00141627 Eh 0.89 kcal/mol

Thermal translational correction ... 0.00141627 Eh 0.89 kcal/mol

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Total thermal energy -384.08707358 Eh

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ENTHALPY

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The enthalpy is H = U + kB\*T

kB is Boltzmann's constant

Total free energy ... -384.08707358 Eh

Thermal Enthalpy correction ... 0.00094421 Eh 0.59 kcal/mol

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Total Enthalpy ... -384.08612937 Eh

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GIBBS FREE ENERGY

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The Gibbs free energy is G = H - T\*S

Total enthalpy ... -384.08612937 Eh

Total entropy correction ... -0.04182688 Eh -26.25 kcal/mol

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Final Gibbs free energy ... -384.12795625 Eh