Supporting Information for

Formation Mechanisms of Naphthalene and Indene: From the Interstellar Medium to Combustion Flames

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Table S1. Parameters of the fitted modified Arrhenius expressions, $A*T^{\alpha}*\exp(-E_a/RT)$, for $C_6H_5 + C_4H_4$ and $C_6H_5C_4H_3 + H$ reactions at pressures of 30 Torr, 1, 10, and 100 atm.

The data are presented in the following order:

/ *p*,atm A, $cm^3\ mol^{-1}\ s^{-1}$ α E_a, $cal\ mol^{-1}$/ ! fit btw. T_1 and T_2 with MAE = mean/max absolute error

The title line for each reaction shows A, α, and E_a at the high-pressure limit.

The fits are provided to a single Arrhenius expression and to a sum of two Arrhenius expressions

$C_6H_5 + C_4H_4$ (R1) → $C_{10}H_9$ (W1) 4.83E+08 0.95 1770.0

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PLOG/3.947E-02   1.75E+36    -7.53   12490.0/          ! fit btw. 500 and 1375 K with MAE of 16.0%, 29.2%
PLOG/1.000E+00   7.10E+20    -2.74   6896.0/           ! fit btw. 500 and 1650 K with MAE of 15.8%, 40.0%
PLOG/1.000E+01   8.52E+10     0.27   2708.0/           ! fit btw. 500 and 1800 K with MAE of 10.4%, 24.8%
PLOG/1.000E+02   4.83E+08     0.95   1770.0/           ! fit btw. 500 and 2250 K with MAE of 9.6%, 35.0%

PLOG/3.947E-02   3.62E+84   -21.48   42190.0/
PLOG/3.947E-02   2.16E+43   -10.07   12890.0/          ! fit btw. 500 and 1375 K with MAE of 1.9%, 4.6%
PLOG/1.000E+00   2.63E+69   -16.52   40770.0/
PLOG/1.000E+00   2.89E+26    -4.68   7584.0/           ! fit btw. 500 and 1650 K with MAE of 2.8%, 6.0%
PLOG/1.000E+01   7.59E+49   -10.65   32900.0/
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PLOG/1.000E+01 1.04E+17 -1.72 4254.0/ ! fit btw. 500 and 1800 K with MAE of 2.5%, 4.6%
PLOG/1.000E+02 1.35E+27 -4.11 18320.0/
PLOG/1.000E+02 1.27E+20 -2.72 5193.0/ ! fit btw. 500 and 2250 K with MAE of 3.7%, 12.1%

$C_6H_5 + C_4H_4$ (R1) → $C_{10}H_9$ (W2) 1.20E+21 -2.54 10670.0

PLOG/3.947E-02 9.74E-01 2.90 -2716.0/ ! fit btw. 500 and 800 K with MAE of 4.3%, 7.4%
PLOG/1.000E+00 5.19E+42 -9.67 16100.0/ ! fit btw. 500 and 1000 K with MAE of 1.6%, 2.7%
PLOG/1.000E+01 5.68E+30 -5.65 13550.0/ ! fit btw. 500 and 1250 K with MAE of 5.8%, 10.0%
PLOG/1.000E+02 1.20E+21 -2.54 10670.0/ ! fit btw. 500 and 1650 K with MAE of 10.1%, 21.8%

PLOG/3.947E-02 9.74E-01 2.90 -2716.0/
PLOG/3.947E-02 0.00E+00 0.00 0.0/ ! fit btw. 500 and 800 K with MAE of 4.3%, 7.4%
PLOG/1.000E+00 5.19E+42 -9.67 16100.0/
PLOG/1.000E+00 0.00E+00 0.00 0.0/ ! fit btw. 500 and 1000 K with MAE of 1.6%, 2.7%
PLOG/1.000E+01 5.11E+71 -17.71 36780.0/
PLOG/1.000E+01 7.14E+25 -4.30 10590.0/ ! fit btw. 500 and 1250 K with MAE of 0.1%, 0.2%
PLOG/1.000E+02 6.21E+50 -10.96 31890.0/
PLOG/1.000E+02 2.19E+26 -4.37 11290.0/ ! fit btw. 500 and 1650 K with MAE of 1.3%, 2.2%

$C_6H_5 + C_4H_4$ (R1) → $C_{10}H_9$ (W3) 8.33E+15 -1.22 6435.0

PLOG/3.947E-02 7.42E+56 -14.00 21160.0/ ! fit btw. 500 and 1250 K with MAE of 14.3%, 24.2%
PLOG/1.000E+00 6.45E+33 -6.75 13200.0/ ! fit btw. 500 and 1375 K with MAE of 15.6%, 28.6%
PLOG/1.000E+01 1.49E+26 -4.34 10660.0/ ! fit btw. 500 and 1650 K with MAE of 18.4%, 45.3%
PLOG/1.000E+02 8.33E+15 -1.22 6435.0/ ! fit btw. 500 and 1800 K with MAE of 12.7%, 21.5%

PLOG/3.947E-02 1.93E+100 -26.66 46050.0/
PLOG/3.947E-02 1.20E+63 -16.41 20390.0/ ! fit btw. 500 and 1250 K with MAE of 0.7%, 2.6%
PLOG/1.000E+00 3.90E+83 -21.12 43890.0/
PLOG/1.000E+00 5.27E+40 -9.21 13650.0/ ! fit btw. 500 and 1375 K with MAE of 1.6%, 3.8%
PLOG/1.000E+01 3.28E+59 -13.82 33050.0/
PLOG/1.000E+01 4.59E+49 -12.04 16650.0/ ! fit btw. 500 and 1650 K with MAE of 4.1%, 11.3%
PLOG/1.000E+02 7.99E+47 -10.20 30490.0/

PLOG/1.000E+02 1.09E+23 -3.60 7851.0/ ! fit btw. 500 and 1800 K with MAE of 2.8%, 8.3%

$C_6H_5 + C_4H_4$ (R1) → $C_{10}H_9$ (W9) 9.41E+18 -1.53 19050.0

PLOG/3.947E-02 3.58E+60 -14.82 25440.0/ ! fit btw. 500 and 1250 K with MAE of 12.5%, 20.1%
PLOG/1.000E+00 1.09E+47 -10.20 24940.0/ ! fit btw. 500 and 1500 K with MAE of 13.3%, 20.4%
PLOG/1.000E+01 1.78E+33 -5.82 22730.0/ ! fit btw. 500 and 1650 K with MAE of 21.2%, 48.6%
PLOG/1.000E+02 9.41E+18 -1.53 19050.0/ ! fit btw. 500 and 2000 K with MAE of 26.4%, 69.0%

PLOG/3.947E-02 1.12E+104 -27.48 50700.0/
PLOG/3.947E-02 5.90E+66 -17.14 25190.0/ ! fit btw. 500 and 1250 K with MAE of 0.5%, 1.5%
PLOG/1.000E+00 1.16E+89 -22.37 50870.0/
PLOG/1.000E+00 2.39E+40 -8.41 20600.0/ ! fit btw. 500 and 1500 K with MAE of 3.0%, 7.7%
PLOG/1.000E+01 1.83E+69 -16.09 46530.0/
PLOG/1.000E+01 6.19E+36 -7.38 20950.0/ ! fit btw. 500 and 1650 K with MAE of 4.6%, 12.6%
PLOG/1.000E+02 2.54E+51 -10.64 42550.0/
PLOG/1.000E+02 1.24E+19 -2.03 15810.0/ ! fit btw. 500 and 2000 K with MAE of 5.6%, 16.9%

$C_6H_5 + C_4H_4$ (R1) → $C_{10}H_9$ (W14) 2.67E+10 0.42 5020.0

PLOG/3.947E-02 5.79E-30 11.82 -14160.0/ ! fit btw. 500 and 800 K with MAE of 7.9%, 13.7%
PLOG/1.000E+00 5.61E+28 -5.59 9901.0/ ! fit btw. 500 and 1000 K with MAE of 2.4%, 5.5%
PLOG/1.000E+01 3.12E+18 -2.15 7614.0/ ! fit btw. 500 and 1250 K with MAE of 2.9%, 5.4%
PLOG/1.000E+02 2.67E+10 0.42 5020.0/ ! fit btw. 500 and 1650 K with MAE of 4.4%, 8.9%

PLOG/3.947E-02 5.79E-30 11.82 -14160.0/
PLOG/3.947E-02 0.00E+00 0.00 0.0/ ! fit btw. 500 and 800 K with MAE of 7.9%, 13.7%
PLOG/1.000E+00 5.61E+28 -5.59 9901.0/
PLOG/1.000E+00 0.00E+00 0.00 0.0/ ! fit btw. 500 and 1000 K with MAE of 2.4%, 5.5%
PLOG/1.000E+01 3.05E+25 -4.19 11700.0/
PLOG/1.000E+01 5.61E+12 -1.02 2055.0/ ! fit btw. 500 and 1250 K with MAE of 0.6%, 1.5%
PLOG/1.000E+02 4.98E+26 -4.17 17780.0/
PLOG/1.000E+02 1.10E+15 -1.16 5818.0/ ! fit btw. 500 and 1650 K with MAE of 0.4%, 0.6%

C_6H_5 + C_4H_4 (R1) → $C_{10}H_9$ (W16) 1.28E+05 2.20 11510.0

PLOG/3.947E-02 8.27E+35 -7.52 15310.0/ ! fit btw. 500 and 1125 K with MAE of 6.9%, 10.6%
PLOG/1.000E+00 5.01E+35 -7.08 19620.0/ ! fit btw. 500 and 1375 K with MAE of 9.9%, 19.0%
PLOG/1.000E+01 8.62E+23 -3.37 17940.0/ ! fit btw. 500 and 1650 K with MAE of 19.3%, 50.9%
PLOG/1.000E+02 1.28E+05 2.20 11510.0/ ! fit btw. 500 and 2000 K with MAE of 19.1%, 40.5%

PLOG/3.947E-02 6.08E+80 -20.63 41150.0/
PLOG/3.947E-02 6.10E+48 -11.78 18430.0/ ! fit btw. 500 and 1125 K with MAE of 1.1%, 2.5%
PLOG/1.000E+00 3.05E+67 -16.24 39650.0/
PLOG/1.000E+00 1.81E+42 -9.42 20090.0/ ! fit btw. 500 and 1375 K with MAE of 3.1%, 6.3%
PLOG/1.000E+01 4.25E+59 -13.53 41900.0/
PLOG/1.000E+01 1.74E+29 -5.40 17340.0/ ! fit btw. 500 and 1650 K with MAE of 7.5%, 24.6%
PLOG/1.000E+02 1.75E+52 -11.34 42480.0/
PLOG/1.000E+02 2.21E-03 4.37 6920.0/ ! fit btw. 500 and 2000 K with MAE of 8.9%, 35.7%

C_6H_5 + C_4H_4 (R1) → total 4.68E+08 1.21 3057.0
PLOG/3.947E-02 5.53E+07 1.46 2386.0/ ! fit btw. 500 and 2500 K with MAE of 4.7%, 9.6%
PLOG/1.000E+00 1.66E+08 1.32 2668.0/ ! fit btw. 500 and 2500 K with MAE of 5.5%, 11.1%
PLOG/1.000E+01 4.02E+08 1.22 2922.0/ ! fit btw. 500 and 2500 K with MAE of 7.3%, 13.0%
PLOG/1.000E+02 4.68E+08 1.21 3057.0/ ! fit btw. 500 and 2500 K with MAE of 9.3%, 16.6%

PLOG/3.947E-02 3.98E+15 -0.77 9299.0/
PLOG/3.947E-02 5.32E+05 1.90 453.3/ ! fit btw. 500 and 2500 K with MAE of 0.2%, 0.4%
PLOG/1.000E+00 2.21E+26 -3.87 16580.0/
PLOG/1.000E+00 1.60E+05 2.12 587.6/ ! fit btw. 500 and 2500 K with MAE of 0.2%, 0.5%
PLOG/1.000E+01 1.90E+34 -6.08 22780.0/
PLOG/1.000E+01 6.20E+05 1.96 955.3/ ! fit btw. 500 and 2500 K with MAE of 0.7%, 1.7%
PLOG/1.000E+02 1.81E+29 -4.54 20720.0/
PLOG/1.000E+02 2.14E+07 1.49 1535.0/ ! fit btw. 500 and 2500 K with MAE of 0.9%, 1.7%

C_6H_5 + C_4H_4 (R1) → indene + H (P1) 8.56E-13 7.21 23420.0

PLOG/3.947E-02 1.37E+52 -11.54 37740.0/ ! fit btw. 500 and 2500 K with MAE of 17.6%, 32.1%

PLOG/1.000E+00 2.74E+59 -13.26 52900.0/ ! fit btw. 600 and 2500 K with MAE of 16.1%, 40.5%
PLOG/1.000E+01 4.52E+49 -10.24 56130.0/ ! fit btw. 600 and 2500 K with MAE of 35.7%, 83.5%
PLOG/1.000E+02 8.56E-13 7.21 23420.0/ ! fit btw. 500 and 2500 K with MAE of 193.0%, 946.9%

PLOG/3.947E-02 3.05E+84 -20.96 56410.0/
PLOG/3.947E-02 1.61E+32 -5.92 26750.0/ ! fit btw. 500 and 2500 K with MAE of 2.0%, 5.3%
PLOG/1.000E+00 5.42E+191 -55.82 91430.0/
PLOG/1.000E+00 1.01E+67 -15.36 58800.0/ ! fit btw. 600 and 2500 K with MAE of 7.5%, 17.2%
PLOG/1.000E+01 2.78E+62 -15.14 52980.0/
PLOG/1.000E+01 3.80E+74 -17.11 76440.0/ ! fit btw. 600 and 2500 K with MAE of 4.3%, 14.0%
PLOG/1.000E+02 3.33E-73 23.50 -16820.0/
PLOG/1.000E+02 5.40E+51 -10.55 70860.0/ ! fit btw. 500 and 2500 K with MAE of 27.1%, 73.7%

C_6H_5 + C_4H_4 (R1) → cis-1-phenyl-vinylacetylene + H (P2) 1.09E+07 2.09 31190.0

PLOG/3.947E-02 1.98E+35 -6.42 28920.0/ ! fit btw. 500 and 2500 K with MAE of 14.1%, 29.2%
PLOG/1.000E+00 3.56E+34 -6.00 34800.0/ ! fit btw. 500 and 2500 K with MAE of 23.3%, 57.8%
PLOG/1.000E+01 1.34E+27 -3.72 36550.0/ ! fit btw. 500 and 2500 K with MAE of 41.5%, 100.5%
PLOG/1.000E+02 1.09E+07 2.09 31190.0/ ! fit btw. 500 and 2500 K with MAE of 55.9%, 134.6%

PLOG/3.947E-02 3.16E+75 -18.09 53030.0/
PLOG/3.947E-02 2.11E+22 -2.77 21620.0/ ! fit btw. 500 and 2500 K with MAE of 0.9%, 2.7%
PLOG/1.000E+00 3.46E+63 -14.19 55500.0/
PLOG/1.000E+00 2.71E+19 -1.87 25250.0/ ! fit btw. 500 and 2500 K with MAE of 2.1%, 4.1%
PLOG/1.000E+01 3.02E+48 -9.65 52910.0/
PLOG/1.000E+01 1.89E+39 -8.51 34000.0/ ! fit btw. 500 and 2500 K with MAE of 5.9%, 10.9%
PLOG/1.000E+02 1.00E-02 4.19 22630.0/
PLOG/1.000E+02 5.28E+50 -10.01 65610.0/ ! fit btw. 500 and 2500 K with MAE of 6.6%, 19.7%

C_6H_5 + C_4H_4 (R1) → trans-1-phenyl-vinylacetylene + H (P3) 3.80E-10 6.78 14680.0

PLOG/3.947E-02 1.30E+34 -5.84 27490.0/ ! fit btw. 500 and 2500 K with MAE of 13.9%, 32.6%
PLOG/1.000E+00 7.09E+28 -4.16 30020.0/ ! fit btw. 500 and 2500 K with MAE of 35.0%, 99.4%
PLOG/1.000E+01 4.29E+12 0.54 24600.0/ ! fit btw. 500 and 2500 K with MAE of 58.7%, 136.0%

PLOG/1.000E+02 3.80E-10 6.78 14680.0/ ! fit btw. 500 and 2500 K with MAE of 49.8%, 138.2%

PLOG/3.947E-02 1.81E+69 -16.03 48640.0/
PLOG/3.947E-02 4.18E+19 -1.76 19320.0/ ! fit btw. 500 and 2500 K with MAE of 1.2%, 3.1%
PLOG/1.000E+00 6.16E+46 -9.15 43460.0/
PLOG/1.000E+00 4.60E+60 -15.29 33300.0/ ! fit btw. 500 and 2500 K with MAE of 5.4%, 12.4%
PLOG/1.000E+01 1.71E+02 2.96 14790.0/
PLOG/1.000E+01 1.53E+53 -10.70 56220.0/ ! fit btw. 500 and 2500 K with MAE of 4.8%, 13.7%
PLOG/1.000E+02 1.23E+47 -8.81 61090.0/
PLOG/1.000E+02 1.37E-13 7.42 10080.0/ ! fit btw. 500 and 2500 K with MAE of 6.3%, 15.6%

C_6H_5 + C_4H_4 (R1) → 4-phenyl-vinylacetylene + H (P4) 2.70E+09 1.49 22140.0

PLOG/3.947E-02 5.12E+31 -5.17 23300.0/ ! fit btw. 500 and 2500 K with MAE of 11.1%, 20.9%
PLOG/1.000E+00 7.58E+32 -5.33 28730.0/ ! fit btw. 500 and 2500 K with MAE of 20.3%, 57.9%
PLOG/1.000E+01 3.43E+24 -2.85 27580.0/ ! fit btw. 500 and 2500 K with MAE of 39.8%, 98.4%
PLOG/1.000E+02 2.70E+09 1.49 22140.0/ ! fit btw. 500 and 2500 K with MAE of 46.6%, 119.5%

PLOG/3.947E-02 9.34E+36 -6.72 25850.0/
PLOG/3.947E-02 4.63E+76 -16.56 96340.0/ ! fit btw. 500 and 2500 K with MAE of 5.0%, 18.5%
PLOG/1.000E+00 6.43E+41 -7.82 35290.0/
PLOG/1.000E+00 1.72E+175 -51.49 69040.0/ ! fit btw. 500 and 2500 K with MAE of 6.7%, 16.3%
PLOG/1.000E+01 6.42E+56 -11.85 52060.0/
PLOG/1.000E+01 7.94E+08 1.28 16580.0/ ! fit btw. 500 and 2500 K with MAE of 3.3%, 7.1%
PLOG/1.000E+02 2.26E+35 -5.68 42490.0/
PLOG/1.000E+02 4.66E+27 -4.96 23290.0/ ! fit btw. 500 and 2500 K with MAE of 10.3%, 28.6%

C_6H_5 + C_4H_4 (R1) → phenyl-butatriene + H (P5) 1.41E+07 1.68 27640.0

PLOG/3.947E-02 3.65E+18 -1.91 22910.0/ ! fit btw. 500 and 2500 K with MAE of 12.6%, 22.6%
PLOG/1.000E+00 1.39E+23 -3.06 29830.0/ ! fit btw. 500 and 2500 K with MAE of 14.4%, 34.3%
PLOG/1.000E+01 7.35E+18 -1.73 30920.0/ ! fit btw. 500 and 2500 K with MAE of 29.1%, 78.0%
PLOG/1.000E+02 1.41E+07 1.68 27640.0/ ! fit btw. 500 and 2500 K with MAE of 43.8%, 91.0%

PLOG/3.947E-02 2.42E+27 -4.54 27070.0/
PLOG/3.947E-02 1.60E+39 -7.04 60180.0/ ! fit btw. 500 and 2500 K with MAE of 2.8%, 10.3%
PLOG/1.000E+00 7.65E+26 -4.11 32520.0/
PLOG/1.000E+00 9.23E+128 -39.42 47670.0/ ! fit btw. 500 and 2500 K with MAE of 8.8%, 18.5%
PLOG/1.000E+01 2.11E+34 -6.03 42520.0/
PLOG/1.000E+01 3.54E+70 -18.97 42100.0/ ! fit btw. 500 and 2500 K with MAE of 5.5%, 12.4%
PLOG/1.000E+02 6.23E+31 -5.14 46860.0/
PLOG/1.000E+02 6.96E+23 -4.33 27970.0/ ! fit btw. 500 and 2500 K with MAE of 8.4%, 14.5%

C_6H_5 + C_4H_4 (R1) → 2-phenyl-vinylacetylene + H (P6) 5.61E-01 3.92 19370.0

PLOG/3.947E-02 4.77E+17 -1.39 21100.0/ ! fit btw. 500 and 2500 K with MAE of 14.5%, 36.4%
PLOG/1.000E+00 1.02E+12 0.30 20560.0/ ! fit btw. 500 and 2500 K with MAE of 19.8%, 37.1%
PLOG/1.000E+01 1.01E+09 1.23 21600.0/ ! fit btw. 500 and 2500 K with MAE of 22.3%, 44.2%
PLOG/1.000E+02 5.61E-01 3.92 19370.0/ ! fit btw. 500 and 2500 K with MAE of 29.3%, 69.0%

PLOG/3.947E-02 1.78E+21 -2.39 23660.0/
PLOG/3.947E-02 7.93E+04 -3.40 -20220.0/ ! fit btw. 500 and 2500 K with MAE of 9.8%, 18.0%
PLOG/1.000E+00 3.35E+49 -10.24 48890.0/
PLOG/1.000E+00 5.51E+04 2.26 15650.0/ ! fit btw. 500 and 2500 K with MAE of 1.4%, 3.9%
PLOG/1.000E+01 6.67E+27 -3.97 36910.0/
PLOG/1.000E+01 6.89E+07 1.14 17980.0/ ! fit btw. 500 and 2500 K with MAE of 2.8%, 5.8%
PLOG/1.000E+02 3.62E+25 -3.21 40420.0/
PLOG/1.000E+02 5.85E-01 3.48 16210.0/ ! fit btw. 500 and 2500 K with MAE of 4.2%, 12.1%

cis-1-phenyl-vinylacetylene + H (P2) → $C_{10}H_9$ (W21) 1.04E+24 -2.80 8378.0

PLOG/3.947E-02 1.04E+74 -18.95 22450.0/ ! fit btw. 500 and 1125 K with MAE of 4.8%, 10.3%
PLOG/1.000E+00 2.25E+43 -8.93 14090.0/ ! fit btw. 500 and 1375 K with MAE of 12.5%, 20.9%
PLOG/1.000E+01 2.00E+35 -6.25 12690.0/ ! fit btw. 500 and 1650 K with MAE of 11.9%, 29.1%
PLOG/1.000E+02 1.04E+24 -2.80 8378.0/ ! fit btw. 500 and 2000 K with MAE of 37.1%, 235.7%

PLOG/3.947E-02 9.29E+86 -22.77 29260.0/
PLOG/3.947E-02 1.89E+68 -18.15 14760.0/ ! fit btw. 500 and 1125 K with MAE of 0.3%, 0.8%

PLOG/1.000E+00 8.60E+81 -20.06 37990.0/
PLOG/1.000E+00 2.37E+49 -11.13 14150.0/ ! fit btw. 500 and 1375 K with MAE of 0.9%, 1.8%
PLOG/1.000E+01 1.44E+79 -18.62 44110.0/
PLOG/1.000E+01 1.87E+61 -14.45 21430.0/ ! fit btw. 500 and 1650 K with MAE of 1.7%, 3.5%
PLOG/1.000E+02 5.97E+26 -3.55 10840.0/
PLOG/1.000E+02 4.11E+21 -3.85 -3820.0/ ! fit btw. 500 and 2000 K with MAE of 31.6%, 154.8%

cis-1-phenyl-vinylacetylene + H (P2) → indene + H (P1) 1.50E+18 -0.95 15430.0

PLOG/3.947E-02 1.39E+35 -6.05 14750.0/ ! fit btw. 500 and 2500 K with MAE of 4.8%, 10.0%
PLOG/1.000E+00 2.40E+41 -7.67 22710.0/ ! fit btw. 500 and 2500 K with MAE of 17.3%, 44.3%
PLOG/1.000E+01 1.28E+33 -5.21 21710.0/ ! fit btw. 500 and 2500 K with MAE of 36.6%, 86.1%
PLOG/1.000E+02 1.50E+18 -0.95 15430.0/ ! fit btw. 500 and 2500 K with MAE of 30.5%, 80.4%

PLOG/3.947E-02 4.42E+38 -7.06 16830.0/
PLOG/3.947E-02 1.18E-15 7.83 -12950.0/ ! fit btw. 500 and 2500 K with MAE of 1.5%, 2.7%
PLOG/1.000E+00 8.21E+48 -9.77 28270.0/
PLOG/1.000E+00 4.88E+190 -55.83 66750.0/ ! fit btw. 500 and 2500 K with MAE of 6.5%, 17.4%
PLOG/1.000E+01 1.39E+66 -14.42 46740.0/
PLOG/1.000E+01 7.98E+18 -1.43 11810.0/ ! fit btw. 500 and 2500 K with MAE of 3.7%, 9.9%
PLOG/1.000E+02 6.77E+22 -2.22 19550.0/
PLOG/1.000E+02 2.36E+20 -2.53 10430.0/ ! fit btw. 500 and 2500 K with MAE of 22.8%, 76.6%

cis-1-phenyl-vinylacetylene + H (P2) → total 3.12E+12 0.64 2479.0

PLOG/3.947E-02 6.13E+11 0.83 1988.0/ ! fit btw. 500 and 2500 K with MAE of 0.9%, 1.6%
PLOG/1.000E+00 8.90E+11 0.78 2082.0/ ! fit btw. 500 and 2500 K with MAE of 1.2%, 2.3%
PLOG/1.000E+01 1.90E+12 0.69 2288.0/ ! fit btw. 500 and 2500 K with MAE of 1.9%, 3.5%
PLOG/1.000E+02 3.12E+12 0.64 2479.0/ ! fit btw. 500 and 2500 K with MAE of 3.5%, 5.8%

PLOG/3.947E-02 9.36E+77 -18.67 43150.0/
PLOG/3.947E-02 2.00E+11 0.97 1712.0/ ! fit btw. 500 and 2500 K with MAE of 0.2%, 0.8%
PLOG/1.000E+00 2.26E+81 -19.57 45790.0/
PLOG/1.000E+00 2.00E+11 0.97 1711.0/ ! fit btw. 500 and 2500 K with MAE of 0.3%, 0.8%

PLOG/1.000E+01 1.37E+74 -17.22 44470.0/
PLOG/1.000E+01 2.18E+11 0.96 1724.0/ ! fit btw. 500 and 2500 K with MAE of 0.3%, 1.0%
PLOG/1.000E+02 4.82E+45 -8.81 29490.0/
PLOG/1.000E+02 4.44E+11 0.86 1837.0/ ! fit btw. 500 and 2500 K with MAE of 0.4%, 1.2%

cis-1-phenyl-vinylacetylene + H (P2) → trans-1-phenyl-vinylacetylene + H (P3) 3.13E+16 0.15 26580.0

PLOG/3.947E-02 1.81E+28 -3.50 22730.0/ ! fit btw. 500 and 2500 K with MAE of 8.5%, 19.7%
PLOG/1.000E+00 3.92E+33 -4.89 29400.0/ ! fit btw. 500 and 2500 K with MAE of 18.6%, 50.6%
PLOG/1.000E+01 6.59E+28 -3.42 30130.0/ ! fit btw. 500 and 2500 K with MAE of 38.1%, 90.5%
PLOG/1.000E+02 3.13E+16 0.15 26580.0/ ! fit btw. 500 and 2500 K with MAE of 48.4%, 125.0%

PLOG/3.947E-02 1.70E+45 -8.35 34740.0/
PLOG/3.947E-02 1.30E+20 -1.29 17590.0/ ! fit btw. 500 and 2500 K with MAE of 0.4%, 0.8%
PLOG/1.000E+00 5.42E+42 -7.44 36170.0/
PLOG/1.000E+00 1.96E+124 -34.58 53260.0/ ! fit btw. 500 and 2500 K with MAE of 3.8%, 9.1%
PLOG/1.000E+01 1.10E+62 -12.69 55370.0/
PLOG/1.000E+01 1.72E+14 0.44 19880.0/ ! fit btw. 500 and 2500 K with MAE of 2.7%, 7.8%
PLOG/1.000E+02 -4.49E+48 -9.39 40650.0/
PLOG/1.000E+02 8.24E+28 -3.42 31610.0/ ! fit btw. 500 and 2500 K with MAE of 17.4%, 41.3%

trans-1-phenyl-vinylacetylene + H (P3) → $C_{10}H_9$ (W1) 9.79E+13 0.01 5337.0

PLOG/3.947E-02 1.32E+38 -7.35 15160.0/ ! fit btw. 500 and 1375 K with MAE of 18.9%, 34.9%
PLOG/1.000E+00 2.86E+22 -2.55 8913.0/ ! fit btw. 500 and 1650 K with MAE of 16.4%, 44.1%
PLOG/1.000E+01 5.63E+14 -0.23 5550.0/ ! fit btw. 500 and 1800 K with MAE of 8.7%, 17.7%
PLOG/1.000E+02 9.79E+13 0.01 5337.0/ ! fit btw. 500 and 2250 K with MAE of 9.2%, 29.1%

PLOG/3.947E-02 3.36E+91 -22.77 47640.0/
PLOG/3.947E-02 1.40E+45 -9.91 15250.0/ ! fit btw. 500 and 1375 K with MAE of 2.2%, 6.2%
PLOG/1.000E+00 3.23E+79 -18.72 48990.0/
PLOG/1.000E+00 3.40E+28 -4.61 9988.0/ ! fit btw. 500 and 1650 K with MAE of 3.2%, 8.6%
PLOG/1.000E+01 2.36E+44 -8.51 28970.0/
PLOG/1.000E+01 3.28E+22 -2.74 7706.0/ ! fit btw. 500 and 1800 K with MAE of 2.2%, 4.4%

PLOG/1.000E+02 2.66E+46 -8.92 34580.0/
PLOG/1.000E+02 2.99E+17 -1.13 6157.0/ ! fit btw. 500 and 2250 K with MAE of 2.5%, 4.4%

trans-1-phenyl-vinylacetylene + H (P3) → $C_{10}H_9$ (W21) 6.16E+23 -2.71 8027.0

PLOG/3.947E-02 2.09E+73 -18.68 22110.0/ ! fit btw. 500 and 1125 K with MAE of 5.0%, 10.6%
PLOG/1.000E+00 4.44E+42 -8.68 13620.0/ ! fit btw. 500 and 1375 K with MAE of 12.4%, 20.8%
PLOG/1.000E+01 5.82E+34 -6.06 12230.0/ ! fit btw. 500 and 1650 K with MAE of 11.7%, 28.8%
PLOG/1.000E+02 6.16E+23 -2.71 8027.0/ ! fit btw. 500 and 2000 K with MAE of 35.2%, 217.5%

PLOG/3.947E-02 5.70E+82 -21.48 26900.0/
PLOG/3.947E-02 2.97E+65 -18.07 8834.0/ ! fit btw. 500 and 1125 K with MAE of 0.7%, 1.3%
PLOG/1.000E+00 2.18E+81 -19.84 37610.0/
PLOG/1.000E+00 5.57E+48 -10.90 13740.0/ ! fit btw. 500 and 1375 K with MAE of 0.9%, 1.6%
PLOG/1.000E+01 4.16E+78 -18.43 43710.0/
PLOG/1.000E+01 1.40E+60 -14.07 20780.0/ ! fit btw. 500 and 1650 K with MAE of 1.7%, 3.7%
PLOG/1.000E+02 5.60E+26 -3.51 10590.0/
PLOG/1.000E+02 3.23E+21 -3.78 -4017.0/ ! fit btw. 500 and 2000 K with MAE of 29.8%, 142.2%

trans-1-phenyl-vinylacetylene + H (P3) → C_6H_5 + C_4H_4 (R1) 2.32E-01 4.84 23210.0

PLOG/3.947E-02 7.96E+42 -7.78 36020.0/ ! fit btw. 500 and 2500 K with MAE of 14.2%, 31.8%
PLOG/1.000E+00 4.33E+37 -6.10 38550.0/ ! fit btw. 500 and 2500 K with MAE of 33.9%, 96.5%
PLOG/1.000E+01 2.62E+21 -1.40 33130.0/ ! fit btw. 500 and 2500 K with MAE of 57.3%, 132.6%
PLOG/1.000E+02 2.32E-01 4.84 23210.0/ ! fit btw. 500 and 2500 K with MAE of 48.5%, 132.8%

PLOG/3.947E-02 1.04E+77 -17.68 56360.0/
PLOG/3.947E-02 5.89E+27 -3.52 27540.0/ ! fit btw. 500 and 2500 K with MAE of 1.1%, 2.7%
PLOG/1.000E+00 1.07E+55 -10.94 51580.0/
PLOG/1.000E+00 1.09E+65 -15.85 40320.0/ ! fit btw. 500 and 2500 K with MAE of 5.5%, 13.5%
PLOG/1.000E+01 9.43E+10 1.05 23380.0/
PLOG/1.000E+01 1.91E+61 -12.45 64220.0/ ! fit btw. 500 and 2500 K with MAE of 4.7%, 13.0%
PLOG/1.000E+02 2.72E+55 -10.63 69290.0/
PLOG/1.000E+02 8.56E-05 5.48 18690.0/ ! fit btw. 500 and 2500 K with MAE of 6.0%, 14.9%

trans-1-phenyl-vinylacetylene + H (P3) → indene + H (P1) 8.49E+31 -4.66 29380.0

PLOG/3.947E-02 1.78E+39 -7.23 16660.0/ ! fit btw. 500 and 2500 K with MAE of 6.2%, 12.9%
PLOG/1.000E+00 4.24E+45 -8.89 24860.0/ ! fit btw. 500 and 2500 K with MAE of 20.8%, 52.4%
PLOG/1.000E+01 1.01E+43 -7.97 28680.0/ ! fit btw. 500 and 2500 K with MAE of 35.3%, 76.3%
PLOG/1.000E+02 8.49E+31 -4.66 29380.0/ ! fit btw. 500 and 2500 K with MAE of 49.8%, 115.4%

PLOG/3.947E-02 9.31E+53 -11.45 27780.0/
PLOG/3.947E-02 1.08E+35 -6.12 13800.0/ ! fit btw. 500 and 2500 K with MAE of 1.3%, 2.0%
PLOG/1.000E+00 3.45E+71 -16.20 43440.0/
PLOG/1.000E+00 4.23E+31 -5.07 15960.0/ ! fit btw. 500 and 2500 K with MAE of 1.3%, 5.7%
PLOG/1.000E+01 1.06E+68 -14.92 48160.0/
PLOG/1.000E+01 1.64E+34 -5.93 20520.0/ ! fit btw. 500 and 2500 K with MAE of 4.4%, 13.2%
PLOG/1.000E+02 2.27E+21 -2.09 20250.0/
PLOG/1.000E+02 1.57E+70 -15.27 59300.0/ ! fit btw. 500 and 2500 K with MAE of 6.4%, 14.7%

trans-1-phenyl-vinylacetylene + H (P3) → cis-1-phenyl-vinylacetylene + H (P2) 2.84E+16 0.12 27310.0

PLOG/3.947E-02 1.64E+28 -3.53 23460.0/ ! fit btw. 500 and 2500 K with MAE of 8.5%, 19.7%
PLOG/1.000E+00 3.55E+33 -4.92 30130.0/ ! fit btw. 500 and 2500 K with MAE of 18.6%, 50.6%
PLOG/1.000E+01 5.97E+28 -3.45 30860.0/ ! fit btw. 500 and 2500 K with MAE of 38.1%, 90.5%
PLOG/1.000E+02 2.84E+16 0.12 27310.0/ ! fit btw. 500 and 2500 K with MAE of 48.4%, 124.9%

PLOG/3.947E-02 1.64E+45 -8.39 35490.0/
PLOG/3.947E-02 1.16E+20 -1.32 18310.0/ ! fit btw. 500 and 2500 K with MAE of 0.4%, 0.8%
PLOG/1.000E+00 4.92E+42 -7.47 36900.0/
PLOG/1.000E+00 2.35E+124 -34.65 54030.0/ ! fit btw. 500 and 2500 K with MAE of 3.8%, 9.2%
PLOG/1.000E+01 2.80E+61 -12.56 55700.0/
PLOG/1.000E+01 1.71E+14 0.39 20590.0/ ! fit btw. 500 and 2500 K with MAE of 2.8%, 7.4%
PLOG/1.000E+02 -4.88E+48 -9.44 41420.0/
PLOG/1.000E+02 6.75E+28 -3.44 32330.0/ ! fit btw. 500 and 2500 K with MAE of 17.4%, 41.4%

trans-1-phenyl-vinylacetylene + H (P3) → total 1.69E+17 -0.72 4581.0

PLOG/3.947E-02 2.77E+15 -0.26 3202.0/ ! fit btw. 500 and 2500 K with MAE of 4.4%, 8.5%
PLOG/1.000E+00 1.71E+16 -0.48 3678.0/ ! fit btw. 500 and 2500 K with MAE of 5.4%, 10.9%
PLOG/1.000E+01 1.52E+17 -0.74 4305.0/ ! fit btw. 500 and 2500 K with MAE of 6.7%, 12.3%
PLOG/1.000E+02 1.69E+17 -0.72 4581.0/ ! fit btw. 500 and 2500 K with MAE of 9.4%, 14.6%

PLOG/3.947E-02 1.97E+38 -7.03 16300.0/
PLOG/3.947E-02 3.34E+09 1.40 -10.3/ ! fit btw. 500 and 2500 K with MAE of 1.1%, 2.6%
PLOG/1.000E+00 1.76E+62 -13.95 31640.0/
PLOG/1.000E+00 2.71E+12 0.59 1531.0/ ! fit btw. 500 and 2500 K with MAE of 2.0%, 4.4%
PLOG/1.000E+01 1.30E+87 -20.81 51830.0/
PLOG/1.000E+01 2.33E+14 0.05 2614.0/ ! fit btw. 500 and 2500 K with MAE of 2.1%, 6.6%
PLOG/1.000E+02 9.96E+27 -3.67 13980.0/
PLOG/1.000E+02 8.73E+31 -5.58 8121.0/ ! fit btw. 500 and 2500 K with MAE of 1.8%, 4.9%

trans-1-phenyl-vinylacetylene + H (P3) → 4-phenyl-vinylacetylene + H (P4) 1.05E+22 -1.49 41080.0

PLOG/3.947E-02 1.85E+52 -10.66 37680.0/ ! fit btw. 500 and 2500 K with MAE of 22.7%, 42.2%
PLOG/1.000E+00 1.63E+55 -11.23 47220.0/ ! fit btw. 500 and 2500 K with MAE of 22.8%, 62.1%
PLOG/1.000E+01 3.86E+44 -8.01 47740.0/ ! fit btw. 500 and 2500 K with MAE of 46.2%, 124.6%
PLOG/1.000E+02 1.05E+22 -1.49 41080.0/ ! fit btw. 500 and 2500 K with MAE of 61.1%, 156.0%

PLOG/3.947E-02 9.93E+63 -14.13 43340.0/
PLOG/3.947E-02 1.10E+83 -18.18 95730.0/ ! fit btw. 500 and 2500 K with MAE of 6.7%, 23.9%
PLOG/1.000E+00 1.29E+63 -13.43 52990.0/
PLOG/1.000E+00 2.96E+188 -54.86 82350.0/ ! fit btw. 500 and 2500 K with MAE of 12.2%, 26.9%
PLOG/1.000E+01 -2.72E+49 -9.75 44900.0/
PLOG/1.000E+01 3.83E+38 -6.37 40810.0/ ! fit btw. 500 and 2500 K with MAE of 33.1%, 122.1%
PLOG/1.000E+02 4.38E+10 1.26 31000.0/
PLOG/1.000E+02 1.89E+66 -13.75 75670.0/ ! fit btw. 500 and 2500 K with MAE of 8.7%, 20.5%

trans-1-phenyl-vinylacetylene + H (P3) → phenyl-butatriene + H (P5) 7.01E+15 0.19 32740.0

PLOG/3.947E-02 1.05E+23 -2.17 26630.0/ ! fit btw. 500 and 2500 K with MAE of 8.1%, 17.4%

PLOG/1.000E+00 8.37E+29 -4.02 33790.0/ ! fit btw. 500 and 2500 K with MAE of 14.4%, 39.6%
PLOG/1.000E+01 1.30E+27 -3.11 35610.0/ ! fit btw. 500 and 2500 K with MAE of 33.8%, 83.8%
PLOG/1.000E+02 7.01E+15 0.19 32740.0/ ! fit btw. 500 and 2500 K with MAE of 48.1%, 119.4%

PLOG/3.947E-02 6.75E+27 -3.51 30280.0/
PLOG/3.947E-02 8.28E+73 -19.01 39310.0/ ! fit btw. 500 and 2500 K with MAE of 0.7%, 1.2%
PLOG/1.000E+00 4.65E+36 -5.90 38760.0/
PLOG/1.000E+00 1.35E+146 -41.89 65670.0/ ! fit btw. 500 and 2500 K with MAE of 3.5%, 7.6%
PLOG/1.000E+01 2.53E+58 -11.85 59030.0/
PLOG/1.000E+01 4.54E+11 1.04 25140.0/ ! fit btw. 500 and 2500 K with MAE of 2.3%, 5.9%
PLOG/1.000E+02 -4.69E+48 -9.57 47060.0/
PLOG/1.000E+02 5.28E+27 -3.24 37500.0/ ! fit btw. 500 and 2500 K with MAE of 17.2%, 39.2%

trans-1-phenyl-vinylacetylene + H (P3) → 2-phenyl-vinylacetylene + H (P6) 2.15E+13 0.81 37660.0

PLOG/3.947E-02 1.80E+38 -6.74 33720.0/ ! fit btw. 500 and 2500 K with MAE of 11.8%, 24.8%
PLOG/1.000E+00 9.41E+39 -7.03 40790.0/ ! fit btw. 500 and 2500 K with MAE of 20.5%, 49.4%
PLOG/1.000E+01 2.24E+33 -4.97 43020.0/ ! fit btw. 500 and 2500 K with MAE of 39.4%, 94.9%
PLOG/1.000E+02 2.15E+13 0.81 37660.0/ ! fit btw. 500 and 2500 K with MAE of 53.2%, 123.3%

PLOG/3.947E-02 2.16E+76 -17.77 57170.0/
PLOG/3.947E-02 2.20E+27 -3.68 27490.0/ ! fit btw. 500 and 2500 K with MAE of 1.1%, 2.6%
PLOG/1.000E+00 1.50E+65 -14.14 58860.0/
PLOG/1.000E+00 1.03E+26 -3.22 31900.0/ ! fit btw. 500 and 2500 K with MAE of 1.7%, 3.3%
PLOG/1.000E+01 -2.07E+30 -3.32 57920.0/
PLOG/1.000E+01 1.26E+11 1.70 32950.0/ ! fit btw. 500 and 2500 K with MAE of 16.8%, 45.7%
PLOG/1.000E+02 3.39E+04 2.86 29300.0/
PLOG/1.000E+02 7.12E+54 -10.69 70370.0/ ! fit btw. 500 and 2500 K with MAE of 6.1%, 18.2%

4-phenyl-vinylacetylene + H (P4) → $C_{10}H_9$ (W3) 4.98E+23 -2.75 9522.0

PLOG/3.947E-02 4.96E+61 -14.63 23130.0/ ! fit btw. 500 and 1250 K with MAE of 14.5%, 24.1%
PLOG/1.000E+00 1.17E+40 -7.84 15570.0/ ! fit btw. 500 and 1375 K with MAE of 15.1%, 27.8%
PLOG/1.000E+01 4.08E+33 -5.79 13510.0/ ! fit btw. 500 and 1650 K with MAE of 17.9%, 43.1%

PLOG/1.000E+02 4.98E+23 -2.75 9522.0/ ! fit btw. 500 and 1800 K with MAE of 13.5%, 32.5%

PLOG/3.947E-02 2.87E+108 -28.25 50010.0/
PLOG/3.947E-02 1.05E+68 -17.03 22610.0/ ! fit btw. 500 and 1250 K with MAE of 0.8%, 1.3%
PLOG/1.000E+00 1.69E+91 -22.60 47230.0/
PLOG/1.000E+00 6.88E+46 -10.23 16120.0/ ! fit btw. 500 and 1375 K with MAE of 1.6%, 3.1%
PLOG/1.000E+01 5.99E+66 -15.22 35840.0/
PLOG/1.000E+01 1.13E+56 -13.15 19190.0/ ! fit btw. 500 and 1650 K with MAE of 4.0%, 10.0%
PLOG/1.000E+02 7.27E+61 -13.48 38160.0/
PLOG/1.000E+02 2.21E+30 -4.98 10860.0/ ! fit btw. 500 and 1800 K with MAE of 2.4%, 4.7%

4-phenyl-vinylacetylene + H (P4) → $C_{10}H_9$ (W9) 1.35E+14 -0.06 6232.0

PLOG/3.947E-02 1.64E+44 -9.28 18250.0/ ! fit btw. 500 and 1250 K with MAE of 18.6%, 30.2%
PLOG/1.000E+00 1.42E+21 -2.21 9022.0/ ! fit btw. 500 and 1500 K with MAE of 10.8%, 23.0%
PLOG/1.000E+01 2.58E+17 -1.06 7571.0/ ! fit btw. 500 and 1650 K with MAE of 10.3%, 29.8%
PLOG/1.000E+02 1.35E+14 -0.06 6232.0/ ! fit btw. 500 and 2000 K with MAE of 6.3%, 15.6%

PLOG/3.947E-02 3.04E+111 -28.88 56820.0/
PLOG/3.947E-02 5.29E+49 -11.38 17660.0/ ! fit btw. 500 and 1250 K with MAE of 1.1%, 2.4%
PLOG/1.000E+00 4.12E+40 -7.80 21160.0/
PLOG/1.000E+00 1.90E+80 -21.25 26740.0/ ! fit btw. 500 and 1500 K with MAE of 5.1%, 20.8%
PLOG/1.000E+01 8.40E+64 -14.47 42510.0/
PLOG/1.000E+01 1.05E+25 -3.52 9724.0/ ! fit btw. 500 and 1650 K with MAE of 3.6%, 6.4%
PLOG/1.000E+02 1.22E+37 -6.46 25920.0/
PLOG/1.000E+02 1.58E+17 -1.09 6788.0/ ! fit btw. 500 and 2000 K with MAE of 1.1%, 1.8%

4-phenyl-vinylacetylene + H (P4) → C_6H_5 + C_4H_4 (R1) 4.86E+16 -0.07 31970.0

PLOG/3.947E-02 9.19E+38 -6.73 33130.0/ ! fit btw. 500 and 2500 K with MAE of 11.5%, 21.8%
PLOG/1.000E+00 1.36E+40 -6.90 38550.0/ ! fit btw. 500 and 2500 K with MAE of 19.9%, 56.9%
PLOG/1.000E+01 6.16E+31 -4.42 37410.0/ ! fit btw. 500 and 2500 K with MAE of 39.3%, 97.2%
PLOG/1.000E+02 4.86E+16 -0.07 31970.0/ ! fit btw. 500 and 2500 K with MAE of 46.0%, 117.0%

PLOG/3.947E-02 2.96E+44 -8.36 35790.0/
PLOG/3.947E-02 4.64E+89 -19.64 112800.0/ ! fit btw. 500 and 2500 K with MAE of 5.1%, 18.4%
PLOG/1.000E+00 6.83E+48 -9.32 44940.0/
PLOG/1.000E+00 1.06E+182 -52.93 78610.0/ ! fit btw. 500 and 2500 K with MAE of 7.0%, 16.7%
PLOG/1.000E+01 7.39E+53 -10.54 54340.0/
PLOG/1.000E+01 1.39E+45 -9.51 35760.0/ ! fit btw. 500 and 2500 K with MAE of 5.2%, 9.0%
PLOG/1.000E+02 -7.05E+48 -9.63 45950.0/
PLOG/1.000E+02 3.53E+28 -3.50 36700.0/ ! fit btw. 500 and 2500 K with MAE of 15.3%, 37.9%

4-phenyl-vinylacetylene + H (P4) → indene + H (P1) 5.78E+02 3.48 31890.0

PLOG/3.947E-02 8.64E+53 -11.63 40880.0/ ! fit btw. 500 and 2500 K with MAE of 26.5%, 50.1%
PLOG/1.000E+00 6.79E+63 -14.12 55930.0/ ! fit btw. 600 and 2500 K with MAE of 16.5%, 31.1%
PLOG/1.000E+01 1.33E+60 -12.81 62180.0/ ! fit btw. 600 and 2500 K with MAE of 23.2%, 60.1%
PLOG/1.000E+02 5.78E+02 3.48 31890.0/ ! fit btw. 500 and 2500 K with MAE of 156.6%, 624.4%

PLOG/3.947E-02 1.39E+68 -15.84 47740.0/
PLOG/3.947E-02 7.19E+65 -14.12 78080.0/ ! fit btw. 500 and 2500 K with MAE of 6.0%, 22.1%
PLOG/1.000E+00 4.15E+215 -53.00 281400.0/
PLOG/1.000E+00 6.17E+70 -16.15 59770.0/ ! fit btw. 600 and 2500 K with MAE of 9.0%, 24.4%
PLOG/1.000E+01 4.44E+204 -58.64 108900.0/
PLOG/1.000E+01 7.00E+72 -16.33 72210.0/ ! fit btw. 600 and 2500 K with MAE of 7.8%, 19.9%
PLOG/1.000E+02 2.39E-56 18.93 -8745.0/
PLOG/1.000E+02 1.94E+54 -10.88 69960.0/ ! fit btw. 500 and 2500 K with MAE of 20.8%, 47.5%

4-phenyl-vinylacetylene + H (P4) → cis-1-phenyl-vinylacetylene + H (P2) 5.34E+22 -1.89 51660.0

PLOG/3.947E-02 4.29E+32 -5.33 37560.0/ ! fit btw. 500 and 2500 K with MAE of 15.0%, 29.1%
PLOG/1.000E+00 1.09E+45 -8.61 51450.0/ ! fit btw. 500 and 2500 K with MAE of 17.9%, 41.7%
PLOG/1.000E+01 5.14E+41 -7.45 56060.0/ ! fit btw. 500 and 2500 K with MAE of 37.6%, 116.4%
PLOG/1.000E+02 5.34E+22 -1.89 51660.0/ ! fit btw. 500 and 2500 K with MAE of 69.7%, 175.1%

PLOG/3.947E-02 1.22E+44 -8.74 42920.0/
PLOG/3.947E-02 3.40E+33 -5.18 52710.0/ ! fit btw. 500 and 2500 K with MAE of 1.8%, 6.8%

PLOG/1.000E+00 7.43E+80 -19.00 72770.0/
PLOG/1.000E+00 1.19E+26 -3.28 40820.0/ ! fit btw. 500 and 2500 K with MAE of 0.8%, 1.8%
PLOG/1.000E+01 3.71E+59 -12.43 69320.0/
PLOG/1.000E+01 6.62E+98 -26.73 66880.0/ ! fit btw. 500 and 2500 K with MAE of 9.1%, 20.9%
PLOG/1.000E+02 3.69E+03 3.14 37750.0/
PLOG/1.000E+02 4.52E+72 -15.77 90010.0/ ! fit btw. 500 and 2500 K with MAE of 7.9%, 23.5%

4-phenyl-vinylacetylene + H (P4) → trans-1-phenyl-vinylacetylene + H (P3) 3.07E+20 -1.11 42380.0

PLOG/3.947E-02 5.45E+50 -10.28 38970.0/ ! fit btw. 500 and 2500 K with MAE of 22.1%, 41.2%
PLOG/1.000E+00 4.78E+53 -10.85 48520.0/ ! fit btw. 500 and 2500 K with MAE of 22.9%, 63.5%
PLOG/1.000E+01 1.14E+43 -7.63 49030.0/ ! fit btw. 500 and 2500 K with MAE of 46.9%, 126.6%
PLOG/1.000E+02 3.07E+20 -1.11 42380.0/ ! fit btw. 500 and 2500 K with MAE of 61.9%, 159.1%

PLOG/3.947E-02 1.16E+62 -13.64 44450.0/
PLOG/3.947E-02 5.08E+83 -18.39 99730.0/ ! fit btw. 500 and 2500 K with MAE of 6.8%, 24.2%
PLOG/1.000E+00 7.21E+61 -13.13 54490.0/
PLOG/1.000E+00 2.03E+187 -54.57 83960.0/ ! fit btw. 500 and 2500 K with MAE of 12.0%, 26.5%
PLOG/1.000E+01 -8.90E+47 -9.38 46240.0/
PLOG/1.000E+01 1.14E+37 -6.00 42120.0/ ! fit btw. 500 and 2500 K with MAE of 33.5%, 126.4%
PLOG/1.000E+02 1.20E+09 1.63 32240.0/
PLOG/1.000E+02 1.24E+65 -13.47 77240.0/ ! fit btw. 500 and 2500 K with MAE of 8.8%, 21.0%

4-phenyl-vinylacetylene + H (P4) → total 8.67E+27 -3.96 11770.0

PLOG/3.947E-02 1.87E+12 0.32 1595.0/ ! fit btw. 500 and 2500 K with MAE of 38.0%, 114.1%
PLOG/1.000E+00 1.13E+22 -2.42 7342.0/ ! fit btw. 500 and 2500 K with MAE of 29.7%, 101.2%
PLOG/1.000E+01 9.78E+26 -3.78 10550.0/ ! fit btw. 500 and 2500 K with MAE of 22.2%, 108.9%
PLOG/1.000E+02 8.67E+27 -3.96 11770.0/ ! fit btw. 500 and 2500 K with MAE of 21.1%, 48.7%

PLOG/3.947E-02 1.24E+47 -10.08 17610.0/
PLOG/3.947E-02 1.75E+54 -10.60 55300.0/ ! fit btw. 500 and 2500 K with MAE of 7.8%, 18.8%
PLOG/1.000E+00 8.56E+36 -6.83 14550.0/
PLOG/1.000E+00 3.22E+136 -32.09 161400.0/ ! fit btw. 500 and 2500 K with MAE of 11.4%, 23.3%

PLOG/1.000E+01 2.94E+41 -7.97 18860.0/
PLOG/1.000E+01 2.32E-26 11.00 -18360.0/ ! fit btw. 500 and 2500 K with MAE of 14.5%, 57.4%
PLOG/1.000E+02 3.43E+106 -25.95 73130.0/
PLOG/1.000E+02 5.91E+23 -2.84 8902.0/ ! fit btw. 500 and 2500 K with MAE of 8.4%, 23.8%

4-phenyl-vinylacetylene + H (P4) → phenyl-butatriene + H (P5) 1.07E+17 -0.39 34660.0

PLOG/3.947E-02 4.94E+25 -3.22 28410.0/ ! fit btw. 500 and 2500 K with MAE of 16.1%, 26.3%
PLOG/1.000E+00 1.13E+31 -4.59 35720.0/ ! fit btw. 500 and 2500 K with MAE of 14.0%, 32.0%
PLOG/1.000E+01 5.24E+27 -3.53 37310.0/ ! fit btw. 500 and 2500 K with MAE of 25.3%, 69.7%
PLOG/1.000E+02 1.07E+17 -0.39 34660.0/ ! fit btw. 500 and 2500 K with MAE of 40.8%, 84.8%

PLOG/3.947E-02 3.19E+39 -7.34 34810.0/
PLOG/3.947E-02 1.70E+39 -6.51 54500.0/ ! fit btw. 500 and 2500 K with MAE of 2.6%, 9.1%
PLOG/1.000E+00 4.36E+33 -5.31 37580.0/
PLOG/1.000E+00 1.01E-03 -6.44 -53030.0/ ! fit btw. 500 and 2500 K with MAE of 11.0%, 21.9%
PLOG/1.000E+01 2.59E+40 -7.06 46770.0/
PLOG/1.000E+01 2.81E+107 -29.67 57790.0/ ! fit btw. 500 and 2500 K with MAE of 6.7%, 14.9%
PLOG/1.000E+02 7.47E+40 -7.00 53240.0/
PLOG/1.000E+02 2.86E+32 -5.99 34670.0/ ! fit btw. 500 and 2500 K with MAE of 6.8%, 12.3%

C_6H_5 + C_4H_4 → *i*-C_4H_3 + C_6H_6 (independent of pressure)

1.97E+02 3.08 4463.1/ ! fit btw. 500 and 2500 K

1.03E+05 2.19 9446.0/
3.91E+02 2.96 4436.3/ ! fit btw. 500 and 2500 K

C_6H_5 + C_4H_4 → *n*-C_4H_3 + C_6H_6 (independent of pressure)

3.41E+02 3.11 8482.7/ ! fit btw. 500 and 2500 K

6.95E+05 2.11 14668./
1.66E+03 2.88 8611.9/ ! fit btw. 500 and 2500 K

Input file for RRKM-ME calculations using the MESS package for the $C_6H_5 + C_4H_4$ and related reactions under combustion-like conditions

```
TemperatureList[K]                    500. 600. 700. 800. 900. 1000.
1125. 1250. 1375. 1500. 1650. 1800. 2000. 2250. 2500.
PressureList[atm]                     0.03947368 1. 10. 100.
EnergyStepOverTemperature             0.2          #Ratio of
discretization energy step to T
ExcessEnergyOverTemperature           50
ModelEnergyLimit[kcal/mol]         400
WellCutoff                            10
ChemicalEigenvalueMax                 0.2
ChemicalEigenvalueMin                 1.e-6          #only for direct
diagonalization method
CalculationMethod                     direct
EigenvalueOutput                        eigenvalue.out
Model
  EnergyRelaxation
    Exponential
      Factor[1/cm]                   424    ! Jasper calc N2
      Power                           0.62
      ExponentCutoff               15
    End
  CollisionFrequency
    LennardJones
        Epsilons[1/cm]          390.  390.    ! N2 , A3/A3a/A6 ! from new
Jasper calc 11/22/15
        Sigmas[angstrom]        4.46  4.46   ! N2 , A3/A3a/A6 ! from new
Jasper calc 11/22/15
        Masses[amu]             28.  129.
    End
OutputTemperatureStep[K]  100
OutputTemperatureSize  24
OutputReferenceEnergy[kcal/mol]  0.
  Well       W1  # [1]
  Species
    RRHO
      Geometry[angstrom]    19
C                  0.397013   -0.371153   -0.299297
C                  1.455304   -1.239729   -0.023651
C                  2.733062   -0.747880    0.241302
C                  2.968224    0.623923    0.233702
C                  1.918366    1.500763   -0.038884
C                  0.644306    1.006660   -0.300367
C                 -1.000420   -0.900298   -0.582712
C                 -1.983549   -0.553980    0.504820
C                 -3.167554    0.100501    0.279867
C                 -4.219722    0.684869    0.068407
H                  1.280046   -2.310977   -0.020116
H                  3.543057   -1.437726    0.451240
H                  3.961098    1.008682    0.437598
```

```
H                   2.093572    2.570947   -0.047949
H                  -0.169717    1.693847   -0.506892
H                  -0.947191   -1.991703   -0.688913
H                  -1.364723   -0.510433   -1.537004
H                  -1.730318   -0.836280    1.522429
H                  -5.136008    1.191581   -0.109512
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CH2CHCCH
        Group                   8 9 10 16 17 18 19
        Axis                    1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  0.577308823 1.63780003 0.690260549 0.  0.62750959 1.631524934
0.683985453
     End
      Rotor     Hindered     ! CHCCH
        Group                   9 10 19
        Axis                    7 8
        Symmetry                1
        Potential[kcal/mol]     8
0.  0.464357097 0.112951726  0.27610422 1.424446769 1.298944851
1.405621482 0.815762467
     End
      Frequencies[1/cm]         49
 132.5999
 184.6433               281.7542               328.4648
 388.2504               415.1299               442.0483
 468.5956               538.6720               573.3504
 635.3959               641.6303               646.8768
 715.8928               763.0779               821.1506
 857.5006               873.9086               924.3247
 979.4135              1001.8757              1017.1025
1024.3944              1051.0540              1102.2450
1143.4895              1181.2519              1191.6946
1203.3011              1212.5840              1296.0048
1338.3716              1360.2516              1401.6663
1473.0430              1485.4996              1527.3186
1626.3529              1645.0458              2013.3618
2999.6668              3067.3910              3150.9445
3154.2940              3159.3586              3168.9537
3177.2390              3188.6452              3468.5381
!23.8404                26.8707
      ZeroEnergy[kcal/mol]           -44.8
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W2  # [2]
  Species
    RRHO
      Geometry[angstrom]    19
C 0.2267454816 -0.0615873481 -0.0309608851
```

```
C -0.8717947185 -0.9240880365 -0.1501037547
C -0.6988004578 -2.3045315244 -0.1034763826
C 0.5733110393 -2.8470027721 0.067053114
C 1.6717071226 -1.9986333288 0.1942840095
C 1.5000865833 -0.6185855788 0.1482568508
C 0.0296325492 1.422077614 -0.1064690182
C 0.8895269631 2.1882063601 -0.755481008
C -1.1666658196 1.9883776584 0.5649845845
C -1.8697689111 3.033630881 0.1276944647
H -1.8628094176 -0.5083907553 -0.293514456
H -1.5589812088 -2.9572544083 -0.203186609
H 0.7069521037 -3.922092479 0.1067348801
H 2.6634905319 -2.4122003888 0.3398458429
H 2.3533015145 0.0382386147 0.272821678
H 1.7995839201 2.0625015115 -1.3228746497
H -1.4703659245 1.4831359087 1.4788453143
H -1.6164112434 3.5369728962 -0.7987395406
H -2.7186392674 3.4119055515 0.685375691
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! HCCCHCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry               1
        Potential[kcal/mol]    8
0. 1.468372441   0.144327206 1.342870523     0. 1.462097345
      0.131777014 1.386796194
     End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   7 9
        Symmetry               1
        Potential[kcal/mol]    8
1.5311234 3.87173417 3.576804663 0.  1.418171673 5.170679022
      2.077056743 1.982930304
     End
      Frequencies[1/cm]        49
 124.6584
 216.7049    276.5393    335.0040
 361.4296    416.7553    465.7166
 520.4471    622.2111    635.8467
 670.0853    715.0269    726.1408
 769.9119    782.8429    812.0572
 858.6645    934.4077    953.4516
 982.9914   1003.3954   1015.5173
1017.0488   1031.8916   1054.9456
1096.1454   1104.7817   1182.2006
1202.5616   1235.6541   1317.1088
1324.5727   1352.4598   1441.5608
1473.1405   1521.2323   1608.1671
1625.6966   1640.7963   1681.9813
3132.5940   3142.3256   3160.7827
3168.0090   3177.5944   3183.4836
```

```
3190.9729   3224.2649   3239.1382
!51.0581     90.0844
      ZeroEnergy[kcal/mol]            -38.3
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W3  # [3]
  Species
    RRHO
      Geometry[angstrom]    19
C 0.5850636927 -0.150901528 0.2451248219
C -0.4173533104 -1.0502647881 -0.148906457
C -0.1363593402 -2.4020770567 -0.2977324856
C 1.1507644465 -2.8865247491 -0.0572179465
C 2.1539881442 -2.0040345574 0.3336761848
C 1.8729131083 -0.6484882019 0.4831123176
C 0.324119378 1.294051302 0.4161905121
C -0.8150386311 1.9121703666 0.2451364298
C -1.980942017 2.5710480857 0.0859375263
C -2.4336968697 3.1533718561 -1.0965397311
H -1.41835051 -0.6786519658 -0.3385128183
H -0.92278133 -3.0834296066 -0.6033972231
H 1.3670490031 -3.9422882871 -0.1745798748
H 3.1571394008 -2.3697298215 0.5229607835
H 2.6583778248 0.0352381629 0.7887138981
H 1.1908119588 1.8875524542 0.718355879
H -2.620209243 2.6491755156 0.9661486364
H -1.8449693542 3.1097082557 -2.0037879762
H -3.3878193583 3.6623209169 -1.1285883371
      Core   RigidRotor
        SymmetryFactor      1
      End
      Rotor     Hindered     ! HCCCHCH2
        Group                 8 9 10 16 17 18 19
        Axis                  1 7
        Symmetry               2
        Potential[kcal/mol]    4
0.  1.937645447  4.681611225  1.884137705
     End
      Frequencies[1/cm]         50
  61.8752              149.2310
 178.1493              265.9593              304.4650
 390.6922              414.3963              502.0931
 524.6942              561.8910              620.5864
 634.4017              707.6551              747.2171
 753.1562              807.5872              829.4960
 855.2265              929.6912              936.0475
 940.0708              978.8394             1000.8616
1015.8955             1049.0252             1084.8187
1104.6899             1181.2884             1191.2935
1198.9789             1218.1761             1287.2454
1343.9766             1358.1570             1409.9284
1485.5755             1491.1886             1525.4680
```

```
1620.9124              1642.0238              1888.5390
3058.4467              3096.6562              3150.5668
3156.0757              3162.1703              3171.8187
3179.2043              3189.4161              3251.4641
!41.8726
      ZeroEnergy[kcal/mol]        -49.7
      ElectronicLevels[1/cm]       1
           0   2
    End
  End
  Well       W4  # [4]
  Species
    RRHO
      Geometry[angstrom]    19
C -0.1601255759 -0.3779815508 -0.3841740674
C -1.0194073821 -1.4057340786 0.042238675
C -0.6272897362 -2.7433324045 -0.0109122131
C 0.6326576 -3.0975110767 -0.4889778014
C 1.5170410872 -2.0986755898 -0.9221310119
C 1.0702380444 -0.8039762052 -0.8419326009
C -0.5520473038 1.0802617232 -0.3159508947
C 0.1505929086 1.8201464857 0.8500063389
C -0.2201823878 3.229619705 0.9299182716
C -0.5424033531 4.3864769455 0.9752882413
H -2.0072285245 -1.1456641062 0.4121376599
H -1.3131037078 -3.5143904764 0.3212553975
H 0.9324550045 -4.1392032154 -0.5301815749
H 2.5015620202 -2.3489904546 -1.3018270903
H -1.6343540484 1.1670296559 -0.1933778721
H -0.2934931568 1.5800108989 -1.2529480448
H 1.235330328 1.7319635473 0.7276735864
H -0.0950732898 1.3229582842 1.7947149716
H -0.8205380334 5.4105221438 1.0223153411
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CH2CH2CCH
        Group                  8 9 10 15 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0. 0.345130275 0.514557864 0.056475863 0.27610422 1.549948687 1.644075126
0.721636028
     End
      Rotor     Hindered     ! CH2CCH
        Group                  9 10 17 18 19
        Axis                   7 8
        Symmetry                1
        Potential[kcal/mol]     8
0. 2.943019977 1.731926468 1.857428386 5.842114283 2.26530962 2.26530962
3.093622279
     End
      Frequencies[1/cm]         49
   84.4242
```

```
  174.2060    274.7379    318.4884
  363.8951    418.5649    444.0764
  527.7844    592.9539    632.9083
  665.5699    676.3962    702.8108
  745.2342    769.3219    823.5543
  853.7827    937.3805    968.4611
  985.4719    988.3490   1007.8768
 1015.0803   1044.7479   1122.9814
 1173.3134   1181.6521   1217.6263
 1268.7484   1294.0143   1313.3082
 1328.0241   1368.7157   1449.3404
 1474.0130   1477.2400   1496.8646
 1574.4753   1634.2350   2221.2866
 3024.4288   3049.3928   3053.3969
 3093.2490   3147.8284   3160.8201
 3173.5756   3186.0225   3478.1833
!31.2260     61.7964
      ZeroEnergy[kcal/mol]            -21.7
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W5  # [5] (mi12)
  Species
    RRHO
      Geometry[angstrom]    19
C                  -1.346495    1.354869   -0.000515
C                   1.368635   -1.300007   -0.300206
C                  -1.152059   -1.416641    0.001007
C                  -2.404450   -0.807630    0.099343
C                  -2.500651    0.580512    0.093838
C                  -0.088935    0.751718   -0.092304
C                   1.156290    1.551663   -0.147413
C                   2.305549    0.937814    0.066890
C                   2.523633   -0.498386    0.354402
C                   0.009777   -0.656770   -0.098947
H                  -1.416941    2.437787    0.004909
H                   1.564774   -1.353751   -1.379143
H                  -1.080886   -2.499985   -0.003120
H                  -3.297634   -1.416983    0.178238
H                  -3.469876    1.061040    0.167254
H                   1.080048    2.622910   -0.311483
H                   3.483834   -0.855019   -0.029454
H                   2.540871   -0.651465    1.442104
H                   1.368045   -2.327392    0.074118
      Core   RigidRotor
        SymmetryFactor          0.5
      End
      Frequencies[1/cm]         51
 132.1257               161.2756               267.7279
 355.6088               372.0623               420.8737
 475.4026               505.4230               532.6353
 592.3354               694.5770               743.0002
 748.4520               756.7483               807.9284
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 834.1999               888.3559               899.7683
 940.7189               949.6858               981.8710
 987.9087              1021.6857              1059.8639
1128.9976              1172.9444              1182.6918
1196.3095              1201.8633              1220.8558
1249.6169              1313.9812              1326.5297
1330.9761              1367.2740              1466.4829
1475.8852              1482.0104              1509.7335
1609.6990              1638.7730              1687.3394
2995.5436              3004.6465              3057.4262
3066.3389              3143.8884              3153.1218
3159.2481              3172.2481              3186.7868
      ZeroEnergy[kcal/mol]           -59.2
      ElectronicLevels[1/cm]       1
           0   2
    End
  End
  Well       W6   # S24 1-H-naphthyl
  Species
    RRHO
      Geometry[angstrom]    19
C       -1.367679       -1.324149       0.000000
C       1.351720        1.378016        0.000000
C       -1.170946       1.446288        0.000000
C       -2.424848       0.839190        0.000000
C       -2.519274       -0.555296       0.000000
C       -0.089006       -0.725145       0.000000
C       1.106951        -1.516899       0.000000
C       2.374959        -0.912706       0.000000
C       2.525747        0.447863        0.000000
C       0.000000        0.691391        0.000000
H       -1.436181       -2.407220       0.000000
H       1.417358        2.052895        0.868000
H       -1.101649       2.530268        0.000000
H       -3.322196       1.447390        0.000000
H       -3.491931       -1.034560       0.000000
H       1.017884        -2.597076       0.000000
H       3.257165        -1.545053       0.000000
H       3.516447        0.889134        0.000000
H       1.417358        2.052895        -0.868000
      Core   RigidRotor
        SymmetryFactor          1
      End
      Frequencies[1/cm]         51
83. 171. 250. 358. 429. 471. 485. 506. 541. 613. 661. 714. 748. 752. 792.
795. 871. 921. 932.
954. 959. 967. 985. 1057. 1092. 1139. 1175. 1179. 1201. 1202. 1234. 1277.
1309. 1356. 1393. 1439.
1445. 1473. 1516. 1559. 1599. 1630. 2955. 2956. 3149. 3152. 3158. 3171.
3172. 3183. 3187.
      ZeroEnergy[kcal/mol]           -89.5
      ElectronicLevels[1/cm]       1
           0   2
    End
```

```
  End
  Well       W7  # [7]
  Species
    RRHO
      Geometry[angstrom]    19
C                  -0.500861   -0.293962   -0.0
C                  -0.939177    1.023554   -0.0
C                  -2.235884    1.457935   -0.0
C                  -3.237485    0.472064    0.0
C                  -2.877139   -0.873950    0.0
C                  -1.537085   -1.253177   -0.0
C                   0.901292   -0.700527   -0.0
C                   1.960521    0.131369   -0.0
C                   3.338548   -0.313972    0.0
C                   4.399126    0.504289    0.0
H                  -2.490993    2.512176   -0.0
H                  -4.282287    0.763117    0.0
H                  -3.647161   -1.636928    0.0
H                  -1.272243   -2.306456   -0.0
H                   1.079649   -1.773673   -0.0
H                   1.788425    1.205726    0.0
H                   3.499673   -1.390395    0.0
H                   4.281429    1.583223    0.0
H                   5.412372    0.121472    0.0
      Core                                      MultiRotor
        SymmetryFactor          1
        InterpolationEnergyMax[kcal/mol]        100
        PotentialEnergySurface[kcal/mol]        c10h9_pva_7.dat
!        QuantumLevelEnergyMax[kcal/mol]         5
        InternalRotation
                Group                           8 9 10 15 16 17 18 19
                Axis                            1 7
                Symmetry                        1
                MassExpansionSize               11
!               PotentialExpansionSize          11
!               HamiltonSizeMin                 13
!               HamiltonSizeMax                 101
                GridSize                        100
        End
        InternalRotation
                Group                           10 17 18 19
                Axis                            8 9
                Symmetry                        1
                MassExpansionSize               11
!               PotentialExpansionSize          11
!               HamiltonSizeMin                 13
!               HamiltonSizeMax                 101
                GridSize                        100
        End
      End
      Frequencies[1/cm]         49
  97.9101              131.4774
 282.2872              299.6277
 338.1474              415.1277              514.7723
```

```
 515.9676               606.6524               632.0399
 653.7285               704.5712               746.7236
 845.6747               855.7314               897.0868
 928.6271               938.0387               960.4544
 978.7726               983.8890               986.3743
1041.5411              1045.3014              1114.3985
1174.0491              1180.9201              1237.4661
1249.0895              1300.7015              1317.4885
1324.7793              1343.5412              1442.1709
1457.9192              1474.0049              1566.1839
1624.9141              1656.1140              1691.2080
3124.2938              3131.6287              3135.9476
3140.4775              3150.8845              3160.3951
3172.7854              3187.0110              3222.3466
!62.1485  174.6722
      ZeroEnergy[kcal/mol]            -39.8
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W8   # [8]
  Species
    RRHO
      Geometry[angstrom]    19
C -0.0405561667 -0.3125822186 -0.0223006004
C -1.1602697369 0.4589439557 -0.3662613609
C -2.4432702095 -0.06012877 -0.226736256
C -2.62607279 -1.3563377297 0.2514128426
C -1.5180595107 -2.1336058663 0.5930540525
C -0.2352810511 -1.61822723 0.4597891617
C 1.2895513091 0.2282243764 -0.175632181
C 2.5746379726 0.1824929665 -0.0196500705
C 2.0476382465 1.4731307391 -0.6497358675
C 2.0015681275 2.7125680278 0.1111697167
H -1.0105767737 1.4663607946 -0.7364752751
H -3.3017146033 0.5462189211 -0.4929293598
H -3.6262667466 -1.7609322952 0.3574054568
H -1.6575858821 -3.1428972611 0.9639977367
H 0.626747938 -2.2202856101 0.7239760841
H 3.4602459621 -0.2922095679 0.3688981071
H 2.1804494409 1.5937235091 -1.7261344797
H 1.8768415338 2.6902426857 1.1874357038
H 2.1125419857 3.6729093174 -0.3768305972
      Core   RigidRotor
        SymmetryFactor          0.5
      End
      Rotor     Hindered     ! CH2CH2CCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  1.738201564  4.235689733 1.713101181
     End
      Rotor     Hindered     ! CH2
```

```
        Group                   18 19
        Axis                    9 10
        Symmetry                 1
        Potential[kcal/mol]      8
0.  2.453562497  5.848389379 1.964105017 0.  2.171183181  5.860939571
     2.491213072
     End
      Frequencies[1/cm]         49
  94.0884    129.2171
 237.6938    347.6153
 384.0412    415.0827    434.7574
 492.7725    537.4190    581.3352
 632.3869    680.8948    700.7773
 714.8421    786.4744    817.9421
 856.2830    905.2641    936.3715
 977.4480    983.3499   1004.5707
1015.5551   1047.3653   1047.7798
1097.7768   1109.6351   1129.2138
1182.5092   1196.3298   1219.5628
1320.9256   1352.6594   1373.9088
1462.5668   1476.6989   1520.3547
1614.3627   1640.3734   1828.8676
3061.2492   3136.1349   3162.6214
3170.6802   3179.9279   3186.7037
3193.3254   3239.9951   3253.4013
!52.2615 277.4009
      ZeroEnergy[kcal/mol]           -24.6
      ElectronicLevels[1/cm]       1
           0   2
    End
  End
  Well       W9   #  [9]
  Species
    RRHO
      Geometry[angstrom]    19
C 0.4829467451 -0.0006451198 -0.124578269
C 1.222407737 -1.2257224544 -0.0496091836
C 2.5967150961 -1.2106302418 0.086120158
C 3.2985299927 -0.0001490002 0.1556810793
C 2.5962504039 1.210143013 0.0862551351
C 1.2219924885 1.2247549477 -0.0494705387
C -0.881537634 -0.0007133994 -0.2473537257
C -2.163140177 0.0001907443 -0.5106688657
C -3.2363783312 0.0001447905 0.4881850769
C -4.5364709115 0.0007470566 0.1813728777
H 0.6822852727 -2.1631247898 -0.1025725308
H 3.1366375396 -2.1497898841 0.1386637885
H 4.3766414894 0.0000718733 0.2628937569
H 3.1358959537 2.1494552968 0.1389102104
H 0.6814428332 2.1619161248 -0.1023339566
H -2.4900677202 0.0003309618 -1.5564588513
H -2.9236513379 -0.0002964845 1.5285201097
H -4.8766459765 0.0012228237 -0.8494622858
H -5.2995214635 0.0008707412 0.9501000148
```

```
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   8 9
        Symmetry                1
        Potential[kcal/mol]     8
0. 3.44738081 6.586845174 3.704317122 2.869807178 3.704317122 6.586845174
3.429253941
     End
      Frequencies[1/cm]         50
  33.0704               67.7926
 183.2880              194.2999              331.8582
 343.9962              408.0400              476.6494
 523.9220              578.8252              626.2389
 644.3007              680.1199              749.4604
 779.0289              821.0821              861.4787
 886.4852              930.3687              934.0306
 971.4889              984.9855              986.1644
1030.5468             1031.9139             1098.5282
1121.4285             1173.2325             1175.2655
1207.5965             1289.9366             1301.6410
1326.1744             1345.6592             1451.1481
1453.5677             1484.8365             1559.6723
1589.3976             1675.6956             1862.5336
3024.7106             3132.9254             3151.5257
3162.9033             3168.5810             3185.7791
3190.6253             3195.7112             3221.6219
!144.4840
      ZeroEnergy[kcal/mol]           -46.3
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W10 # [10] (A4a')
  Species
    RRHO
      Geometry[angstrom]    19
C -0.1469245393 -0.3765489178 0.0149917187
C -1.5047660561 -0.0414013849 0.1701116757
C -2.4749324804 -1.0276282929 0.282447433
C -2.1207350473 -2.3776253781 0.2431680791
C -0.7823651682 -2.7291409361 0.0896477288
C 0.1896735909 -1.7404197006 -0.0229010151
C 0.9227720879 0.6144243449 -0.1080153206
C 0.804680817 1.9545574325 -0.0844003225
C 1.9139327761 2.9030281378 -0.2126969601
C 3.195112327 2.6407744353 -0.3736741315
H -1.8053489771 0.9991481592 0.2024209222
H -3.5151433804 -0.7449186402 0.4011172912
H -2.8819225441 -3.1443876261 0.3311435311
H -0.4940746238 -3.7739339996 0.0573103301
H 1.2308031213 -2.0217640085 -0.1422948148
```

```
H 1.921314418 0.2005152102 -0.231051212
H -0.1740703692 2.4076721211 0.0384155978
H 1.6266010823 3.9603528346 -0.1671659529
H 4.1131514275 3.1971975078 -0.4819690053
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CHCHCHCH
        Group                   8 9 10 16 17 18 19
        Axis                    1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  1.39307129   4.706321925 1.311495043 0.  1.405621482  4.706321925
      1.298944851
      End
      Frequencies[1/cm]         50
  65.1776    119.9631
 160.6696    237.9482    276.2382
 403.4759    410.7570    501.0509
 506.8672    613.0833    634.3697
 643.5950    702.9644    761.4077
 812.7380    819.9126    844.9994
 892.3864    898.0926    926.4539
 974.6197    994.6827   1008.7185
1011.3572   1022.9882   1052.3058
1104.9515   1182.3957   1203.5158
1234.8256   1269.1467   1310.2178
1346.8753   1353.5849   1365.7512
1480.4270   1527.0676   1610.3147
1618.6712   1644.2183   1684.0991
3015.9270   3132.2808   3157.1332
3158.2857   3164.8677   3174.4964
3183.0682   3191.0856   3248.7269
!15.9436
      ZeroEnergy[kcal/mol]            -37.5
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W11 # [11]
  Species
    RRHO
      Geometry[angstrom]    19
C -0.3033113007 0.0436361227 0.1570032649
C -1.4766567331 -0.3599504415 0.8001641449
C -1.7447812455 -1.7100138666 1.0232574826
C -0.8382119144 -2.679139108 0.6038345557
C 0.3369270065 -2.2892035755 -0.0394237142
C 0.6012322116 -0.9417187489 -0.2603358792
C -0.0208692341 1.5086960462 -0.080514018
C 0.4183478777 1.9466803742 -1.491203546
C 1.636212292 2.4267470378 -1.0086798208
C 1.3662698154 2.0556776042 0.3088736194
H -2.1878295344 0.3910734774 1.1296869566
```

```
H -2.6612089322 -2.0022693727 1.5241855344
H -1.0432589652 -3.7298983513 0.7755305519
H 1.0482419873 -3.0386803559 -0.3691673058
H 1.5163804055 -0.6447381605 -0.7608862391
H -0.8438590415 2.1128810663 0.3163161988
H -0.0550462169 1.8793712244 -2.4608440972
H 2.4774983724 2.9193882 -1.481540064
H 1.8981292729 2.1044036049 1.2488619283
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CHCHCHCH
        Group                   8 9 10 16 17 18 19
        Axis                    1 7
        Symmetry                 2
        Potential[kcal/mol]      4
0.  0.953814577  1.957829921 1.01029044
      End
      Frequencies[1/cm]         50
 134.0486    135.3907
 313.5121    319.0044    390.0329
 416.4847    523.7129    531.1833
 572.8625    635.1523    667.7236
 714.4975    770.9981    833.9609
 856.3047    900.0967    911.2812
 925.8140    940.9082    957.2956
 960.5248    978.4799   1000.5867
1017.3260   1051.0724   1100.9036
1139.1060   1168.0349   1181.0979
1200.5547   1202.8714   1223.1079
1286.9222   1324.5343   1346.9842
1370.9550   1443.6516   1485.5054
1526.6706   1624.4922   1644.6548
3032.7177   3152.1823   3159.4398
3169.4634   3177.6653   3182.3038
3187.0956   3213.8857   3226.8684
!40.7168
      ZeroEnergy[kcal/mol]           -46.1
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W12 # [12] (A4b)
  Species
    RRHO
      Geometry[angstrom]    19
C                  0.349152    0.534603    0.216532
C                  1.474080    1.230577   -0.258043
C                  2.686322    0.582630   -0.465034
C                  2.810551   -0.777117   -0.183026
C                  1.714335   -1.476470    0.317204
C                  0.498697   -0.829355    0.519153
C                 -0.910299    1.267912    0.419649
C                 -2.176446    0.847073    0.229456
```

```
C                  -2.609614   -0.431087   -0.325029
C                  -3.862979   -0.833051   -0.398257
H                   1.385556    2.289656   -0.476987
H                   3.536948    1.139430   -0.842200
H                   3.756789   -1.282904   -0.337947
H                   1.808904   -2.528004    0.564895
H                  -0.331086   -1.374947    0.950941
H                  -0.786044    2.297592    0.746259
H                  -2.977623    1.539649    0.468784
H                  -1.834687   -1.083298   -0.738683
H                  -4.401555   -1.691461   -0.770695
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CHCHCHCH
        Group                   8 9 10 16 17 18 19
        Axis                    1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  1.351055758 0.304534797 1.872642984
      End
      Rotor     Hindered     ! vinyl
        Group                   10 18 19
        Axis                    8 9
        Symmetry                1
        Potential[kcal/mol]     8
0.  4.350788797 6.353178173 4.872771354 3.387549026 4.121831882
6.353165623 2.529745926
      End
      Frequencies[1/cm]         49
 161.1444
 204.3905               261.5355               341.3204
 411.9998               421.1128               506.5448
 522.6694               633.5929               658.0906
 702.5250               715.2594               756.2717
 784.2090               805.1112               835.8422
 856.4963               870.0258               937.5725
 983.4297              1000.7009              1005.7591
1015.3298              1049.9470              1082.7450
1106.2995              1182.4379              1203.7940
1211.7962              1246.8644              1273.3742
1333.6849              1355.9091              1431.0181
1476.6738              1525.0476              1610.0571
1623.9886              1641.9457              1669.0710
3045.5370              3131.8837              3158.1937
3160.7704              3165.3865              3175.3778
3186.3915              3194.0528              3242.0541
!  49.9576               95.2209
      ZeroEnergy[kcal/mol]           -38.2
      ElectronicLevels[1/cm]       1
           0   2
    End
  End
  Well       W13 # [13] (A5)
```

```
  Species
    RRHO
      Geometry[angstrom]    19
H       1.648587        -0.520319       0.000000
C       0.535192        -0.641408       0.000000
C       0.000000        0.777145        0.000000
C       -0.221521       1.406662        1.234810
C       -0.221521       1.406662        -1.234810
C       -0.221210       0.697827        2.414916
C       -0.221210       0.697827        -2.414916
C       -0.067147       -0.727814       2.404998
C       -0.067147       -0.727814       -2.404998
C       0.235228        -1.388157       1.269343
C       0.235228        -1.388157       -1.269343
H       -0.464470       2.462997        1.241098
H       -0.464470       2.462997        -1.241098
H       -0.425816       1.201714        3.349586
H       -0.425816       1.201714        -3.349586
H       -0.227968       -1.276630       3.324412
H       -0.227968       -1.276630       -3.324412
H       0.336292        -2.466247       1.256992
H       0.336292        -2.466247       -1.256992
      Core   RigidRotor
        SymmetryFactor          1
      End
      Frequencies[1/cm]         51
117. 153. 327. 353. 442. 470. 471. 515. 567. 610. 668.
684. 711. 772. 789. 798. 875. 918. 940. 966. 982. 985.
997. 999. 1070. 1072. 1110. 1161. 1174. 1184. 1203.
1259. 1262. 1336. 1342. 1404. 1420. 1471. 1508. 1515.
1628. 1630. 2684. 3146. 3150. 3152. 3154. 3170. 3172.
3186. 3186.
      ZeroEnergy[kcal/mol]            -65.8
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W14 # [14]
  Species
    RRHO
      Geometry[angstrom]    19
C 0.175611594 0.0831555282 -0.2067885345
C -0.4668373252 -0.9275087805 0.5136205008
C 0.0038793866 -2.2362755595 0.4641367608
C 1.1203217448 -2.5533421503 -0.3083616678
C 1.7655740935 -1.5510934701 -1.0283460676
C 1.2945420619 -0.2407335794 -0.9770891383
C -0.3653130313 1.5254794982 -0.214728224
C -1.474879171 1.6443061375 -1.2250022188
C -0.7909209937 1.9794127494 1.1128299084
C -1.156253173 2.3590485452 2.1925050293
H -1.3277212762 -0.6828025513 1.1254052414
H -0.4998885671 -3.0101273551 1.0327995994
H 1.4869798574 -3.5729385893 -0.3443258039
```

```
H 2.6395129561 -1.786273531 -1.6257072382
H 1.8049992873 0.5371901872 -1.536341279
H 0.4641863657 2.1694778573 -0.5340761316
H -2.503369181 1.4957620959 -0.924147963
H -1.229662862 1.6566760103 -2.2794437196
H -1.4693876998 2.6983423633 3.1491792047
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CH2CHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0. 0.533383152 1.593874359 0.470632192 0.451806905 0.509520217
1.493472824 0.458082001
     End
      Rotor     Hindered     ! CH2
        Group                  17 18
        Axis                   7 8
        Symmetry                1
        Potential[kcal/mol]     8
0. 0.175702685 0.48945748 0.332580083 0.069026055 0.194527973 0.52083296
0.269829124
     End
      Frequencies[1/cm]         49
 103.9539
 158.9172    195.2578    280.9014
 316.8738    411.7523    412.9700
 483.7882    527.9116    570.8359
 634.4594    644.0121    673.6199
 675.7857    712.6981    775.9286
 783.0436    854.0604    876.2601
 927.1266    978.9335   1001.6670
1018.0452   1047.9645   1060.2529
1080.5496   1107.5971   1181.4417
1184.6360   1203.5258   1239.6676
1317.6854   1345.1205   1364.6303
1445.1633   1484.7190   1522.9301
1626.6730   1640.4305   2220.4897
3002.7889   3142.9825   3153.7095
3163.0121   3172.5021   3181.2409
3189.6452   3259.2566   3477.5829
!27.4523 133.2678
      ZeroEnergy[kcal/mol]           -33.0
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W15 # [15]
  Species
    RRHO
      Geometry[angstrom]    19
C  0.3751111698 0.0618800253 -0.0163243666
```

```
C -0.6076725701 -0.7472119063 -0.6033280404
C -0.305579055 -2.0367691241 -1.0270231224
C 0.9818493729 -2.5488349897 -0.8674602717
C 1.9639341118 -1.7582142857 -0.2770750996
C 1.6617191627 -0.4657396955 0.1450848463
C 0.095008381 1.4537646742 0.4303886902
C -0.7988822433 2.4056429748 -0.3636596945
C -1.2879026208 1.8700757139 0.915295749
C -2.1964687044 1.7543954623 1.8141854636
H -1.6194339594 -0.3718773245 -0.7108060608
H -1.0799063914 -2.6478201093 -1.477683633
H 1.2139592829 -3.5555102693 -1.1958372478
H 2.9678200897 -2.1460560646 -0.1438144117
H 2.4337793933 0.1445617518 0.6023865521
H 0.915739047 1.9302177923 0.9591220706
H -1.2463021166 2.0233794027 -1.2769029017
H -0.507625211 3.4512816302 -0.4023905932
H -2.3647321626 1.2378900962 2.7454213021
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CH2CHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0. 0.778111892   1.305219947 0.803212275 0. 0.771836796   1.324045235
      0.809487371
     End
      Frequencies[1/cm]         50
  98.5003    169.5641
 235.7917    309.1201    365.1639
 412.5426    414.8875    539.5605
 549.8937    633.7097    672.2437
 700.5404    710.4861    742.2476
 775.5159    785.9991    850.0934
 878.4408    902.3981    934.8822
 976.0729    998.5173   1011.6432
1017.9453   1049.0110   1056.8217
1075.9297   1093.2421   1125.3272
1181.9034   1204.3893   1224.4227
1311.3784   1351.2653   1378.7105
1452.4326   1485.6807   1528.1934
1621.7874   1645.0605   1787.5008
3092.1506   3130.1643   3156.1261
3161.5898   3171.0427   3176.8270
3178.6306   3189.2594   3256.2249
!29.8608
      ZeroEnergy[kcal/mol]           -23.4
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W16 # [16]
```

```
  Species
    RRHO
      Geometry[angstrom]    19
C 0.3932433805 0.221599492 0.
C 0.9525816834 -1.087487386 0.
C 2.3247562654 -1.2770266641 0.
C 3.1958738532 -0.1836202892 0.
C 2.6713264216 1.1144310311 0.
C 1.3038415408 1.3169050484 0.
C -0.9979641668 0.4613873241 0.
C -2.0391393377 -0.6259855043 0.
C -3.410662282 -0.122413999 0.
C -4.5353943146 0.2983069573 0.
H 0.2982939431 -1.9512509482 0.
H 2.7257105148 -2.2847913491 0.
H 4.2682525836 -0.3397888366 0.
H 3.3411705101 1.9673081136 0.
H 0.9040236263 2.3254313344 0.
H -1.348602298 1.4864722651 0.
H -1.9033406193 -1.2821885624 0.8728702514
H -1.9033406193 -1.2821885624 -0.8728702514
H -5.531691685 0.6665875354 0.
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CH2CCH
        Group                  9 10 17 18 19
        Axis                   7 8
        Symmetry                1
        Potential[kcal/mol]     8
0.  0.426706521  0.558483535 1.769577044     3.319525731 1.769577044
      0.558483535 0.432981617
     End
      Frequencies[1/cm]         50
 102.1059              114.7180
 210.2181              234.5908              323.1762
 371.4645              410.2228              478.2050
 488.0338              610.5176              612.8485
 627.9984              659.1584              682.6465
 689.0400              765.0389              827.5961
 851.5629              892.3266              913.4571
 964.3279              972.0364              990.8252
 993.9108             1038.5004             1068.2605
1117.2053             1176.7843             1188.5926
1214.5752             1235.3845             1299.0511
1333.6213             1352.6089             1426.0768
1457.3638             1482.1350             1506.5489
1579.9868             1603.1075             2228.9863
2968.8485             2979.6146             3159.0362
3164.5793             3175.2869             3183.0197
3184.0061             3192.2049             3478.2585
!30.9503
      ZeroEnergy[kcal/mol]           -44.0
      ElectronicLevels[1/cm]        1
```

```
          0   2
    End
  End
  Well       W17 # [17]
  Species
    RRHO
      Geometry[angstrom]    19
C 0.4293858489 -0.3418141256 -0.2657983746
C -0.8592349871 -0.9268847183 -0.149649254
C -1.0659317106 -2.177469943 0.3747653797
C 0.0918847563 -2.8672214573 0.7971473464
C 1.3726457794 -2.3031623468 0.6816912469
C 1.5815865788 -1.0313760766 0.1475693842
C -0.0846501279 0.850542623 -0.8351206813
C -1.5296730456 0.3207742373 -0.7765635119
C -2.5541323165 1.0440091788 0.0517349054
C -2.3592336772 2.1899145743 0.6966784343
H -2.0466256143 -2.630532339 0.469286655
H -0.006286318 -3.8602123091 1.2212830866
H 2.2251611484 -2.881219588 1.0219207938
H 2.5781482216 -0.6128481795 0.0676374364
H 0.3456768517 1.7702717197 -1.20696017
H -1.9512998609 0.1038891135 -1.7677529406
H -3.5282987124 0.5606905917 0.1065081057
H -1.4035242053 2.7026950917 0.6703540789
H -3.1485675783 2.6515473933 1.2789986711
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   8 9
        Symmetry                2
        Potential[kcal/mol]     4
1.424446769 3.099897375 1.524848304 0. 3.037146416 2.208833757
1.838603099 2.867718826
     End
      Frequencies[1/cm]         50
 120.1056              158.1866
 261.0116              294.3082              389.5210
 429.9400              516.2146              519.7110
 540.4187              596.8057              642.1241
 684.8521              729.0565              757.4019
 833.1849              855.8417              882.4536
 921.3500              934.9576              946.9480
 978.7454              983.7075             1009.9194
1031.7490             1077.8055             1097.7006
1121.4407             1159.3936             1177.5504
1201.1100             1232.5117             1310.6126
1315.4366             1329.5743             1387.5455
1443.1015             1445.7775             1490.7138
1573.8941             1630.8790             1702.1866
2993.2657             3119.3862             3134.8050
3159.3769             3169.1705             3180.0149
```

```
3187.4105              3211.2648              3214.8731
!70.7669
      ZeroEnergy[kcal/mol]            -41.1
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W18  # [18']
  Species
    RRHO
      Geometry[angstrom]    19
C                  0.408010   -0.548316   -0.0
C                  1.650245   -1.224983    0.0
C                  2.857745   -0.533648    0.0
C                  2.881546    0.860181    0.0
C                  1.671304    1.571250    0.0
C                  0.517146    0.834641   -0.0
C                 -0.834243   -1.321328   -0.0
C                 -2.113456   -0.889529   -0.0
C                 -2.589860    0.479635    0.0
C                 -3.887936    0.810617    0.0
H                  1.649262   -2.311018    0.0
H                  3.789304   -1.088014    0.0
H                  3.824591    1.395913    0.0
H                  1.661792    2.655861   -0.0
H                 -0.680858   -2.396961    0.0
H                 -2.888722   -1.652577   -0.0
H                 -1.841159    1.267486    0.0
H                 -4.210864    1.844692    0.0
H                 -4.666346    0.053485   -0.0
      Core   MultiRotor
        SymmetryFactor          1
        InterpolationEnergyMax[kcal/mol]        100
        PotentialEnergySurface[kcal/mol]        c10h9_pva_18.dat
!        QuantumLevelEnergyMax[kcal/mol]         5
        InternalRotation
                Group                           8 9 10 15 16 17 18 19
                Axis                            1 7
                Symmetry                        1
                MassExpansionSize               11
!               PotentialExpansionSize          11
!               HamiltonSizeMin                 13
!               HamiltonSizeMax                 101
                GridSize                        100
        End
        InternalRotation
                Group                           10 17 18 19
                Axis                            8 9
                Symmetry                        1
                MassExpansionSize               11
!               PotentialExpansionSize          11
!               HamiltonSizeMin                 13
!               HamiltonSizeMax                 101
                GridSize                        100
```

```
        End
      End
      Frequencies[1/cm]         49
 113.2672
 170.5873               268.5193               350.5420
 372.1737               415.5944               518.0314
 521.4308               626.6929               652.5916
 713.5941               713.9168               751.2289
 804.4919               821.6647               860.3607
 935.3704               939.2281               942.8331
 980.4010               986.9728               993.1368
1039.8542              1043.6909              1116.5497
1147.7880              1176.7178              1215.3708
1245.5041              1296.0415              1316.5398
1327.7207              1406.9601              1442.6252
1472.2358              1483.7737              1564.8904
1620.2862              1645.6514              1686.7714
3123.1897              3130.6947              3135.9956
3150.0273              3154.0143              3161.1453
3173.2693              3187.0179              3219.0318
!44.7268                119.6404
      ZeroEnergy[kcal/mol]           -38.2
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W19 # [19]
  Species
    RRHO
      Geometry[angstrom]    19
C 0.2956820346 0.7034620021 -1.3230830644
 C -0.5178414775 -0.4818118509 -1.6571384871
 C 0.0228554305 -1.7390760703 -1.6774776292
 C 1.3882971731 -1.957981618 -1.3833507577
 C 2.2121097361 -0.8545648679 -1.063733013
 C 1.7144980606 0.4202625699 -1.0310524888
 C -0.3864481076 1.9172531734 -0.6361277695
 C -0.1010173269 2.0803971966 -1.8871944552
 C -0.9122091012 2.3400769904 0.6382950978
 C -1.4867684772 3.527778556 0.8568133543
 H -1.5664685393 -0.3239000301 -1.8865850238
 H -0.6085503214 -2.5864353056 -1.9259759595
 H 1.7990884843 -2.9596307735 -1.405188309
 H 3.261208594 -1.0227907792 -0.8411592879
 H 2.3552145822 1.2611569085 -0.7869499329
 H -0.0858261822 2.6814109275 -2.7828352353
 H -0.8221258744 1.6244891761 1.4502159918
 H -1.5928768538 4.2624277726 0.0661407061
 H -1.8671908668 3.7953979594 1.8356172561
      Core   RigidRotor
        SymmetryFactor          1
      End
!      Rotor     Hindered     ! vinyl
!        Group                  10 17 18 19
```

```
!        Axis                    7 9
!        Symmetry                 1
!        Potential[kcal/mol]      8
!
!     End
      Frequencies[1/cm]         51
  24.2941                70.1137                120.3237
 186.4550               293.4023                295.5015
 390.3312               427.6676                461.7996
 498.9798               598.9898                607.5480
 631.7433               655.1742                727.2360
 747.2008               756.5625                778.8115
 813.2310               914.9120                947.7689
 956.8432               962.5053                969.5831
 989.1907               997.4866               1022.9027
1085.0832              1091.1541               1113.6429
1139.8172              1198.0972               1270.1392
1323.4447              1325.8122               1408.8794
1442.2897              1455.3599               1535.0814
1586.7316              1662.7870               1827.0245
3137.9457              3149.7491               3151.8470
3155.6989              3170.9063               3171.1144
3192.8421              3226.2568               3234.3204
!
      ZeroEnergy[kcal/mol]            -14.4
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Well       W20 # [20]
  Species
    RRHO
      Geometry[angstrom]    19
C                  0.363846   -0.593772   -0.00
C                  1.639120   -1.212440    0.00
C                  2.806068   -0.465816    0.00
C                  2.746723    0.929740    0.00
C                  1.501750    1.562158   -0.00
C                  0.328651    0.821500   -0.00
C                 -0.798737   -1.433984   -0.00
C                 -2.176372   -1.098642   -0.00
C                 -2.786343    0.090761    0.00
C                 -3.457383    1.204507    0.00
H                  1.693718   -2.296262    0.00
H                  3.766993   -0.968431    0.00
H                  3.658303    1.516230    0.00
H                  1.447731    2.645457   -0.00
H                 -0.623719    1.332674   -0.00
H                 -0.595621   -2.500036   -0.000
H                 -2.854310   -1.952149   -0.000
H                 -3.748517    1.6992265   0.9253915
H                 -3.748517    1.6992265  -0.9253915
      Core   RigidRotor
        SymmetryFactor          1
```

```
      End
      Rotor     Hindered     ! CHCHCCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  3.175198525  7.749743437  3.005770936
     End
      Frequencies[1/cm]         50
 118.4600              137.0140
 226.3050              255.3546              308.4895
 379.3045              411.4924              494.7862
 524.8081              543.3135              629.6090
 693.4713              731.8260              740.4519
 789.0267              802.5947              841.0340
 880.5937              911.8557              916.0046
 974.6881              979.7133              990.5591
 995.7770             1008.8681             1046.1161
1108.8460             1158.9066             1180.0123
1196.9721             1249.7005             1327.4114
1353.4873             1385.0767             1436.2701
1463.7534             1494.4555             1515.1049
1595.9553             1618.3201             1932.7109
3076.5320             3102.6598             3138.4032
3155.3064             3160.7061             3164.7509
3174.5894             3188.0549             3216.0293
!43.6257
      ZeroEnergy[kcal/mol]           -53.4
      ElectronicLevels[1/cm]       1
           0   2
    End
  End
  Well       W21 # [21, (20-trans)]
  Species
    RRHO
      Geometry[angstrom]    19
C 0.2847901212 -0.6430007369 0.1099367044
C 1.5134779094 -1.3489731566 0.1444101528
C 2.7287691518 -0.6889963833 0.0574719351
C 2.7689147656 0.7016602428 -0.0673177333
C 1.5707345427 1.4202205548 -0.103492417
C 0.3516125811 0.7670592146 -0.0170741081
C -0.9416704519 -1.3757114975 0.2035012375
C -2.2486587157 -0.8312636828 0.1839510441
C -3.3712525987 -1.548037649 0.2739925845
C -4.4668131195 -2.2408593787 0.361227835
H 1.4918723576 -2.4294986651 0.2411303507
H 3.6519898289 -1.2572519155 0.086695327
H 3.7190031185 1.2185772295 -0.1353676089
H 1.5922735208 2.5002582364 -0.2000682267
H -0.5604410873 1.350963609 -0.0476996418
H -0.861328366 -2.4538379199 0.2985515163
H -2.3686014627 0.2459774159 0.0893801197
H -4.9710666864 -2.6305128601 -0.5215880645
```

```
H -4.9294734094 -2.4641236575 1.3212209932
      Core   RigidRotor
        SymmetryFactor          1
      End
      Rotor     Hindered     ! CHCHCCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0. 3.595629951   9.155364918 3.501503512
     End
      Frequencies[1/cm]         50
  69.9259              103.2749
 225.3209              230.0342              296.3701
 376.9712              410.8597              494.6996
 509.1355              546.0657              627.1816
 634.8426              691.5510              752.1307
 805.2838              834.7425              859.2114
 883.1174              901.6249              913.5049
 971.2917              990.7804              992.0434
1000.7318             1040.9754             1059.3960
1100.3365             1173.3714             1184.3795
1192.1831             1242.1007             1300.0938
1338.1518             1354.6966             1430.3385
1467.0837             1499.0125             1511.8115
1592.3224             1614.9859             1948.0879
3079.3071             3125.0561             3140.9994
3157.1752             3161.1132             3164.4790
3174.6407             3183.0281             3191.8164
!95.6777
      ZeroEnergy[kcal/mol]           -54.8
      ElectronicLevels[1/cm]        1
           0   2
    End
  End
  Bimolecular      R1    # C6H5+C4H4
     Fragment        C6H5
      RRHO
        Geometry[angstrom]     11
C     0.000000     0.000000     1.390346
C     0.000000     1.221722     0.769740
C     0.000000     -1.221722     0.769740
C     0.000000     1.208778     -0.629525
C     0.000000     -1.208778     -0.629525
C     0.000000     0.000000     -1.319309
H     0.000000     2.153977     1.319039
H     0.000000     -2.153977     1.319039
H     0.000000     2.145530     -1.172910
H     0.000000     -2.145530     -1.172910
H     0.000000     0.000000     -2.401057
         Core     RigidRotor
         SymmetryFactor       2
         End
         Frequencies[1/cm]      27
```

```
402. 428. 602. 621. 672. 726. 820. 903. 979. 1001. 1009.
1017. 1052. 1073. 1177. 1177. 1303. 1326. 1464. 1473.
1570. 1627. 3154. 3160. 3173. 3175. 3186.
         ZeroEnergy[kcal/mol]         0.
         ElectronicLevels[1/cm]        1
             0   2
    End
     Fragment        C4H4
      RRHO
        Geometry[angstrom]     8
C                    -0.121777   -1.696291    0.000000
C                     0.577127   -0.556570    0.000000
H                     0.380759   -2.655833    0.000000
H                    -1.205246   -1.698019    0.000000
C                     0.000000    0.743633    0.000000
H                     1.663858   -0.592912    0.000000
C                    -0.451683    1.860294    0.000000
H                    -0.861371    2.840371    0.000000
        Core     RigidRotor
          SymmetryFactor        1
        End
        Frequencies[1/cm]       18
 224.5636               317.2210               558.0616
 649.0310               680.5666               704.0299
 892.5128               955.0465              1010.7565
1111.7851              1321.1849              1443.6994
1668.9159              2205.5991              3136.5225
3147.7200              3236.6300              3477.4967
        ZeroEnergy[kcal/mol]          0.
        ElectronicLevels[1/cm]        1
             0   1
      End
      GroundEnergy[kcal/mol]       0.0
   End
  Bimolecular      P1    # N1 + H
     Fragment        Naphthalene
       RRHO
       Geometry[angstrom]      18
C       0.000000        0.000000        0.715661
C       0.000000        0.000000        -0.715661
C       0.000000        1.243465        1.400275
C       0.000000        -1.243465       1.400275
C       0.000000        1.243465        -1.400275
C       0.000000        -1.243465       -1.400275
C       0.000000        2.429373        0.707395
C       0.000000        -2.429373       0.707395
C       0.000000        2.429373        -0.707395
C       0.000000        -2.429373       -0.707395
H       0.000000        1.241873        2.485452
H       0.000000        -1.241873       2.485452
H       0.000000        1.241873        -2.485452
H       0.000000        -1.241873       -2.485452
H       0.000000        3.372182        1.242827
H       0.000000        -3.372182       1.242827
```

```
H       0.000000        3.372182        -1.242827
H       0.000000        -3.372182       -1.242827
       Core      RigidRotor
         SymmetryFactor       4
       End
       Frequencies[1/cm]       48
174.  186. 366. 396.  480.  488.  519.  520.  635.  636.
729.  773.  787.  799.  809.  850.  897.  951.  957.  974.
993.  1000.  1036.  1046.  1151.  1169.  1172.  1185.  1232.
1270.  1287.  1391.  1399.  1418.  1491.  1492.  1549.  1614.
1641.  1671.  3156.  3158.  3160.  3164.  3174.  3175.
3187.  3188.
       ZeroEnergy[kcal/mol]        0.
       ElectronicLevels[1/cm]      1
         0    1
       End
     Fragment     H
       Atom
         Mass[amu]   1
         ElectronicLevels[1/cm]      1
            0    2
       End
     GroundEnergy[kcal/mol]             -63.3
   End
  Bimolecular      P2    # A19 (cis-1-phenyl-vinylacetylene) + H
     Fragment        C6H5CHCHCCH-cis
       RRHO
       Geometry[angstrom]      18
C                  0.000000    0.634987    0.000000
C                  0.809169    1.786273    0.000000
C                  2.195677    1.696039    0.000000
C                  2.811035    0.446045    0.000000
C                  2.025500   -0.706454    0.000000
C                  0.638684   -0.618852    0.000000
C                 -1.450217    0.825119    0.000000
C                 -2.467720   -0.063875    0.000000
C                 -2.412870   -1.479395    0.000000
C                 -2.458772   -2.685057    0.000000
H                  0.335711    2.762742    0.000000
H                  2.795530    2.599219    0.000000
H                  3.892500    0.369650    0.000000
H                  2.498072   -1.682477    0.000000
H                  0.046277   -1.522660    0.000000
H                 -1.753322    1.868785    0.000000
H                 -3.475696    0.342851    0.000000
H                 -2.481987   -3.747096    0.000000
       Core      RigidRotor
         SymmetryFactor       1
       End
      Rotor     Hindered     ! CHCHCCH
        Group                  8 9 10 16 17 18
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
```

```
0.  1.569527614 4.403995962 1.4762138
      End
       Frequencies[1/cm]       47
 122.8633               156.4537
 233.5966               304.2421               380.9169
 413.1899               435.3553               517.5030
 583.0498               631.1568               633.2581
 674.6979               704.8687               739.6807
 748.1223               801.4766               806.1642
 852.0880               933.9045               971.9751
 978.6414               993.6595              1006.0081
1016.1663              1052.1990              1110.8271
1183.6446              1205.1384              1212.6300
1273.1152              1344.5664              1364.1269
1444.9712              1481.6265              1527.7432
1611.5487              1641.1000              1658.0564
2188.6240              3131.5827              3150.5173
3157.8087              3165.9620              3176.1038
3188.5743              3219.4263              3475.5412
!32.9329
       ZeroEnergy[kcal/mol]           0.
       ElectronicLevels[1/cm]      1
         0    1
       End
     Fragment     H
       Atom
         Mass[amu]   1
         ElectronicLevels[1/cm]      1
            0    2
       End
     GroundEnergy[kcal/mol]             -7.7
   End
 Bimolecular      P3    # A18 (trans-1-phenyl-vinylacetylene) + H
     Fragment        C6H5CHCHCCH-trans
       RRHO
       Geometry[angstrom]      18
C                   -0.382320   -0.190952   -0.000415
C                   -0.933945    1.102927   -0.000542
C                   -2.309164    1.290582   -0.000124
C                   -3.172688    0.193485    0.000381
C                   -2.644594   -1.094721    0.000410
C                   -1.266320   -1.282738   -0.000016
C                    1.056992   -0.454906   -0.000714
C                    2.051683    0.454558    0.000638
C                    3.427248    0.115680    0.000209
C                    4.606627   -0.136088    0.000160
H                   -0.283847    1.969858   -0.001108
H                   -2.712895    2.296905   -0.000255
H                   -4.246075    0.344594    0.000687
H                   -3.305538   -1.954164    0.000748
H                   -0.860830   -2.289142    0.000012
H                    1.337164   -1.504723   -0.002041
H                    1.827786    1.517714    0.002220
H                    5.643108   -0.368000   -0.000187
```

```
       Core      RigidRotor
         SymmetryFactor       1
       End
      Rotor     Hindered     ! CHCHCCH
        Group                  8 9 10 16 17 18
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0. 1.474647537   4.812998555 1.462097345
      End
       Frequencies[1/cm]       47
   88.1859    105.4856
  236.9909    246.5241    377.6284
  407.8833    420.1650    492.2572
  534.0235    622.4087    632.4259
  637.0955    680.6630    703.2350
  767.3202    845.4647    858.4914
  870.2819    926.5100    977.1610
  989.0688   1004.4865   1014.4175
 1033.2707   1052.1850   1106.7065
 1183.5622   1205.0301   1233.4754
 1295.7938   1328.6642   1350.8106
 1364.0935   1480.6248   1527.6530
 1615.3155   1641.3240   1668.8536
 2195.3287   3141.7539   3152.5224
 3160.8428   3166.8618   3175.7304
 3183.6745   3192.3435   3477.2991
!43.9705
       ZeroEnergy[kcal/mol]           0.
       ElectronicLevels[1/cm]      1
         0    1
       End
     Fragment     H
       Atom
         Mass[amu]   1
         ElectronicLevels[1/cm]      1
            0    2
       End
     GroundEnergy[kcal/mol]             -8.55
   End
 Bimolecular      P4    # 4-phenyl-vinylacetylene + H
     Fragment        C6H5CCCHCH2
       RRHO
       Geometry[angstrom]      18
C                    0.484021   -0.078692    0.000924
C                    1.300122   -1.224860    0.000402
C                    2.684087   -1.103027   -0.000547
C                    3.279738    0.157874   -0.000935
C                    2.480687    1.300693   -0.000356
C                    1.095861    1.188333    0.000607
C                   -0.933812   -0.199451    0.001718
C                   -2.140981   -0.297415    0.000361
C                   -3.549967   -0.450839   -0.000680
C                   -4.430629    0.558646   -0.000742
```

```
H                     0.834825   -2.203106    0.000685
H                     3.300766   -1.994756   -0.000980
H                     4.359873    0.249273   -0.001659
H                     2.938748    2.283358   -0.000654
H                     0.472519    2.074293    0.001064
H                    -3.916409   -1.475017   -0.001470
H                    -4.108826    1.593245    0.000073
H                    -5.496256    0.365136   -0.001568
       Core      RigidRotor
         SymmetryFactor       1
       End
      Rotor     Hindered     ! vinyl
        Group                  10 16 17 18
        Axis                   8 9
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.470632192  0.953814577 0.476907288
      End
       Frequencies[1/cm]       47
   71.0509     90.8319
  200.9453    235.1965    375.1708
  394.2995    411.0865    508.1349
  547.9912    583.4041    638.6494
  695.1720    705.3333    717.7347
  775.5331    853.0463    932.6650
  940.2360    950.3620    981.3560
 1002.9667   1006.9362   1014.7197
 1048.5179   1100.6273   1102.5990
 1182.7522   1199.9772   1296.4159
 1310.3475   1320.1664   1351.4984
 1448.5387   1473.0906   1524.4206
 1607.8032   1638.4190   1665.4240
 2299.3394   3130.9663   3146.4054
 3164.3692   3172.5552   3184.0910
 3191.6309   3196.0085   3235.9421
!40.1661
       ZeroEnergy[kcal/mol]           0.
       ElectronicLevels[1/cm]      1
         0    1
       End
     Fragment     H
       Atom
         Mass[amu]   1
         ElectronicLevels[1/cm]      1
            0    2
       End
     GroundEnergy[kcal/mol]             -10.0
   End
 Bimolecular      P5    # phenylbutatriene + H
     Fragment        C6H5CHCCCH2
       RRHO
       Geometry[angstrom]      18
C                  -0.451861   -0.465416   -0.0
C                  -0.584437    0.934044   -0.0
```

```
C                  -1.840044    1.524536   -0.0
C                  -2.992140    0.734812    0.0
C                  -2.875836   -0.653188    0.0
C                  -1.618115   -1.247287   -0.0
C                   0.853509   -1.126664    0.0
C                   2.036840   -0.529469   -0.0
C                   3.170346    0.024077   -0.0
C                   4.355482    0.599773    0.0
H                   0.308384    1.548829   -0.0
H                  -1.925539    2.605508   -0.0
H                  -3.971245    1.200083    0.0
H                  -3.764963   -1.273677    0.0
H                  -1.531136   -2.328935   -0.0
H                   0.834309   -2.215492    0.0
H                   5.268109    0.012381    0.0
H                   4.459627    1.680000   -0.0
       Core      RigidRotor
         SymmetryFactor       1
       End
      Rotor     Hindered     ! CHCCCCH2
        Group                  8 9 10 16 17 18
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0. 2.779867484   6.752003188 2.804967867
      End
       Frequencies[1/cm]       47
  75.8972              193.0238
 239.4403              252.8587              338.4970
 413.8440              418.8752              430.6240
 539.8037              597.7979              628.7253
 633.8635              706.5575              774.9405
 824.3220              851.6566              860.1551
 882.2726              935.5073              948.9032
 981.6315             1003.6833             1015.2817
1029.2404             1048.8969             1105.5992
1182.1287             1198.5828             1228.6799
1298.6171             1348.9246             1361.6210
1445.9315             1486.1146             1523.7681
1615.4188             1639.0391             1676.8023
2182.9480             3115.0328             3120.3898
3158.6155             3165.4352             3174.6737
3182.8000             3191.2877             3196.5284
!53.0287
       ZeroEnergy[kcal/mol]           0.
       ElectronicLevels[1/cm]      1
         0    1
       End
     Fragment     H
       Atom
         Mass[amu]   1
         ElectronicLevels[1/cm]      1
            0    2
       End
```

```
     GroundEnergy[kcal/mol]             -2.2
   End
 Bimolecular      P6    # 2-phenyl-vinylacetylene + H
     Fragment        2-phenyl-vinylacetylene
       RRHO
       Geometry[angstrom]      18
C -0.6656465244 -0.5377507864 0.0377525794
C -0.9382337215 -1.5152457076 1.0037676911
C -0.3055505578 -2.7540218478 0.9610303863
C 0.6216796366 -3.0348181068 -0.039523857
C 0.9153485927 -2.0635396482 -0.995296808
C 0.2810909708 -0.8266815125 -0.955376811
C -1.3732354696 0.7746209541 0.0652975546
C -1.634072041 1.4888045646 -1.0443320057
C -1.8006122179 1.2684626191 1.3405657527
C -2.1568466172 1.6714631301 2.4178140429
H -1.6556051102 -1.3010774031 1.7869340001
H -0.5365519551 -3.5002198741 1.7130453718
H 1.1194163719 -3.9974693928 -0.0690109609
H 1.6500293925 -2.2649615696 -1.7669356511
H 0.541172534 -0.0690988864 -1.6851949387
H -2.1393091752 2.4439031503 -0.9865675589
H -1.3620342808 1.1240171385 -2.0266785206
H -2.4684961188 2.0380918365 3.3649189822
       Core      RigidRotor
         SymmetryFactor       1
       End
      Rotor     Hindered     ! CHCCCCH2
        Group                  8 9 10 16 17 18
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0. 2.045681263 1.154617646 0.200803069  0. 2.045681263 1.123242166
0.200803069
      End
       Frequencies[1/cm]       47
 118.6846              161.3469
 250.4095              292.5531              395.0883
 415.5910              419.7688              487.9697
 619.4421              632.3565              639.0731
 654.6454              685.7325              706.7321
 731.0242              741.9694              793.3808
 856.3705              915.6116              928.3757
 938.5337              982.9370             1003.4459
1017.1670             1049.9358             1103.8487
1127.0601             1183.1760             1206.6794
1295.8079             1331.6798             1356.7784
1431.3453             1478.4705             1526.4856
1615.7464             1643.1610             1650.6728
2203.6069             3155.6348             3162.0157
3170.5053             3180.8446             3188.0538
3193.4202             3246.0761             3476.2262
!46.5850
       ZeroEnergy[kcal/mol]          0.
```

```
       ElectronicLevels[1/cm]      1
         0    1
       End
     Fragment     H
       Atom
         Mass[amu]   1
         ElectronicLevels[1/cm]      1
            0    2
       End
     GroundEnergy[kcal/mol]             -7.6
   End
   Barrier      B1   R1   W1    #  ts [0]-[1]
   Variational
     RRHO
       Geometry[angstrom]     19        # 2.51
C 0.9397097498 -0.3859231857 -0.0225709981
C 2.1339654764 -1.0613630272 -0.1501865574
C 3.3091597305 -0.3177551643 0.0307400971
C 3.2377946309 1.0441171398 0.3268473095
C 2.000886726 1.6800250607 0.4460379306
C 0.8148628916 0.9540096415 0.2697506643
C -1.277392643 -1.487277592 -0.451937797
C -2.1371027682 -0.8407722066 0.3570895908
C -2.7985311578 0.3651610196 -0.0059562506
C -3.3650468955 1.3973171318 -0.286972189
H 2.1781387206 -2.1197946591 -0.3810558307
H 4.273578694 -0.8057140938 -0.0599319754
H 4.1500926843 1.6119025601 0.465558716
H 1.953864074 2.7388716642 0.6763153692
H -0.1549952275 1.4296299463 0.3594815973
H -0.8289916483 -2.4218397785 -0.142144420
H -1.1199685286 -1.1689356429 -1.473743746
H -2.317974327 -1.2115528125 1.3608309741
H -3.8642331592 2.2977659188 -0.5470367523
       Core     RigidRotor
         SymmetryFactor    1
       End
!       Tunneling      Eckart
!         ImaginaryFrequency[1/cm]    173.7179
!         WellDepth[kcal/mol]         36.9
!         WellDepth[kcal/mol]         13.9
!       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.547166481 1.011041123 0.564948315
     End
       Frequencies[1/cm]     49
  45.2803
  56.0485               98.9485              187.8237
 224.8482              353.8820              397.9512
 422.5669              555.3380              592.4263
```

```
 605.6434               624.2435               629.6627
 675.9243               715.5847               726.9212
 828.0266               887.4137               897.1396
 914.8523               948.6886               955.5230
 985.9601              1003.6297              1027.6809
1056.3805              1081.8762              1118.7599
1180.3294              1185.6609              1317.8613
1322.6590              1342.0603              1447.9433
1468.4332              1480.6534              1588.9775
1642.1842              1652.5305              2207.2099
3175.3644              3177.9258              3183.2142
3184.3696              3195.0304              3200.5629
3211.5082              3274.4249              3496.9318
!20.7395
        ZeroEnergy[kcal/mol]          -0.34
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.49
C                         -0.60147  -0.53158   0.03633
C                         -1.76411  -1.26529   0.13129
C                         -2.97206  -0.55394   0.09321
C                         -2.963     0.83548  -0.0369
C                         -1.75633   1.53099  -0.13035
C                         -0.53853   0.83788  -0.09522
C                          1.64547  -1.59382   0.22536
C                          2.44899  -0.82316  -0.53324
C                          3.09521   0.34765  -0.04968
C                          3.64766   1.35354   0.33551
H                         -1.76001  -2.34477   0.2327
H                         -3.91328  -1.08821   0.16473
H                         -3.90033   1.37815  -0.0659
H                         -1.75767   2.61091  -0.23126
H                          0.40866   1.35991  -0.16779
H                          1.21179  -2.49855  -0.17937
H                          1.53556  -1.41531   1.28661
H                          2.58895  -1.05793  -1.58344
H                          4.13533   2.22936   0.68586
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0. 0.552208439 1.022840632 0.577308823
     End
       Frequencies[1/cm]     49
  47.1562
  59.2459               102.2249               191.9457
 225.1736               356.8476               397.9187
 423.3156               555.0312               588.9783
```

```
 605.9861               623.3603               629.8926
 676.0239               715.7603               728.1653
 828.3602               887.5139               896.5882
 909.0543               948.6279               955.4949
 986.1252              1001.3382              1027.7637
1056.4738              1082.0337              1118.9761
1180.3798              1185.7908              1317.9387
1320.6980              1342.3134              1446.5736
1468.5948              1480.7984              1588.8832
1641.5380              1644.3532              2206.1204
3175.3896              3177.7936              3183.2146
3184.2201              3194.8292              3200.2929
3211.4489              3274.4694              3496.9854
!21.0428
        ZeroEnergy[kcal/mol]          -0.29
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.47
C                  -0.594413   -0.526754    0.040958
C                  -1.755356   -1.263412    0.136107
C                  -2.965487   -0.556077    0.094911
C                  -2.960724    0.833041   -0.038635
C                  -1.756066    1.532011   -0.132399
C                  -0.536306    0.842661   -0.094296
C                   1.630490   -1.590512    0.219007
C                   2.437646   -0.819722   -0.538270
C                   3.091906    0.343781   -0.049733
C                   3.651814    1.343763    0.340348
H                  -1.748164   -2.342625    0.240415
H                  -3.905093   -1.093153    0.166603
H                  -3.899712    1.372699   -0.070116
H                  -1.760634    2.611662   -0.236047
H                   0.409340    1.367474   -0.167396
H                   1.195135   -2.493174   -0.188552
H                   1.531020   -1.421497    1.282847
H                   2.571351   -1.048460   -1.590580
H                   4.145731    2.214394    0.694831
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.552208439 1.029115728 0.583583919
     End
       Frequencies[1/cm]     49
  48.5445
  63.2250               105.7086               196.5140
 225.6190               359.9084               397.8872
 424.2520               554.5666               585.1918
```

```
 606.3628               622.2785               630.0742
 676.1179               715.9505               729.3653
 828.6971               887.6459               894.8019
 904.0192               948.5743               955.4407
 986.2688               998.7362              1027.8651
1056.5771              1082.2424              1119.2169
1180.4273              1185.9725              1316.8887
1319.5231              1342.5630              1445.1128
1468.7433              1480.9854              1588.7570
1633.9768              1642.6432              2204.7564
3175.3722              3177.6532              3183.2176
3184.0600              3194.5886              3200.0218
3211.3887              3274.3729              3497.0339
!21.3664
        ZeroEnergy[kcal/mol]          -0.26
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.45
C                  -0.587518   -0.522008    0.044309
C                  -1.746707   -1.261655    0.139813
C                  -2.958989   -0.558273    0.096504
C                  -2.958537    0.830608   -0.039633
C                  -1.755939    1.533059   -0.133904
C                  -0.534235    0.847422   -0.093811
C                   1.615344   -1.586714    0.213935
C                   2.426828   -0.816747   -0.542484
C                   3.088848    0.339879   -0.049939
C                   3.655959    1.334244    0.344385
H                  -1.736382   -2.340652    0.246299
H                  -3.896963   -1.098159    0.168511
H                  -3.899176    1.367287   -0.072783
H                  -1.763749    2.612490   -0.239645
H                   0.409874    1.374966   -0.167591
H                   1.178957   -2.487944   -0.195695
H                   1.526306   -1.426366    1.280046
H                   2.554807   -1.040436   -1.596554
H                   4.156002    2.199926    0.702369
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.552208439 1.041665919 0.589859015
     End
       Frequencies[1/cm]     49
  49.6823
  67.5618               109.3800               201.0007
 226.0508               363.0542               397.8791
 425.3331               553.9321               581.1795
```

```
 606.7750               620.9677               630.3465
 676.1823               716.1621               730.5466
 829.0649               887.7770               890.2924
 901.3493               948.5341               955.4033
 986.2968               995.9329              1027.9706
1056.7039              1082.4475              1119.4949
1180.4788              1186.1415              1314.3195
1319.5818              1342.8535              1443.4806
1468.9256              1481.1837              1588.4673
1624.8932              1642.6038              2203.0576
3175.2894              3177.5260              3183.2509
3183.9206              3194.3782              3199.7444
3211.3334              3274.2615              3497.0546
!21.6447
        ZeroEnergy[kcal/mol]          -0.2456
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.43
C                  -0.581062   -0.518901    0.046879
C                  -1.739433   -1.260092    0.142606
C                  -2.952956   -0.559081    0.097756
C                  -2.955050    0.829612   -0.040323
C                  -1.753630    1.534024   -0.134996
C                  -0.530851    0.850530   -0.093439
C                   1.600164   -1.583272    0.210108
C                   2.416171   -0.814281   -0.546027
C                   3.084727    0.336349   -0.050436
C                   3.657975    1.325802    0.347767
H                  -1.727313   -2.338921    0.250703
H                  -3.889979   -1.100594    0.169988
H                  -3.896647    1.364537   -0.074708
H                  -1.763306    2.613288   -0.242309
H                   0.412370    1.379626   -0.167765
H                   1.164576   -2.484345   -0.200759
H                   1.521522   -1.430912    1.278225
H                   2.539191   -1.034009   -1.601481
H                   4.163255    2.187190    0.708731
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.558483535 1.054216111 0.602409206
     End
       Frequencies[1/cm]     49
  50.9426
  72.4902              113.4440              205.8570
 226.7046              366.3267              397.9037
 426.6009              553.0077              577.0407
```

```
 607.2277               619.3551               630.6992
 676.1760               716.4029               731.6642
 829.4636               883.5561               888.0695
 900.4181               948.5085               955.3865
 985.9572               993.0546              1028.0845
1056.8612              1082.6814              1119.8454
1180.5363              1186.3400              1310.9346
1319.9386              1343.1758              1441.5766
1469.1379              1481.4058              1587.8177
1615.5264              1642.6721              2200.9482
3175.0732              3177.4263              3183.3046
3183.8291              3194.2321              3199.5524
3211.2710              3274.0667              3497.0437
!22.1771
        ZeroEnergy[kcal/mol]          -0.2486
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.41
C                  -0.574188   -0.515378    0.049950
C                  -1.731571   -1.258433    0.145765
C                  -2.946568   -0.560264    0.099040
C                  -2.951688    0.828217   -0.041138
C                  -1.751677    1.534990   -0.136064
C                  -0.527617    0.854062   -0.092753
C                   1.585089   -1.580098    0.205731
C                   2.404725   -0.811097   -0.550155
C                   3.080267    0.332871   -0.050922
C                   3.660211    1.316909    0.351424
H                  -1.717325   -2.337070    0.255663
H                  -3.882452   -1.103732    0.171388
H                  -3.894425    1.361040   -0.077006
H                  -1.763581    2.614063   -0.245071
H                   0.414515    1.385070   -0.167600
H                   1.150316   -2.480764   -0.206929
H                   1.518393   -1.437338    1.276002
H                   2.521464   -1.025463   -1.607383
H                   4.171210    2.173520    0.715672
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.564758631 1.073041399 0.621234494
     End
       Frequencies[1/cm]     49
  52.0818
  77.4974               117.5304               210.3406
 227.2406               369.5445               397.9466
 428.0526               551.7043               573.0761
```

```
 607.7214               617.4581               631.1002
 676.1519               716.6675               732.7199
 829.9070               876.4699               888.3073
 900.0088               948.4991               955.3664
 984.6847               990.8505              1028.2095
1057.0333              1082.9452              1120.2250
1180.5996              1186.5613              1307.3105
1320.3975              1343.5339              1439.6125
1469.3671              1481.6759              1586.5380
1607.4776              1642.7581              2198.4921
3174.8350              3177.3219              3183.3740
3183.7649              3194.0637              3199.3457
3211.2094              3273.8441              3497.0300
!22.4538
        ZeroEnergy[kcal/mol]          -0.274
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.39
C                  -0.567883   -0.512809    0.052399
C                  -1.724848   -1.256881    0.148290
C                  -2.940815   -0.560694    0.100145
C                  -2.948022    0.827618   -0.041693
C                  -1.748927    1.535904   -0.136880
C                  -0.524079    0.856664   -0.092250
C                   1.569888   -1.576656    0.202183
C                   2.394128   -0.808281   -0.553759
C                   3.076018    0.329453   -0.051570
C                   3.662172    1.308434    0.354645
H                  -1.709225   -2.335366    0.259609
H                  -3.875908   -1.105508    0.172612
H                  -3.891520    1.359021   -0.078698
H                  -1.762266    2.614823   -0.247236
H                   0.417313    1.388965   -0.167596
H                   1.137087   -2.477812   -0.211571
H                   1.514833   -1.442895    1.274315
H                   2.505447   -1.018326   -1.612396
H                   4.178438    2.160586    0.721901
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.564758631 1.085591591 0.62750959
     End
       Frequencies[1/cm]     49
  53.2118
  82.8464               121.8477               215.1755
 228.0527               372.7922               398.0187
 429.7413               549.7647               569.5237
```

```
 608.2459               615.2540               631.5698
 676.0731               716.9664               733.6970
 830.3899               869.1902               888.6308
 899.7304               948.5207               955.3647
 981.7846               989.9506              1028.3492
1057.2290              1083.2531              1120.6693
1180.6622              1186.8208              1303.0097
1320.9266              1343.9186              1437.4097
1469.6130              1481.9897              1583.6082
1600.8928              1642.8432              2195.5920
3174.4060              3177.2377              3183.4028
3183.7842              3193.9208              3199.1417
3211.1531              3273.3938              3496.9676
!22.9807
        ZeroEnergy[kcal/mol]          -0.326
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.37
C                  -0.561818   -0.510554    0.054651
C                  -1.718536   -1.255392    0.150590
C                  -2.935308   -0.560896    0.101177
C                  -2.944287    0.827261   -0.042160
C                  -1.745953    1.536794   -0.137585
C                  -0.520471    0.858958   -0.091773
C                   1.554590   -1.573084    0.198936
C                   2.383942   -0.805494   -0.557241
C                   3.071864    0.326074   -0.052301
C                   3.664043    1.300090    0.357739
H                  -1.701755   -2.333731    0.263185
H                  -3.869735   -1.106837    0.173746
H                  -3.888423    1.357463   -0.080183
H                  -1.760485    2.615570   -0.249162
H                   0.420308    1.392315   -0.167588
H                   1.124634   -2.475244   -0.215713
H                   1.511482   -1.448374    1.272749
H                   2.490152   -1.011549   -1.617141
H                   4.185413    2.147856    0.727906
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.571033727 1.110691974 0.640059782
     End
       Frequencies[1/cm]     49
  54.3053
  88.3662              126.2658              220.0265
 229.0924              375.9955              398.1261
 431.6584              547.1274              566.6489
```

```
 608.7893               612.6985               632.1128
 675.9156               717.2673               734.5578
 830.8892               862.1311               888.9780
 899.3824               948.5498               955.3642
 977.7710               989.9009              1028.4951
1057.4509              1083.5682              1121.1871
1180.7307              1187.0770              1298.1393
1321.4813              1344.3472              1435.0083
1469.8966              1482.3309              1578.1412
1597.0755              1642.9746              2192.2203
3173.8548              3177.1938              3183.4110
3183.9322              3193.8350              3198.9939
3211.1096              3272.8404              3496.8981
!23.5600
        ZeroEnergy[kcal/mol]          -0.406
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.35
C                  -0.555909   -0.508653    0.056774
C                  -1.712592   -1.253959    0.152702
C                  -2.929988   -0.560849    0.102109
C                  -2.940394    0.827168   -0.042579
C                  -1.742644    1.537652   -0.138183
C                  -0.516703    0.860909   -0.091277
C                   1.539240   -1.569521    0.195968
C                   2.374068   -0.802713   -0.560643
C                   3.067614    0.322803   -0.053141
C                   3.665554    1.291979    0.360734
H                  -1.694901   -2.332159    0.266455
H                  -3.863887   -1.107683    0.174736
H                  -3.885034    1.356410   -0.081553
H                  -1.758102    2.616298   -0.250868
H                   0.423594    1.395087   -0.167518
H                   1.113163   -2.473266   -0.219393
H                   1.508493   -1.454020    1.271291
H                   2.475398   -1.005023   -1.621693
H                   4.191796    2.135466    0.733755
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                 8 9 10 16 17 18 19
        Axis                  1 7
        Symmetry               2
        Potential[kcal/mol]    4
0.  0.577308823 1.129517262 0.65888507
     End
       Frequencies[1/cm]     49
  55.3896
  94.0099               130.7537               224.6313
 230.5819               379.0896               398.2715
 433.8053               543.9504               564.5256
```

```
 609.0218               610.1082               632.7294
 675.6911               717.5731               735.2789
 831.4202               855.6105               889.3585
 898.8529               948.5964               955.3701
 973.2379               990.2185              1028.6525
1057.7011              1083.9066              1121.7877
1180.8087              1187.3451              1292.6903
1322.0732              1344.8250              1432.4423
1470.2194              1482.7143              1570.9188
1595.4279              1643.1423              2188.3402
3173.1304              3177.1769              3183.4153
3184.1715              3193.7906              3198.8830
3211.0636              3272.1055              3496.7954
!24.1883
        ZeroEnergy[kcal/mol]          -0.5285
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.33
C                  -0.550017   -0.508237    0.047939
C                  -0.513540    0.860231   -0.111625
C                  -1.739903    1.536498   -0.151145
C                  -2.936439    0.826855   -0.036274
C                  -2.924012   -0.559846    0.120541
C                  -1.706019   -1.252173    0.163860
C                   1.523964   -1.567740    0.177644
C                   2.367905   -0.793885   -0.568028
C                   3.062932    0.321592   -0.044308
C                   3.663210    1.282885    0.385103
H                   0.425827    1.393909   -0.201732
H                  -1.756751    2.614154   -0.272714
H                  -3.881565    1.355633   -0.069437
H                  -3.856905   -1.106139    0.208499
H                  -1.686847   -2.329297    0.287091
H                   1.105558   -2.469859   -0.249081
H                   1.500748   -1.471978    1.255161
H                   2.470359   -0.982864   -1.631386
H                   4.191087    2.119363    0.771345
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                 8 9 10 16 17 18 19
        Axis                  1 7
        Symmetry               2
        Potential[kcal/mol]    4
0.  0.59613411 1.160892741 0.621234494
     End
       Frequencies[1/cm]     49
  56.1783
 100.0474               135.1940               228.4469
 233.4550               381.7740               398.5878
 435.9216               540.6031               562.9486
```

```
 606.2784               610.2270               633.3840
 675.3906               717.6765               735.9180
 831.9545               849.6496               889.7692
 898.0867               948.6982               955.3689
 968.4164               990.7053              1028.8253
1057.9608              1084.2627              1122.5299
1180.8873              1187.5910              1286.5669
1322.6670              1345.3731              1429.7948
1470.5916              1483.1480              1563.1475
1594.8251              1643.4065              2183.9708
3172.2354              3177.2258              3183.4665
3184.3207              3193.8268              3198.8309
3211.0371              3271.1980              3496.6884
!25.0185
        ZeroEnergy[kcal/mol]          -0.70
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.31
C                  -0.544448   -0.507055    0.050060
C                  -0.509426    0.861667   -0.109354
C                  -1.735878    1.537484   -0.150192
C                  -2.932281    0.827376   -0.036940
C                  -2.919210   -0.559363    0.119613
C                  -1.700973   -1.250924    0.164306
C                   1.508506   -1.563971    0.177217
C                   2.358706   -0.791997   -0.570477
C                   3.058589    0.318394   -0.046253
C                   3.664148    1.275696    0.385596
H                   0.429768    1.395820   -0.198543
H                  -1.753008    2.615149   -0.271585
H                  -3.877629    1.355695   -0.071192
H                  -3.851907   -1.106189    0.206270
H                  -1.681490   -2.328034    0.287477
H                   1.096138   -2.469486   -0.248450
H                   1.498490   -1.476062    1.255695
H                   2.456747   -0.979362   -1.634482
H                   4.196488    2.108629    0.773354
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.602409206 1.179718029 0.640059782
     End
       Frequencies[1/cm]     49
  57.2723
 105.7256               139.7111               230.6031
 237.6933               384.5253               398.8182
 438.4239               537.5483               561.8791
```

```
 602.4553               610.9040               634.1507
 674.9792               717.9403               736.3024
 832.5577               844.9738               890.1414
 896.8998               948.7804               955.3629
 963.7955               991.4103              1029.0192
1058.2795              1084.6659              1123.3099
1180.9800              1187.9042              1279.9472
1323.3504              1345.9540              1427.0047
1470.9855              1483.6458              1555.5764
1594.7077              1643.6253              2178.9474
3171.0916              3177.2799              3183.5369
3184.6896              3193.8747              3198.8134
3211.0105              3269.9598              3496.5257
!25.7407
        ZeroEnergy[kcal/mol]          -0.925
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.29
C                  -0.539095   -0.506163    0.052191
C                  -0.505298    0.862824   -0.107068
C                  -1.731696    1.538434   -0.149248
C                  -2.928111    0.828109   -0.037633
C                  -2.914667   -0.558670    0.118664
C                  -1.696332   -1.249700    0.164754
C                   1.492975   -1.560160    0.176866
C                   2.349845   -0.789972   -0.573005
C                   3.054391    0.315245   -0.048280
C                   3.665138    1.268537    0.386182
H                   0.433821    1.397273   -0.195322
H                  -1.748884    2.616110   -0.270464
H                  -3.873572    1.356159   -0.072989
H                  -3.847272   -1.105846    0.204010
H                  -1.676738   -2.326792    0.287863
H                   1.087597   -2.469493   -0.247699
H                   1.496712   -1.480419    1.256125
H                   2.443582   -0.975792   -1.637613
H                   4.201853    2.097895    0.775553
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.614959398 1.211093509 0.658885069
     End
       Frequencies[1/cm]     49
  58.3061
 111.3339               144.1510               232.3773
 242.4924               387.0289               399.0978
 441.0404               535.1040               561.0793
```

```
 598.1340               611.6546               634.9947
 674.4758               718.1559               736.4608
 833.1793               841.4566               890.2998
 895.3831               948.8767               955.2850
 959.6139               992.2793              1029.2420
1058.6418              1085.1013              1124.2029
1181.0809              1188.2369              1272.7660
1324.0759              1346.5960              1424.1692
1471.4188              1484.2072              1548.4076
1594.8510              1643.8763              2173.3240
3169.6989              3177.3747              3183.6482
3185.0965              3193.9803              3198.8444
3210.9984              3268.4125              3496.3296
!26.4804
        ZeroEnergy[kcal/mol]          -1.22
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.27
C                  -0.533969   -0.505527    0.054359
C                  -0.501205    0.863741   -0.104742
C                  -1.727424    1.539351   -0.148308
C                  -2.923980    0.829022   -0.038365
C                  -2.910396   -0.557799    0.117685
C                  -1.692092   -1.248496    0.165216
C                   1.477365   -1.556269    0.176580
C                   2.341338   -0.787796   -0.575628
C                   3.050414    0.312117   -0.050396
C                   3.666301    1.261356    0.386858
H                   0.437920    1.398335   -0.192025
H                  -1.744476    2.617038   -0.269352
H                  -3.869461    1.356968   -0.074858
H                  -3.843000   -1.105165    0.201696
H                  -1.672554   -2.325568    0.288263
H                   1.079868   -2.469785   -0.246845
H                   1.495363   -1.484956    1.256416
H                   2.430892   -0.972154   -1.640793
H                   4.207344    2.087081    0.777942
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.621234494 1.229918796 0.671435261
     End
       Frequencies[1/cm]     49
  59.2713
 116.7951               148.4506               234.1869
 247.4369               389.2549               399.4286
 443.6990               533.5111               560.4514
```

```
 593.3156               612.4561               635.9158
 673.8667               718.2938               736.3369
 833.8102               839.2108               889.6083
 894.0949               948.9787               954.6650
 956.6396               993.3261              1029.5043
1059.0548              1085.5727              1125.2195
1181.1912              1188.5903              1265.0772
1324.8455              1347.2997              1421.3376
1471.8914              1484.8362              1541.7565
1595.1686              1644.1517              2167.0729
3168.0338              3177.5070              3183.8060
3185.5362              3194.1379              3198.9412
3210.9916              3266.5132              3496.1012
!27.2387
        ZeroEnergy[kcal/mol]          -1.5976
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.25
C                  -0.529079   -0.505100    0.056616
C                  -0.497196    0.864470   -0.102321
C                  -1.723137    1.540238   -0.147362
C                  -2.919938    0.830077   -0.039165
C                  -2.906407   -0.556788    0.116652
C                  -1.688236   -1.247309    0.165708
C                   1.461673   -1.552252    0.176351
C                   2.333176   -0.785456   -0.578363
C                   3.046740    0.308979   -0.052615
C                   3.667772    1.254084    0.387602
H                   0.441999    1.399090   -0.188563
H                  -1.739892    2.617936   -0.268239
H                  -3.865362    1.358048   -0.076857
H                  -3.839082   -1.104219    0.199275
H                  -1.668888   -2.324355    0.288693
H                   1.072831   -2.470236   -0.245909
H                   1.494365   -1.489556    1.256529
H                   2.418668   -0.968450   -1.644040
H                   4.213146    2.076085    0.780496
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                 8 9 10 16 17 18 19
        Axis                  1 7
        Symmetry               2
        Potential[kcal/mol]    4
0.  0.633784686 1.261294276 0.690260549
     End
       Frequencies[1/cm]     49
  60.1433
 122.0170               152.5319               236.1301
 252.3820               391.1617               399.8099
 446.3195               532.8967               559.9365
```

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 588.0170               613.2996               636.9120
 673.1499               718.2969               735.8720
 834.4433               838.2807               887.2774
 893.8481               949.0479               952.6879
 955.9518               994.5651              1029.8207
1059.5289              1086.0747              1126.3643
1181.3091              1188.9606              1256.9707
1325.6515              1348.0616              1418.5643
1472.3975              1485.5316              1535.6665
1595.6145              1644.4467              2160.2312
3166.1034              3177.6898              3184.0222
3185.9881              3194.3703              3199.1174
3211.0072              3264.2593              3495.8471
!27.9904
        ZeroEnergy[kcal/mol]          -2.078
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.23
C                  -0.524578   -0.505014    0.059018
C                  -0.493213    0.864881   -0.099742
C                  -1.718690    1.541113   -0.146419
C                  -2.915938    0.831447   -0.040070
C                  -2.902847   -0.555466    0.115548
C                  -1.685015   -1.246126    0.166270
C                   1.445781   -1.548186    0.176199
C                   2.325327   -0.782783   -0.581376
C                   3.043556    0.305763   -0.055005
C                   3.669864    1.246525    0.388519
H                   0.446181    1.399302   -0.184809
H                  -1.734843    2.618822   -0.267150
H                  -3.861153    1.359703   -0.079060
H                  -3.835744   -1.102708    0.196715
H                  -1.666097   -2.323141    0.289201
H                   1.066214   -2.470838   -0.244928
H                   1.493421   -1.494162    1.256484
H                   2.406861   -0.964487   -1.647528
H                   4.219677    2.064588    0.783424
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.646334878 1.286394659 0.702810741
     End
       Frequencies[1/cm]     49
  60.9704
 127.2154               156.4407               238.5312
 257.4511               392.7957               400.2390
 448.8484               533.2613               559.5086
```

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 582.1464               614.1821               637.9824
 672.2805               718.0722               734.9840
 835.1240               838.4438               883.8673
 894.2826               948.9991               951.1793
 955.8921               995.9981              1030.2074
1060.0709              1086.6209              1127.6332
1181.4356              1189.3524              1247.9656
1326.4995              1348.8866              1415.7043
1472.9399              1486.2889              1529.7740
1596.1661              1644.7500              2152.6269
3163.7018              3177.9157              3184.2977
3186.4603              3194.6815              3199.3796
3211.0443              3261.4778              3495.5630
!29.0646
        ZeroEnergy[kcal/mol]          -3.565
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.21
C                  -0.520043   -0.504956    0.060403
C                  -0.489449    0.865276   -0.098292
C                  -1.714534    1.541888   -0.145823
C                  -2.912108    0.832655   -0.040415
C                  -2.899247   -0.554289    0.115142
C                  -1.681672   -1.244994    0.166720
C                   1.429978   -1.543905    0.175966
C                   2.318061   -0.780229   -0.584061
C                   3.040460    0.302655   -0.056958
C                   3.671621    1.239266    0.389928
H                   0.450040    1.399568   -0.182819
H                  -1.730237    2.619592   -0.266486
H                  -3.857179    1.361125   -0.080098
H                  -3.832267   -1.101393    0.195569
H                  -1.663048   -2.321970    0.289640
H                   1.060385   -2.471416   -0.243984
H                   1.491819   -1.498161    1.256117
H                   2.396569   -0.961100   -1.650527
H                   4.225512    2.053550    0.786926
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.658885069 1.305219947 0.715360933
     End
       Frequencies[1/cm]     49
  61.6194
 131.7067               159.8670               240.7240
 262.1979               393.9747               400.6829
 451.0984               534.6910               559.1714
```

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 576.0604               615.0798               639.0985
 671.3727               717.4813               733.7429
 835.9121               839.8579               880.4057
 894.9937               948.8368               950.7618
 955.9252               997.6622              1030.7031
1060.7180              1087.1846              1129.0083
1181.5680              1189.7539              1239.4898
1327.3686              1349.7594              1413.2178
1473.4938              1487.1230              1524.8940
1596.8273              1645.0560              2144.8524
3161.1938              3178.1750              3184.6198
3186.9069              3195.0278              3199.7068
3211.0967              3258.4444              3495.2621
!29.7556
        ZeroEnergy[kcal/mol]          -4.546
        ElectronicLevels[1/cm]        1
           0   2
   End
 End
   Barrier B2   W1   W4    #  ts [1]-[4]
     RRHO
       Geometry[angstrom]     19        #
C -0.7180426841 -0.1505898857 0.1802973618
C -1.7979011378 -1.0351219275 0.2242134851
C -1.5562451116 -2.4013967669 0.3756476549
C -0.2539108646 -2.8940787323 0.4843892023
C 0.8391234802 -2.0190970277 0.4444366489
C 0.5586818532 -0.6772489187 0.2906668056
C -0.739747775 1.3549629925 0.00349863
C 0.7198820929 1.8102191407 0.23021152
C 1.3287853615 2.6556259215 -0.7429675232
C 1.8613310962 3.3426993931 -1.5805577499
H -2.8167551984 -0.668002225 0.1432169953
H -2.3917996597 -3.0916302817 0.410801316
H -0.0862901311 -3.9596169617 0.6013473841
H 1.8535103677 -2.39320451 0.5293657093
H 1.2381337711 0.6383331597 0.217624677
H -1.4222541599 1.8452768592 0.7042555337
H -1.0684770536 1.6222218647 -1.0047329826
H 0.9165127134 2.1364287024 1.2534288175
H 2.3256814851 3.9543482595 -2.3143236642
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1656.0928
         WellDepth[kcal/mol]         36.9
         WellDepth[kcal/mol]         13.9
       End
       Frequencies[1/cm]     50
   47.2747    115.0999
  186.2009    217.9082    325.8150
  388.9331    410.0068    445.5467
  495.7675    546.3780    593.6036
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  621.5433    657.5229    666.8208
  699.9458    746.6017    808.9133
  842.1979    866.5311    939.2222
  947.2080    990.3629   1002.3964
 1023.6414   1037.1343   1074.6656
 1128.1235   1174.2266   1188.4479
 1208.9596   1247.4230   1293.6276
 1311.7097   1331.4712   1362.2136
 1462.2760   1477.0736   1485.1689
 1597.5131   1628.9939   1663.5902
 2168.4297   3038.1219   3067.9072
 3084.7765   3150.5119   3159.0901
 3172.4900   3183.4987   3475.0595
        ZeroEnergy[kcal/mol]       -7.9
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier  B3   W4   W5    #  ts [4]-[5]
     RRHO
       Geometry[angstrom]     19        #
C -0.6594058903 0.0693377389 0.1125526818
C -1.6079047412 -0.8112483556 -0.428386598
C -1.2854049333 -2.1418631457 -0.6974695621
C -0.0052226317 -2.6235976087 -0.4369150163
C 0.9646928446 -1.7634548902 0.0953454904
C 0.5999290377 -0.4616587531 0.3570853887
C -1.013826047 1.5060893695 0.4414431842
C -0.0166845212 2.5491032545 -0.1375491519
C 1.3399155741 2.1567804858 0.2342007602
C 2.1496923758 1.3057432101 0.5663877847
H -2.6111577016 -0.4487960966 -0.6352001655
H -2.0373460195 -2.8015338251 -1.1156870481
H 0.2450870807 -3.6581222926 -0.6484851001
H 1.9689625292 -2.1249095683 0.2932402665
H -1.0293332188 1.6311302744 1.5293156368
H -2.0190411394 1.7333003866 0.0760812399
H -0.0969653802 2.589911187 -1.2295377337
H -0.27000511 3.5450059837 0.2386029007
H 3.0551125546 0.8226261179 0.8515002328
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    374.5283
         WellDepth[kcal/mol]         8.0
         WellDepth[kcal/mol]         45.65
       End
       Frequencies[1/cm]     50
   78.2883    120.4949
  203.9925    290.4802    334.1191
  370.7779    425.2855    489.1239
  490.5034    597.5770    619.1957
  655.4261    710.1131    735.4917
  745.6243    771.1574    848.0252
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  858.7684    932.0761    935.1675
  972.8113    981.8491    990.8556
 1023.5512   1048.7560   1122.0942
 1176.0809   1185.7414   1206.8485
 1218.6564   1285.1584   1321.0580
 1326.3108   1367.1263   1450.5148
 1470.7020   1477.4634   1484.0688
 1582.2452   1625.8222   2064.7784
 3026.0241   3027.8148   3060.3661
 3075.5177   3142.6905   3149.0250
 3163.8174   3181.9267   3434.1769
       ZeroEnergy[kcal/mol]       -13.75
       ElectronicLevels[1/cm]       1
           0   2
   End
   Barrier      B4   W5   W6    #  ts [5]-[6] (tsmi20)
     RRHO
       Geometry[angstrom]     19        #
C                  1.312909    1.376875    0.001282
C                 -1.335865   -1.362234    0.304201
C                  1.187464   -1.402259   -0.012735
C                  2.422810   -0.759317   -0.112685
C                  2.482779    0.633560   -0.097178
C                  0.061881    0.745143    0.097498
C                 -1.192347    1.481219    0.208737
C                 -2.315029    0.877371   -0.299992
C                 -2.436143   -0.528856   -0.325451
C                  0.008858   -0.672872    0.100248
H                  1.354770    2.461106   -0.001775
H                 -1.517085   -1.482198    1.382058
H                  1.146143   -2.487216   -0.011375
H                  3.331429   -1.344384   -0.197988
H                  3.440315    1.137540   -0.167464
H                 -1.192321    2.496942    0.588931
H                 -3.274943    0.247664    0.349820
H                 -3.145774   -0.990175   -1.008506
H                 -1.326433   -2.371056   -0.117249
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1706.9714
         WellDepth[kcal/mol]         42.3
         WellDepth[kcal/mol]         72.6
       End
       Frequencies[1/cm]     50
 118.6829              174.0298
 267.7454              355.7880              419.8821
 448.7010              496.0452              499.6531
 547.1800              608.9357              691.8280
 715.4890              737.8448              759.8139
 766.1107              794.6103              868.4985
 900.1124              914.1004              949.8657
 986.4100              987.0639             1056.6070
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1082.3913              1124.1530              1180.6098
1185.2146              1188.7651              1210.2844
1226.0019              1266.6665              1287.0724
1329.7221              1348.0942              1388.2136
1438.6859              1459.3220              1481.6577
1512.5174              1601.4381              1628.1264
2085.7563              2981.1012              3062.5794
3128.3505              3152.8276              3160.0331
3163.4442              3173.3605              3187.2700
        ZeroEnergy[kcal/mol]          -16.9
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B5   W6   P1    #  ts [6]-naphthalene (tsmi34, S24-NP)
     RRHO
       Geometry[angstrom]     19        #
C       -1.290042       1.402102        0.046057
C       1.253427        -1.355938       -0.042243
C       -1.237357       -1.394194       -0.068217
C       -2.43776        -0.723187       -0.046207
C       -2.464036       0.6884  0.0141
C       -0.03571        0.739602        0.018314
C       1.195175        1.44918 0.023361
C       2.397911        0.782533        -0.046104
C       2.430979        -0.623417       -0.102225
C       -0.011778       -0.687789       -0.035574
H       -1.307449       2.486124        0.08998
H       1.272031        -2.428367       -0.198449
H       -1.215993       -2.478359       -0.104629
H       -3.369923       -1.276121       -0.07252
H       -3.416244       1.206388        0.034545
H       1.171756        2.533084        0.065342
H       3.327173        1.340625        -0.064286
H       3.382405        -1.138825       -0.163082
H       1.351379        -1.908297       1.84553
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    650.
         WellDepth[kcal/mol]         31.8
         WellDepth[kcal/mol]         5.6
       End
       Frequencies[1/cm]     50
169. 177. 274. 347. 372. 414. 482. 511. 518. 521. 629. 638. 737. 772.
788. 800. 808.
863. 901. 948. 961. 979. 996. 1003. 1037. 1048. 1145. 1166. 1169. 1185.
1227. 1265.
1285. 1382. 1390. 1416. 1484. 1488. 1544. 1600. 1623. 1661. 3159. 3161.
3164. 3170.
3176. 3179. 3189. 3191.
        ZeroEnergy[kcal/mol]          -57.7
        ElectronicLevels[1/cm]        1
           0   2
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   End
   Barrier      B6   W1    P3    #  ts [1]-trans-phenyl-vinylacetylene p3
     RRHO
       Geometry[angstrom]     19        #
C 0.6955278673 -0.4822748527 0.7172924558
C 1.6280930731 -1.5269703068 0.6272998988
C 2.9914421148 -1.2859758904 0.7619332409
C 3.4527859562 0.0094644012 0.9814060221
C 2.5387292154 1.0610512602 1.0606317626
C 1.1775119194 0.8200604233 0.927625125
C -0.7340591895 -0.7988702893 0.5933949689
C -1.7661292132 0.0026164649 0.9694004465
C -3.122190398 -0.3845808302 0.9085243403
C -4.2901907195 -0.6854405412 0.86898931
H 1.2746233484 -2.5380042157 0.4540696986
H 3.6932099967 -2.1094956113 0.6931637999
H 4.5147310023 0.2014978487 1.0832436383
H 2.8909891657 2.0740329745 1.2198356966
H 0.4859885395 1.6533439696 0.972330885
H -0.9673605337 -1.8241764114 0.3237527153
H -0.8630138675 -0.5732908594 -1.4965861705
H -1.5720317859 1.0078183488 1.3319426779
H -5.3159513983 -0.9586054159 0.830282235
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    538.6839
         WellDepth[kcal/mol]         39.9
         WellDepth[kcal/mol]         3.5
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  0.928714193 4.329816171 2.334335675 0.  0.834587755 4.279615404
2.284134908
     End
       Frequencies[1/cm]     49
  88.2396
 103.7725              204.1246              238.5574
 305.6976              323.3131              379.9293
 411.6392              425.4617              495.3811
 533.0669              623.0493              632.5254
 636.6777              679.6917              705.3358
 769.4249              846.2931              856.2688
 857.5141              927.6629              978.4094
 986.6972             1004.2304             1015.3272
1037.3996             1052.8781             1106.6608
1183.6034             1204.7521             1225.8030
1291.5020             1313.0712             1345.7731
1361.2462             1479.9824             1526.8617
1605.3051             1628.0955             1642.5919
```

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2183.0739              3147.9940              3160.0443
3162.2220              3167.2895              3176.1654
3184.0781              3192.6864              3475.6720
!59.9406
        ZeroEnergy[kcal/mol]          -4.9
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B7   R1    W3    #  ts [0]-[3]
   Variational
     RRHO
       Geometry[angstrom]     19        #  2.507
C 0.3933706615 -0.1305870995 0.7172852348
C -0.298095098 -1.2719126842 1.0582112407
C 0.452677504 -2.4300514351 1.2990756516
C 1.842605542 -2.3995438818 1.1856102726
C 2.4978511699 -1.2201453114 0.8316436886
C 1.7622908391 -0.0530192545 0.5871900784
C -0.9157048792 1.9783128094 0.3623424547
C -1.2613915758 2.0516807625 -0.7997959521
C -1.584120613 2.0711920524 -2.1762217698
C -2.7029973101 1.5544647961 -2.7057174221
H -1.3797646127 -1.2839491704 1.1385921788
H -0.0513063168 -3.3516053231 1.5724684614
H 2.4176656898 -3.2995963747 1.3719042691
H 3.5794232116 -1.2040006942 0.7424239117
H 2.2601132038 0.8688626634 0.3060166292
H -0.7495188953 2.1407004103 1.399477965
H -0.8563852201 2.5496953351 -2.8274586988
H -3.4514650495 1.0708343345 -2.0896606314
H -2.8876794526 1.606714296 -3.7715049496
       Core     RigidRotor
         SymmetryFactor    1
       End
!      Tunneling      Eckart
!        ImaginaryFrequency[1/cm]    206.1321
!        WellDepth[kcal/mol]         1.2
!        WellDepth[kcal/mol]         50.9
!      End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.039051804 0.027622972 0.058181434
     End
       Frequencies[1/cm]     49
  30.1278
  53.5515               79.8242              106.8325
 230.5916              327.9586              399.1705
 431.6920              560.9478              565.4770
 608.2951              666.7505              669.8322
 683.9382              697.5842              723.8023
 825.8071              895.9096              898.4387
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 938.9466               963.3056               976.0413
 992.5424              1001.5129              1016.3524
1049.3908              1074.0961              1111.7342
1175.6284              1176.9377              1307.6808
1315.4499              1323.1449              1440.8953
1462.5992              1471.6361              1576.8867
1627.0476              1642.0757              2115.1932
3135.0059              3148.3547              3150.3470
3155.9210              3167.8913              3170.5300
3184.1278              3238.7560              3457.4010
!12.0698
        ZeroEnergy[kcal/mol]          1.2
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        #  2.487
C                  -0.706861   -0.495844   -0.013221
C                  -0.696446    0.873123   -0.152295
C                  -1.933254    1.529319   -0.132861
C                  -3.112050    0.798954    0.021942
C                  -3.071440   -0.587973    0.159061
C                  -1.841673   -1.260142    0.141921
C                   1.509959   -1.622302   -0.076689
C                   2.390529   -0.794300   -0.212216
C                   3.327061    0.243873   -0.411789
C                   3.919305    0.939811    0.572573
H                   0.229174    1.426045   -0.270439
H                  -1.972232    2.608796   -0.238474
H                  -4.066354    1.313274    0.035952
H                  -3.991285   -1.151299    0.279144
H                  -1.803687   -2.339775    0.247794
H                   0.983131   -2.536968    0.052487
H                   3.573311    0.468947   -1.447137
H                   3.703001    0.742606    1.615630
H                   4.634166    1.721261    0.346492
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.050200767 0.006275096 0.031375479
     End
       Frequencies[1/cm]     49
  37.3149
  62.3507               86.3195              125.3559
 229.0059              336.2311              400.8317
 429.4012              559.8769              567.5303
 609.0298              658.4147              677.1367
 683.7119              699.4683              722.9308
 824.5483              894.3834              900.0818
```

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 935.4069               962.7737               974.4517
 991.9066               999.6605              1017.2927
1049.7912              1076.5250              1112.1828
1175.8524              1178.5366              1310.6885
1313.7337              1324.8568              1439.9563
1463.7900              1475.2176              1577.5893
1629.5952              1632.6799              2100.6296
3131.8470              3147.5766              3147.9728
3154.8011              3164.7542              3171.8295
3184.5285              3238.8421              3447.6377
!12.1509
        ZeroEnergy[kcal/mol]          1.281
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.467
C                  -0.701429   -0.494493   -0.014673
C                  -0.692909    0.874583   -0.153447
C                  -1.930176    1.529693   -0.132534
C                  -3.108157    0.798248    0.023363
C                  -3.066026   -0.588661    0.160118
C                  -1.835665   -1.259565    0.141551
C                   1.495542   -1.615879   -0.077449
C                   2.382979   -0.793387   -0.212992
C                   3.321512    0.241850   -0.411660
C                   3.917475    0.934594    0.573538
H                   0.232116    1.428360   -0.272427
H                  -1.970245    2.609154   -0.237867
H                  -4.062926    1.311676    0.038518
H                  -3.985191   -1.152900    0.281085
H                  -1.796526   -2.339183    0.247142
H                   0.980179   -2.537554    0.051211
H                   3.567502    0.468035   -1.446856
H                   3.701796    0.736304    1.616498
H                   4.634421    1.714207    0.347800
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.069026055 0.043925671 0.056475863
     End
       Frequencies[1/cm]     49
  38.4671
  65.6618                91.0102               129.6793
 229.7809               335.7793               400.9566
 429.9648               559.7726               564.7449
 609.4021               657.2120               677.9142
 684.2062               699.8648               723.3127
 825.0114               894.7127               900.6980
```

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 933.3556               962.8635               973.8134
 991.9903               998.4776              1017.3421
1049.8456              1076.7560              1112.1996
1175.8962              1178.6999              1311.1444
1312.8540              1325.0638              1439.4974
1464.0341              1475.4838              1577.8424
1628.2256              1630.5697              2090.2308
3131.5528              3147.6239              3147.9809
3154.7612              3164.7216              3171.6540
3184.4966              3239.0650              3441.7581
!13.8451
        ZeroEnergy[kcal/mol]          1.384
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.447
C                  -0.696293   -0.493403   -0.016050
C                  -0.689424    0.875789   -0.154464
C                  -1.927023    1.530039   -0.132199
C                  -3.104338    0.797740    0.024740
C                  -3.060932   -0.589160    0.161179
C                  -1.830120   -1.259037    0.141153
C                   1.481103   -1.609157   -0.078258
C                   2.375696   -0.792392   -0.213770
C                   3.316119    0.239858   -0.411576
C                   3.916102    0.929234    0.574476
H                   0.235141    1.430229   -0.274141
H                  -1.967971    2.609490   -0.237252
H                  -4.059478    1.310449    0.040939
H                  -3.979524   -1.154137    0.282992
H                  -1.789997   -2.338652    0.246375
H                   0.978352   -2.538333    0.049911
H                   3.561660    0.467295   -1.446633
H                   3.701310    0.729639    1.617350
H                   4.635169    1.706959    0.349064
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.094126439 0.081576247 0.081576247
     End
       Frequencies[1/cm]     49
  39.6012
  69.0676                96.0165               134.2836
 230.6064               335.3742               401.1147
 430.6237               558.9974               562.8935
 609.7965               656.1029               678.3437
 684.7336               700.7593               723.7586
 825.5144               895.0970               901.3587
```

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 931.0512               962.9824               973.1755
 992.0825               997.1444              1017.3888
1049.9001              1077.0019              1112.2111
1175.9386              1178.8698              1311.4826
1311.9703              1325.2801              1438.9665
1464.3010              1475.7620              1578.1233
1624.3371              1630.5701              2079.0401
3131.2469              3147.6777              3148.0249
3154.7346              3164.7121              3171.4740
3184.4748              3239.3025              3435.0549
!15.4162
        ZeroEnergy[kcal/mol]          1.4766
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.427
C                  -0.691373   -0.492384   -0.017471
C                  -0.686115    0.876906   -0.155660
C                  -1.924031    1.530332   -0.131983
C                  -3.100688    0.797230    0.026108
C                  -3.056043   -0.589654    0.162284
C                  -1.824805   -1.258537    0.140847
C                   1.466657   -1.602093   -0.079005
C                   2.368726   -0.791301   -0.214548
C                   3.311305    0.237540   -0.411435
C                   3.914808    0.924060    0.575509
H                   0.237981    1.431968   -0.276223
H                  -1.965823    2.609768   -0.236840
H                  -4.056180    1.309243    0.043410
H                  -3.974075   -1.155340    0.285012
H                  -1.783684   -2.338124    0.245842
H                   0.977451   -2.539093    0.048546
H                   3.557311    0.465523   -1.446300
H                   3.700020    0.723914    1.618263
H                   4.636356    1.699542    0.350408
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.112951726 0.125501918 0.100401534
     End
       Frequencies[1/cm]     49
  40.6788
  72.5532               101.2815               139.1694
 231.5409               335.1243               401.3076
 431.3799               557.3059               562.3070
 610.2168               654.9558               678.3065
 685.2918               702.2548               724.2671
 826.0418               895.5132               902.1008
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 928.4486               963.1306               972.5463
 992.1900               995.6788              1017.4408
1049.9625              1077.2507              1112.2411
1175.9898              1179.0423              1310.5551
1312.2108              1325.5292              1438.3552
1464.6003              1476.0523              1578.4268
1619.7786              1630.8488              2067.0397
3130.8459              3147.7014              3148.1223
3154.7331              3164.7230              3171.3400
3184.4679              3239.5440              3427.7032
!16.8769
        ZeroEnergy[kcal/mol]          1.555
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.407
C                  -0.686684   -0.491531   -0.018746
C                  -0.682827    0.877850   -0.156714
C                  -1.920978    1.530597   -0.131748
C                  -3.097078    0.796840    0.027405
C                  -3.051384   -0.590026    0.163351
C                  -1.819811   -1.258076    0.140608
C                   1.452162   -1.594819   -0.079848
C                   2.361917   -0.790062   -0.215508
C                   3.306544    0.235294   -0.411348
C                   3.913881    0.918684    0.576610
H                   0.240883    1.433392   -0.278126
H                  -1.963470    2.610018   -0.236413
H                  -4.052859    1.308278    0.045731
H                  -3.968934   -1.156303    0.286907
H                  -1.777790   -2.337621    0.245425
H                   0.977672   -2.540054    0.047022
H                   3.552819    0.464171   -1.445996
H                   3.699329    0.717686    1.619229
H                   4.637890    1.691935    0.351852
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.131777014 0.175702685 0.131777014
     End
       Frequencies[1/cm]     49
  41.7531
  76.1482               106.7780               144.3178
 232.7195               335.1801               401.5296
 432.2439               555.4823               562.3620
 610.6658               653.9025               677.7279
 685.8835               704.5653               724.8352
 826.5845               895.9685               902.8995
```

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 925.4909               963.2944               971.9322
 992.3048               994.0374              1017.5040
1050.0351              1077.5122              1112.2649
1176.0513              1179.2121              1309.1849
1312.7074              1325.8209              1437.6420
1464.9475              1476.3543              1578.7593
1614.6634              1631.2315              2054.0482
3130.3836              3147.7349              3148.3123
3154.8019              3164.7958              3171.2652
3184.4720              3239.8173              3419.5480
!18.3683
        ZeroEnergy[kcal/mol]          1.6154
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.387
C                  -0.682225   -0.490773   -0.019784
C                  -0.679685    0.878700   -0.157560
C                  -1.918036    1.530830   -0.131501
C                  -3.093640    0.796482    0.028545
C                  -3.046985   -0.590368    0.164275
C                  -1.815115   -1.257651    0.140437
C                   1.437644   -1.587220   -0.080648
C                   2.355384   -0.788706   -0.216515
C                   3.302141    0.232882   -0.411340
C                   3.913319    0.913294    0.577645
H                   0.243694    1.434652   -0.279688
H                  -1.961154    2.610234   -0.236002
H                  -4.049684    1.307396    0.047738
H                  -3.964098   -1.157189    0.288521
H                  -1.772233   -2.337144    0.245086
H                   0.978941   -2.540971    0.045499
H                   3.548988    0.462365   -1.445766
H                   3.698759    0.711733    1.620134
H                   4.639977    1.684099    0.353162
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.156877397 0.225903452 0.156877397
     End
       Frequencies[1/cm]     49
  42.8024
  79.8257               112.4239               149.7149
 234.0562               335.5425               401.7902
 433.2335               553.9924               562.6352
 611.1440               652.9072               676.6189
 686.5130               707.7977               725.4769
 827.1587               896.4749               903.7584
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 922.1656               963.4880               971.3520
 992.1485               992.5002              1017.5727
1050.1166              1077.7883              1112.2887
1176.1201              1179.3872              1307.5762
1313.2365              1326.1398              1436.8222
1465.3321              1476.6757              1579.1257
1609.0485              1631.6732              2040.3444
3129.8666              3147.7659              3148.5773
3154.9184              3164.9174              3171.2265
3184.4851              3240.1110              3410.7156
!19.8121
        ZeroEnergy[kcal/mol]          1.6527
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.367
C                  -0.677950   -0.490106   -0.020938
C                  -0.676678    0.879451   -0.158581
C                  -1.915192    1.531019   -0.131343
C                  -3.090312    0.796141    0.029738
C                  -3.042746   -0.590688    0.165336
C                  -1.810629   -1.257262    0.140311
C                   1.423113   -1.579376   -0.081493
C                   2.349077   -0.787212   -0.217587
C                   3.298027    0.230352   -0.411285
C                   3.912940    0.907923    0.578828
H                   0.246395    1.435738   -0.281544
H                  -1.958892    2.610402   -0.235718
H                  -4.046595    1.306572    0.049856
H                  -3.959437   -1.157995    0.290393
H                  -1.766882   -2.336686    0.244869
H                   0.981233   -2.541867    0.043870
H                   3.545794    0.460240   -1.445455
H                   3.698064    0.706031    1.621164
H                   4.642417    1.676110    0.354646
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.188252877 0.27610422 0.188252877
     End
       Frequencies[1/cm]     49
  43.8188
  83.5579              118.1355              155.3235
 235.6284              336.3067              402.0873
 434.3607              553.0443              563.0242
 611.6536              652.0571              675.0384
 687.1818              712.1317              726.2025
 827.7711              897.0360              904.6774
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 918.4364               963.7138               970.8228
 990.1806               992.6067              1017.6553
1050.2099              1078.0879              1112.3091
1176.2008              1179.5711              1305.7092
1313.8007              1326.4956              1435.8861
1465.7622              1477.0233              1579.5414
1602.9609              1632.1771              2025.9923
3129.2926              3147.8055              3148.9108
3155.0844              3165.0944              3171.2368
3184.5117              3240.4314              3401.1408
!21.2429
        ZeroEnergy[kcal/mol]          1.6613
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.347
C                  -0.674015   -0.489310   -0.022024
C                  -0.674211    0.880334   -0.159514
C                  -1.912988    1.531144   -0.131134
C                  -3.087519    0.795554    0.030908
C                  -3.038834   -0.591246    0.166374
C                  -1.806372   -1.256919    0.140212
C                   1.408584   -1.570738   -0.082419
C                   2.343228   -0.785407   -0.218763
C                   3.294737    0.227619   -0.411268
C                   3.913605    0.902174    0.580050
H                   0.248463    1.437099   -0.283320
H                  -1.957423    2.610499   -0.235373
H                  -4.044117    1.305355    0.051923
H                  -3.955014   -1.159191    0.292189
H                  -1.761566   -2.336256    0.244701
H                   0.984229   -2.541970    0.042100
H                   3.543705    0.457749   -1.445153
H                   3.698172    0.700113    1.622215
H                   4.646261    1.667376    0.356178
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.213353261 0.338855179 0.219628356
     End
       Frequencies[1/cm]     49
  44.7311
  87.2141               123.7747               161.0924
 237.2287               337.4466               402.4247
 435.6302               552.6440               563.4565
 612.1928               651.3211               673.1065
 687.8868               717.7028               727.0183
 828.4182               897.6493               905.6403
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 914.3308               963.9766               970.3768
 988.0152               992.7750              1017.7498
1050.3208              1078.4033              1112.3293
1176.2891              1179.7640              1303.6006
1314.3886              1326.8894              1434.8363
1466.2326              1477.4033              1579.9956
1596.5565              1632.7438              2011.5402
3128.6717              3147.8419              3149.2946
3155.3054              3165.3211              3171.3008
3184.5595              3240.7747              3391.0092
!22.5097
        ZeroEnergy[kcal/mol]          1.633
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.327
C                  -0.670125   -0.488716   -0.023045
C                  -0.671612    0.881021   -0.160437
C                  -1.910540    1.531254   -0.130974
C                  -3.084589    0.795142    0.032078
C                  -3.034987   -0.591640    0.167392
C                  -1.802299   -1.256603    0.140128
C                   1.394035   -1.562247   -0.083295
C                   2.337288   -0.783463   -0.219957
C                   3.291240    0.224884   -0.411279
C                   3.914173    0.896528    0.581275
H                   0.250785    1.438071   -0.284994
H                  -1.955544    2.610576   -0.235119
H                  -4.041428    1.304451    0.053964
H                  -3.950743   -1.160069    0.293968
H                  -1.756575   -2.335854    0.244478
H                   0.988240   -2.542330    0.040354
H                   3.541518    0.455122   -1.444889
H                   3.698153    0.694449    1.623287
H                   4.650083    1.658628    0.357641
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.24472874 0.395331042 0.251003836
     End
       Frequencies[1/cm]     49
  45.6784
  91.0046               129.3357               166.9845
 239.2640               339.1637               402.7960
 437.0612               552.8428               563.9759
 612.7651               650.6236               670.9399
 688.6365               724.5002               727.9519
 829.1017               898.3113               906.6445
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 909.7816               964.2673               970.0191
 985.6517               992.9570              1017.8623
1050.4450              1078.7511              1112.3412
1176.3867              1179.9725              1301.1396
1315.0234              1327.3144              1433.6466
1466.7481              1477.8182              1580.5101
1589.7236              1633.3575              1996.6711
3127.9644              3147.8923              3149.7561
3155.6213              3165.6329              3171.4329
3184.6331              3241.1348              3380.2645
!23.8528
        ZeroEnergy[kcal/mol]          1.559
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.307
C                  -0.666401   -0.488177   -0.023926
C                  -0.669138    0.881663   -0.161249
C                  -1.908203    1.531327   -0.130824
C                  -3.081802    0.794712    0.033122
C                  -3.031318   -0.592037    0.168361
C                  -1.798420   -1.256317    0.140119
C                   1.379477   -1.553500   -0.084167
C                   2.331446   -0.781269   -0.221231
C                   3.288084    0.221940   -0.411343
C                   3.915045    0.890828    0.582515
H                   0.253001    1.438960   -0.286520
H                  -1.953750    2.610613   -0.234907
H                  -4.038871    1.303552    0.055771
H                  -3.946664   -1.160940    0.295631
H                  -1.751776   -2.335467    0.244381
H                   0.992794   -2.542287    0.038580
H                   3.540109    0.451942   -1.444652
H                   3.698034    0.689114    1.624364
H                   4.654508    1.649493    0.359091
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.27610422 0.458082001 0.288654411
     End
       Frequencies[1/cm]     49
  46.6019
  94.8297               134.6901               172.9300
 241.6351               341.4525               403.2051
 438.6567               553.5399               564.5699
 613.3680               649.8370               668.8105
 689.4269               728.7933               732.8511
 829.8240               898.9930               904.7198
```

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 907.7966               964.5947               969.7807
 983.1301               993.1633              1017.9939
1050.5876              1079.1241              1112.3579
1176.4990              1180.1965              1298.3279
1315.6907              1327.7792              1432.3139
1467.3099              1478.2715              1580.9087
1582.7808              1634.0307              1981.8455
3127.1925              3147.9462              3150.2581
3156.0050              3166.0085              3171.6408
3184.7204              3241.5281              3368.9776
!25.2012
        ZeroEnergy[kcal/mol]          1.424
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.287
C                  -0.662819   -0.487658   -0.024767
C                  -0.666841    0.882297   -0.162028
C                  -1.906047    1.531359   -0.130665
C                  -3.079192    0.794230    0.034160
C                  -3.027806   -0.592482    0.169325
C                  -1.794691   -1.256057    0.140136
C                   1.364929   -1.544474   -0.085072
C                   2.325620   -0.778737   -0.222580
C                   3.285230    0.218867   -0.411439
C                   3.916397    0.884917    0.583800
H                   0.255029    1.439847   -0.288004
H                  -1.952154    2.610606   -0.234693
H                  -4.036494    1.302590    0.057556
H                  -3.942726   -1.161878    0.297274
H                  -1.747095   -2.335096    0.244318
H                   0.997603   -2.541662    0.036712
H                   3.539263    0.448437   -1.444426
H                   3.698170    0.683782    1.625476
H                   4.659721    1.639804    0.360566
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.307479699 0.527108056 0.326304987
     End
       Frequencies[1/cm]     49
  47.4980
  98.6337               139.7505               178.8217
 244.3051               344.2953               403.6479
 440.4153               554.6359               565.2247
 613.9989               648.6611               667.0652
 690.2554               729.8963               742.3782
 830.5815               898.7541               900.2837
```

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 908.8976               964.9532               969.6824
 980.4883               993.3873              1018.1456
1050.7494              1079.5224              1112.3762
1176.6212              1180.4380              1295.1519
1316.3940              1328.2754              1430.8436
1467.9076              1478.7719              1575.2064
1581.8648              1634.7483              1967.4449
3126.3833              3148.0090              3150.7964
3156.4559              3166.4630              3171.9193
3184.8398              3241.9480              3357.2961
!26.5143
        ZeroEnergy[kcal/mol]          1.2125
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.267
C                  -0.659338   -0.487131   -0.025558
C                  -0.664717    0.882954   -0.162746
C                  -1.904086    1.531358   -0.130475
C                  -3.076752    0.793670    0.035190
C                  -3.024413   -0.593001    0.170269
C                  -1.791062   -1.255819    0.140164
C                   1.350404   -1.535200   -0.086009
C                   2.319735   -0.775833   -0.223994
C                   3.282641    0.215679   -0.411571
C                   3.918244    0.878759    0.585103
H                   0.256863    1.440789   -0.289395
H                  -1.950788    2.610562   -0.234440
H                  -4.034306    1.301516    0.059310
H                  -3.938884   -1.162928    0.298866
H                  -1.742465   -2.334739    0.244255
H                   1.002389   -2.540362    0.034762
H                   3.538887    0.444634   -1.444226
H                   3.698622    0.678402    1.626603
H                   4.665742    1.629505    0.362031
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.338855179 0.589859015 0.35140537
     End
       Frequencies[1/cm]     49
  48.3655
 102.3795               144.4559               184.5554
 247.2676               347.6736               404.1203
 442.3318               556.0191               565.9382
 614.6548               646.7595               666.0598
 691.1194               731.0504               753.1880
 831.3742               893.2782               900.7191
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 910.0436               965.3410               969.7212
 977.7992               993.6326              1018.3200
1050.9306              1079.9464              1112.3972
1176.7568              1180.6992              1291.6149
1317.1350              1328.8008              1429.2495
1468.5378              1479.3244              1567.9711
1582.5616              1635.5037              1953.7554
3125.5240              3148.0881              3151.3523
3156.9721              3166.9804              3172.2638
3184.9711              3242.3965              3345.2817
!27.7809
        ZeroEnergy[kcal/mol]          0.911
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.247
C                  -0.655758   -0.486924   -0.026409
C                  -0.662212    0.883307   -0.163589
C                  -1.901574    1.531354   -0.130375
C                  -3.073939    0.793420    0.036232
C                  -3.020979   -0.593217    0.171292
C                  -1.787571   -1.255572    0.140243
C                   1.335906   -1.526384   -0.086924
C                   2.313300   -0.772627   -0.225429
C                   3.279682    0.212449   -0.411689
C                   3.919662    0.872711    0.586503
H                   0.259196    1.441204   -0.290958
H                  -1.948605    2.610518   -0.234333
H                  -4.031617    1.300990    0.061098
H                  -3.935136   -1.163434    0.300631
H                  -1.738220   -2.334377    0.244282
H                   1.006965   -2.539008    0.032756
H                   3.538448    0.440520   -1.443993
H                   3.698335    0.673439    1.627816
H                   4.671535    1.619058    0.363574
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.370230658 0.652609974 0.389055946
     End
       Frequencies[1/cm]     49
  49.2767
 106.1734               148.8033               190.0704
 250.6256               351.5694               404.6140
 444.4017               557.6144               566.7323
 615.3328               643.9292               665.8223
 692.0173               732.2719               764.9380
 832.2029               887.0553               901.5285
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 911.2213               965.7518               969.8068
 975.1711               993.8931              1018.5183
1051.1239              1080.4069              1112.4239
1176.9040              1180.9904              1287.6583
1317.9254              1329.3414              1427.5189
1469.1898              1479.9344              1560.7528
1583.3691              1636.2633              1940.8998
3124.6291              3148.1780              3151.9011
3157.5456              3167.5522              3172.6839
3185.1210              3242.8763              3333.3453
!29.0831
        ZeroEnergy[kcal/mol]          0.49
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.227
C                  -0.652340   -0.486411   -0.027169
C                  -0.660311    0.883993   -0.164235
C                  -1.899858    1.531294   -0.130119
C                  -3.071712    0.792743    0.037287
C                  -3.017715   -0.593850    0.172224
C                  -1.784047   -1.255358    0.140258
C                   1.321482   -1.516804   -0.087921
C                   2.307056   -0.768947   -0.226931
C                   3.277435    0.209093   -0.411874
C                   3.922265    0.866067    0.587840
H                   0.260762    1.442240   -0.292221
H                  -1.947541    2.610411   -0.233987
H                  -4.029667    1.299745    0.062871
H                  -3.931388   -1.164650    0.302188
H                  -1.733634   -2.334041    0.244156
H                   1.011081   -2.536338    0.030648
H                   3.538739    0.436205   -1.443830
H                   3.699232    0.667933    1.628970
H                   4.678891    1.607573    0.365035
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.401606138 0.715360933 0.420431425
     End
       Frequencies[1/cm]     49
  50.0847
 109.6854               152.7086               195.2322
 254.0447               355.8623               405.1264
 446.6051               559.3074               567.5762
 616.0252               640.3747               666.5175
 692.9374               733.5680               777.9579
 833.0626               880.6030               902.3865
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 912.3949               966.1805               969.5423
 973.1660               994.1706              1018.7421
1051.3374              1080.8852              1112.4590
1177.0583              1181.2999              1283.4575
1318.7477              1329.9048              1425.7365
1469.8597              1480.6042              1553.9456
1584.2513              1637.0386              1929.4116
3123.7213              3148.2813              3152.4478
3158.1454              3168.1695              3173.1482
3185.2935              3243.3572              3321.1321
!30.2012
        ZeroEnergy[kcal/mol]          -0.068
        ElectronicLevels[1/cm]        1
           0   2
   End
     RRHO
       Geometry[angstrom]     19        # 2.207
C                  -0.648953   -0.485876   -0.027914
C                  -0.658575    0.884731   -0.164795
C                  -1.898337    1.531204   -0.129785
C                  -3.069645    0.791972    0.038371
C                  -3.014528   -0.594577    0.173124
C                  -1.780568   -1.255152    0.140226
C                   1.307127   -1.507003   -0.088957
C                   2.300591   -0.764811   -0.228442
C                   3.275416    0.205665   -0.412087
C                   3.925429    0.859063    0.589140
H                   0.262124    1.443405   -0.293319
H                  -1.946726    2.610273   -0.233521
H                  -4.027906    1.298349    0.064668
H                  -3.927680   -1.166018    0.303678
H                  -1.729043   -2.333719    0.243913
H                   1.014444   -2.532819    0.028494
H                   3.539289    0.431688   -1.443709
H                   3.700650    0.662209    1.630100
H                   4.687107    1.595336    0.366406
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.432981617 0.778111892 0.445531809
     End
       Frequencies[1/cm]     49
  50.8672
 113.0394               156.2113               200.0152
 257.6147               360.5250               405.6467
 448.9232               561.0210               568.5071
 616.7282               636.2692               667.8377
 693.8784               734.9272               791.9836
 833.9500               873.9588               903.2698
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 913.5557                966.5604                968.0277
 972.7904                994.4595               1018.9959
1051.5666               1081.3888               1112.5055
1177.2195               1181.6356               1279.0014
1319.6131               1330.4782               1423.9057
1470.5359               1481.3375               1547.5436
1585.2174               1637.8015               1919.2836
3122.8228               3148.4096               3152.9789
3158.7628               3168.8066               3173.6599
3185.4851               3243.8594               3309.0771
!31.2415
        ZeroEnergy[kcal/mol]          -1.629
        ElectronicLevels[1/cm]        1
           0   2
   End
  End
   Barrier      B8   W3    W7    #  ts [3]-[7]
     RRHO
       Geometry[angstrom]     19        #
C 0.7041432133 -0.0034886803 0.1966500229
C -0.3377501017 -0.9063532951 0.4285551438
C -0.1520377715 -2.1983894635 0.8430060696
C 1.1778345976 -2.6151900979 1.0635372727
C 2.2366005928 -1.7394768978 0.8486850368
C 2.0121962222 -0.4267482542 0.4101833439
C 0.1744297674 1.2919366668 -0.2660117433
C -1.1574874233 1.28385307 -0.3706643712
C -2.1898653303 2.1703130737 -0.8178501714
C -2.2104342569 2.7752467705 -2.0181834379
H -1.3715916721 0.0210157579 0.072089846
H -0.9781244406 -2.8814108735 1.0085727428
H 1.3714402557 -3.6258884093 1.4067661845
H 3.2522707284 -2.077707661 1.0209063029
H 2.8487333329 0.2425872509 0.2357257821
H 0.8014452424 2.1547328382 -0.4701069527
H -3.0282262396 2.3221320986 -0.139306765
H -1.4188199099 2.6192120931 -2.742243951
H -3.0229043558 3.4351095511 -2.2998461851
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1942.3374
         WellDepth[kcal/mol]         34.9
         WellDepth[kcal/mol]         22.0
       End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   8 9
        Symmetry                1
        Potential[kcal/mol]     8
0.  0.48945748 0.156877397 0.081576247 0.  0.495732576 0.169427589
0.081576247
     End
```

```
       Frequencies[1/cm]     49
   92.0816
  166.3041    215.2011    278.3669
  361.3415    399.9219    409.5042
  536.6811    552.2659    628.3050
  645.8508    688.9791    712.6056
  754.2678    849.7895    854.7150
  883.7234    930.3071    936.3080
  981.1898    983.3830   1004.9704
 1016.7555   1030.7393   1049.0651
 1098.9793   1118.9185   1176.3803
 1186.4619   1240.5490   1300.8789
 1314.5057   1364.7869   1436.8546
 1455.9281   1473.1769   1599.5593
 1613.6065   1627.7660   1666.5738
 1732.5818   3114.8403   3137.5287
 3154.4328   3158.9839   3161.2555
 3171.9663   3184.2303   3227.1270
!71.6011
        ZeroEnergy[kcal/mol]          -14.8
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B9   W3    P4    #  ts [3]-p4 (4-phenyl-vinylacetylene)
     RRHO
       Geometry[angstrom]     19        #
C -0.2413536228 -0.4022553945 0.2316133098
C -1.5902461569 -0.6055482468 0.6390530588
C -2.0901469656 -1.908035644 0.8131164765
C -1.2588174832 -3.024662084 0.5884802657
C 0.0798109715 -2.8349691185 0.1877606102
C 0.5898254021 -1.5368225458 0.010797859
C 0.2757660007 0.9508516488 0.0240670377
C 0.6122176029 2.046056248 -0.4058121195
C 1.0307803972 3.361669683 -0.8245623682
C 2.2445170994 3.644615219 -1.3481269664
H -2.2363097513 0.2652003085 0.8138945985
H -3.1331002731 -2.0534297143 1.1255342496
H -1.6530903156 -4.0405387733 0.7260302599
H 0.7291692471 -3.7033578221 0.0124920758
H 1.632313425 -1.3874360009 -0.3007632519
H 0.9405261321 1.0686941198 1.9680063357
H 0.2889120866 4.1684125582 -0.7022840911
H 3.0104862646 2.8722194405 -1.4879497562
H 2.5069737132 4.6648372928 -1.6532834016
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    604.6093
         WellDepth[kcal/mol]         44.5
         WellDepth[kcal/mol]         4.8
       End
      Rotor     Hindered     ! CHCCCHCH2
```

```
        Group                   8 9 10 16 17 18 19
        Axis                    1 7
        Symmetry                 1
        Potential[kcal/mol]      8
0.  0.48945748 0.156877397 0.081576247 0.  0.495732576 0.169427589
0.081576247
     End
      Rotor     Hindered     ! vinyl
        Group                   10 17 18 19
        Axis                    8 9
        Symmetry                 1
        Potential[kcal/mol]      8
0.  0.131777014 0.464357097 0.414156329 0.069026055 0.056475863
0.97891496 0.715360933
     End
       Frequencies[1/cm]     48
 102.7685    117.0418    202.0436
 244.0326    368.9774    392.5277
 411.4554    449.8235    513.9452
 552.5296    586.8397    638.0547
 693.4695    704.9136    720.3052
 773.9929    852.7354    933.3010
 940.1109    953.4927    981.6565
1000.1766   1003.2463   1015.5599
1049.4620   1100.6033   1102.6597
1183.1538   1200.9547   1284.3097
1313.2260   1316.4017   1351.8285
1446.1335   1473.7340   1523.6578
1610.5144   1635.8318   1647.8349
2225.1800   3132.1196   3148.2898
3165.2403   3174.3376   3185.4177
3193.7243   3197.6361   3239.1251
! 35.9618     62.1656
        ZeroEnergy[kcal/mol]          -5.3
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B10  W3    P5    #  ts [3]-p5 phenylbutatriene
     RRHO
       Geometry[angstrom]     19        #
C                   0.494439   -0.464397   -0.0
C                   0.643126    0.933217   -0.0
C                   1.906980    1.506597   -0.0
C                   3.048583    0.702211    0.0
C                   2.915244   -0.684348    0.0
C                   1.650311   -1.262165    0.0
C                  -0.816398   -1.116212   -0.0
C                  -2.006803   -0.538062   -0.0
C                  -3.113731    0.095944    0.0
C                  -4.396968    0.414438    0.0
H                  -0.240163    1.562262   -0.0
H                   2.005782    2.586317   -0.0
H                   4.033536    1.154974    0.0
H                   3.796379   -1.316051    0.0
```

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H                   1.549513   -2.342554    0.0
H                  -0.797710   -2.206143   -0.0
H                  -2.408179    1.966205    0.0
H                  -5.148290   -0.369363   -0.0
H                  -4.739565    1.441025    0.0
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    604.6791
         WellDepth[kcal/mol]         53.9
         WellDepth[kcal/mol]         6.4
       End
      Rotor     Hindered     ! CHCCCHCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  2.585339511 6.457073681 2.610439894
     End
       Frequencies[1/cm]     49
  67.7888
  93.9546               194.8191               256.1073
 267.5271               353.3758               413.1267
 449.9986               479.2179               519.9138
 557.0246               591.6972               632.8562
 636.4844               705.9664               772.0274
 818.6379               851.9032               871.4348
 877.8159               936.8796               943.3014
 982.2137              1005.3597              1015.1765
1031.2219              1049.6229              1107.1416
1182.9117              1201.3434              1226.1127
1295.2908              1348.3435              1363.3181
1445.5039              1485.5470              1524.1537
1615.1520              1638.0476              1668.0391
2100.3740              3102.0424              3129.0728
3158.9853              3162.8593              3171.7390
3180.0015              3191.0430              3218.6161
!49.3622
        ZeroEnergy[kcal/mol]          4.2
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B11  W7    W17   #  ts [7]-[17]
     RRHO
       Geometry[angstrom]     19        #
C 0.2378184396 -0.3304309063 -0.1878509912
C -0.957215628 -0.9703826656 0.1760485349
C -1.0183031689 -2.2606713181 0.6547064938
C 0.2105286332 -2.9286083283 0.7967658074
C 1.422454418 -2.308291478 0.454841762
C 1.4605615569 -1.0111148783 -0.0464436491
C -0.2060194338 0.9646080428 -0.5903998758
C -1.6162901671 0.8305093213 -0.8060842293
```

```
C -2.5973086977 1.8552716448 -0.4693326147
C -2.4033788166 2.8206556397 0.4401710637
H -1.9485154291 -2.7480518712 0.9249941287
H 0.22371375 -3.9410973424 1.1875084649
H 2.3477435586 -2.8589574038 0.584267047
H 2.403727759 -0.5454061253 -0.3119614888
H 0.3226840785 1.9075714975 -0.5140144927
H -1.9270957385 0.1267739529 -1.5707038124
H -3.5497466108 1.8102651418 -0.9918719842
H -1.4918776729 2.8731795329 1.0259679167
H -3.1549080614 3.5776758056 0.6307308053
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    540.9819
         WellDepth[kcal/mol]         32.1
         WellDepth[kcal/mol]         33.4
       End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   8 9
        Symmetry                1
        Potential[kcal/mol]     8
0.439256713 2.78614258 6.41314801 4.398842226 0.  1.593874359 5.779363324
3.288150252
     End
       Frequencies[1/cm]     49
 111.6126
 180.4999               256.9315               297.1546
 401.9328               410.8667               489.1318
 554.4017               571.3185               608.4107
 667.4413               687.0385               727.7816
 749.2477               766.1873               858.4607
 869.1899               937.6761               949.6286
 975.3691               983.1798               999.1075
1019.1528              1024.8307              1052.4321
1121.1004              1163.2865              1179.0844
1224.3039              1247.5488              1310.8058
1329.2166              1358.5127              1433.0902
1445.9498              1457.9856              1475.6447
1570.1305              1599.7891              1657.1286
3132.0541              3138.5007              3152.4285
3152.6860              3163.2509              3172.7496
3181.0030              3182.1692              3223.8606
!78.7919
        ZeroEnergy[kcal/mol]          -7.7
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B12  W17   W18   #  ts [17]-[18]
     RRHO
       Geometry[angstrom]     19        #
C 0.5005143756 0.8727365708 -0.066463776
```

```
C 0.2059913675 -0.4153438639 -0.5383943844
C 1.1017838265 -1.4618112843 -0.5188833164
C 2.380861251 -1.1713767226 -0.0141240672
C 2.709659093 0.1125416021 0.4481367265
C 1.7836001678 1.1511495482 0.4362037621
C -0.7029246298 1.5878031038 -0.3495781342
C -1.7284214623 0.6036785081 -0.5347857414
C -2.2770926033 -0.2346983579 0.5287513708
C -3.4685615464 -0.8418254278 0.4532196311
H 0.8570274286 -2.4554519257 -0.8771166427
H 3.1333523447 -1.9530973928 0.0099583669
H 3.7104555022 0.2932897424 0.8246060272
H 2.0493784343 2.137566047 0.8006978574
H -0.7794579801 2.6094740786 -0.7057934983
H -2.4366152646 0.7641832599 -1.3520936063
H -1.6785593869 -0.3294378999 1.4298962368
H -4.0903007736 -0.7670406912 -0.4331265498
H -3.8516361444 -1.4347868947 1.2745397379
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    618.2649
         WellDepth[kcal/mol]         37.2
         WellDepth[kcal/mol]         34.3
       End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   8 9
        Symmetry                1
        Potential[kcal/mol]     8
3.557979375 8.270576396     5.722887461 0.  5.515809296 8.653357246
      8.245476013 6.821029243
     End
       Frequencies[1/cm]     49
 85.3201               140.3922129
 269.6242              334.5118
 374.2997              416.6569              473.4535
 522.6421              593.6824              638.1026
 649.4275              689.8181              722.2629
 765.2312              847.6720              864.2708
 901.1956              915.0762              939.9850
 952.5986              958.6377              985.9787
1019.4259             1032.1364             1083.1591
1121.3451             1170.1320             1208.3051
1230.6650             1250.3640             1314.2116
1315.6262             1368.7956             1388.4461
1440.6257             1463.6608             1477.6113
1569.7189             1599.6105             1653.3478
3072.6244             3133.4142             3154.1053
3155.8156             3165.8101             3168.8884
3175.5655             3183.7804             3222.0281
!109.3765 and 180.2030 are replaced with their geometric mean
        ZeroEnergy[kcal/mol]         -3.9
```

```
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B13  W18   W6    #  ts [18]-[6]
     RRHO
       Geometry[angstrom]     19        #
C                    0.6433   -0.19386   0.03856
C                    1.16717  -1.49301  -0.14392
C                    0.33085  -2.59982  -0.24441
C                   -1.05442  -2.45223  -0.16797
C                   -1.60704  -1.17726   0.01914
C                   -0.74412  -0.11168   0.1083
C                    1.55014   0.95434   0.08339
C                    1.2213    2.25967  -0.05776
C                   -0.13539   2.75707  -0.17031
C                   -1.17151   2.27822   0.5571
H                    2.244    -1.6217   -0.20614
H                    0.76122  -3.5853   -0.38227
H                   -1.703    -3.31854  -0.2463
H                   -2.68218  -1.0477    0.08916
H                    2.60651   0.70181   0.11536
H                    2.03057   2.97308  -0.19413
H                   -0.32476   3.50651  -0.93637
H                   -2.189     2.59709   0.35972
H                   -1.00956   1.73387   1.47737
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    256.7451
         WellDepth[kcal/mol]         4.8
         WellDepth[kcal/mol]         57.4
       End
       Frequencies[1/cm]     50
  87.4142              139.2657
 226.1307              258.4703              380.9825
 404.4556              423.0168              504.9426
 547.9785              591.7376              639.4866
 707.4830              735.9871              768.8099
 795.8965              828.2484              860.6750
 877.4613              940.3918              957.0187
 973.1230              979.6621              987.6868
 992.7687             1043.7448             1082.5197
1126.4168             1175.1690             1192.3405
1228.2094             1275.4679             1294.2883
1328.2598             1418.5718             1444.8748
1463.2684             1477.5651             1567.0742
1585.5384             1616.4527             1645.5138
3120.8872             3131.0517             3144.9918
3146.9665             3152.5228             3154.4580
3167.4274             3183.7627             3229.4964
        ZeroEnergy[kcal/mol]          -32.0
        ElectronicLevels[1/cm]        1
           0   2
```

```
   End
   Barrier      B14  R1    W2    #  ts [0]-[2]
     RRHO
       Geometry[angstrom]     19        #
C 0.3042339651 -0.1907513022 0.0791405558
C -0.3936002062 -1.1048097458 -0.6822443161
C -0.0703875626 -2.4584601859 -0.528761553
C 0.9279240212 -2.8432581561 0.3662974629
C 1.6138026292 -1.8850655575 1.1125042274
C 1.3056588112 -0.5272142921 0.9653525398
C -0.1562753682 2.0464850936 -0.2103208653
C 0.9021712862 2.5533843806 -0.5577936223
C -1.5498682461 1.9769848191 0.1368323896
C -2.5274489697 2.4732259222 -0.6264023259
H -1.1722942634 -0.7952104593 -1.3714060411
H -0.5990416328 -3.2077856016 -1.1093381533
H 1.1737251393 -3.8930260336 0.4807320839
H 2.3906003173 -2.1896767393 1.806637814
H 1.8387893382 0.2286177234 1.5321173262
H 1.9006937975 2.7751380455 -0.8492917851
H -1.7878749643 1.477822007 1.0704966328
H -2.3190057826 2.9586665321 -1.5723925722
H -3.5628541094 2.4023286705 -0.3151822623
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    373.7196
         WellDepth[kcal/mol]         4.1
         WellDepth[kcal/mol]         40.9
       End
     Rotor     Hindered     ! HCCCHCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0. 0.269829124 0.24472874 1.374246002 0.476907288 0.043925671 0.282379316
1.374246002
     End
     Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   7 9
        Symmetry                1
        Potential[kcal/mol]     8
0.017914144 1.199855439     0.602081019  0.  1.082051809 0.629801255
0.083091055 0.355668043
     End
       Frequencies[1/cm]     48
  63.6036    102.6017    190.7743
 227.5940    282.4249    399.5234
 440.7641    504.2073    544.6837
 610.5741    612.0670    678.1479
 688.6733    692.0872    727.6076
 832.6358    878.0771    901.0814
```

```
 949.9144    965.4862    972.9822
 993.1417   1013.2996   1016.6921
1049.5364   1076.7424   1105.9009
1175.7836   1179.0736   1312.7078
1321.1698   1322.9156   1436.6013
1463.0300   1474.9021   1580.5909
1626.1849   1660.7326   2042.0132
3142.9854   3149.8932   3155.4157
3162.0155   3166.9385   3169.9080
3183.5021   3234.0393   3453.0202
!19.8359     45.8467
        ZeroEnergy[kcal/mol]          4.1
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B15  W2    W8    #  ts [2]-[8]
     RRHO
       Geometry[angstrom]     19        #
C -0.0066344881 -0.2959372936 -0.0190760542
C -1.1201762211 0.4838875967 -0.3555412679
C -2.4066846173 -0.0317848262 -0.2261104266
C -2.5961461017 -1.3315263295 0.2380983171
C -1.4913251317 -2.1163529096 0.574070862
C -0.2067016005 -1.6044289959 0.4466932081
C 1.3403274485 0.2482507223 -0.1625068489
C 2.5911381384 -0.0168009886 0.0409045904
C 1.8704051311 1.5523709957 -0.6679046827
C 1.9195456333 2.7166111358 0.0859489441
H -0.9677979462 1.4962462207 -0.711866943
H -3.2619010663 0.5812384188 -0.4876766519
H -3.5981619365 -1.7332574264 0.337861318
H -1.6353423688 -3.1289994205 0.9341493756
H 0.6533952964 -2.2129476121 0.704005444
H 3.4084985897 -0.5969072187 0.4306289303
H 2.0977607424 1.612861575 -1.7281914762
H 1.6406545201 2.7190085103 1.133080532
H 2.3004050226 3.6370223094 -0.3394503776
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    594.4365
         WellDepth[kcal/mol]         19.6
         WellDepth[kcal/mol]         7.4
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  2.164908085  5.578560255 2.37198625 0.  2.177458277 5.553459871
2.434737209
     End
       Frequencies[1/cm]     49
```

```
 97.4589
 141.8659    226.9607    329.0379
 372.5506    415.1638    444.6813
 474.3365    518.9307    569.2500
 633.0051    642.8142    672.0132
 710.0732    735.4633    742.0261
 784.0983    857.4815    935.4639
 956.4283    963.5465    983.6168
1004.2750   1016.0699   1047.1844
1099.3325   1118.2150   1182.0928
1195.1966   1205.8354   1289.7501
1326.7751   1353.2399   1380.9255
1478.6194   1495.1266   1522.6917
1618.1303   1642.2514   1771.8012
3134.8943   3140.4408   3160.8914
3168.1931   3176.5396   3183.6318
3191.1217   3233.1033   3286.1156
!55.4692
        ZeroEnergy[kcal/mol]          -17.3
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B16  W8    W9    #  ts [8]-[9]
     RRHO
       Geometry[angstrom]     19        #
C -0.2388366873 -0.0314758754 0.2892121912
C -0.7606585905 -0.6661889835 -0.8566914266
C -1.4565779818 -1.8615496857 -0.7408431137
C -1.6418378076 -2.4561480077 0.5082824514
C -1.1215544226 -1.8416354653 1.6472535203
C -0.425320428 -0.6439172201 1.5458921595
C 0.4970716323 1.1832918002 0.1817475227
C 0.8806214304 2.406189706 0.2927472562
C 1.9714837451 1.8372991722 -0.5521686547
C 2.0301043252 1.9882279877 -1.9471048375
H -0.6109658391 -0.2105369579 -1.8279715397
H -1.8563925019 -2.3350527996 -1.6306618101
H -2.1847133941 -3.3904125486 0.5923133741
H -1.2605463413 -2.2975897004 2.6212670192
H -0.0206206672 -0.1683259712 2.4313460038
H 0.57250402 3.3806778132 0.6522464312
H 2.8604723318 1.4723183928 -0.0440919178
H 1.2089335722 2.4337958084 -2.4962364267
H 2.8843575283 1.6305653929 -2.5081735464
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    527.0097
         WellDepth[kcal/mol]         6.5
         WellDepth[kcal/mol]         28.1
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
```

```
        Axis                    1 7
        Symmetry                 1
        Potential[kcal/mol]     8
0.  1.123242166  1.5311234 0.62750959 0.  1.160892741 1.537398495
0.658885069
     End
       Frequencies[1/cm]     49
  79.2230
 117.3086    241.0358    288.6640
 404.1271    411.3605    440.0655
 466.3494    522.4888    525.9684
 633.5119    678.4618    702.5005
 737.8488    757.7506    767.4084
 846.4283    893.9730    916.1767
 958.5914    976.3084    996.6787
1008.6913   1044.9791   1062.7949
1101.3096   1128.6993   1181.0261
1184.4988   1206.8292   1232.2573
1306.3609   1352.4693   1373.7331
1469.9052   1484.1239   1511.2621
1597.9071   1628.6138   1888.1744
3120.7207   3138.9310   3163.1199
3166.0944   3170.4984   3183.2791
3189.4651   3194.7485   3236.4217
!39.0392
        ZeroEnergy[kcal/mol]          -18.2
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B17  W9    W10   #  ts [9]-[10]
     RRHO
       Geometry[angstrom]     19        #
C -0.2066025523 -0.2202248251 0.0421342691
C -1.5682376922 0.127767059 -0.0756107254
C -2.5582311919 -0.8418030835 0.0205349008
C -2.2170922573 -2.1801314923 0.2179910267
C -0.8740808226 -2.5428334442 0.3171941426
C 0.1205742454 -1.5771761671 0.2264664208
C 0.8278051814 0.778360458 -0.037855983
C 0.9817052767 2.0650889993 0.2864392909
C 2.2944340041 2.5921827614 -0.1669929062
C 3.0248959899 1.6658870345 -0.7754946853
H -1.8352150525 1.1632957093 -0.2520604493
H -3.6004162835 -0.5554705444 -0.0687709484
H -2.9918943115 -2.9353256561 0.2847976677
H -0.6025630145 -3.582256144 0.4641690335
H 1.1641932923 -1.8604890855 0.3032337289
H 2.0748136397 0.6223718599 -0.6133464477
H 0.2576825636 2.6630825086 0.8315503338
H 2.5975305425 3.6228998714 -0.007090353
H 3.9848475363 1.6591876804 -1.2713170722
       Core     RigidRotor
         SymmetryFactor    1
       End
```

```
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    2000.9575
         WellDepth[kcal/mol]         35.3
         WellDepth[kcal/mol]         26.5
       End
      Rotor     Hindered     ! CHCHCHCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  0.759286604  0.370230658  0.131777014  0.  0.796937179 0.338855179
0.131777014
     End
       Frequencies[1/cm]     49
   96.5416
  112.3423    275.4386    340.6682
  381.5563    411.1753    438.2259
  514.0811    607.8732    629.8959
  647.5174    705.2437    721.7364
  770.0634    835.8202    851.6187
  892.0312    912.6963    925.9598
  934.0376    980.4461    995.4077
 1001.4786   1012.5644   1047.9852
 1059.0866   1100.6198   1180.4728
 1181.9183   1201.3913   1252.8162
 1291.1108   1314.5865   1351.2823
 1470.5484   1512.8072   1591.4101
 1603.0048   1631.7531   1672.1264
 1727.6358   3147.0416   3161.4733
 3162.7467   3168.4319   3179.0719
 3184.8943   3191.9650   3229.8732
!39.6180
        ZeroEnergy[kcal/mol]          -11.0
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B18  W10   W11   #  ts [10]-[11]
     RRHO
       Geometry[angstrom]     19        #
C 0.2540608459 -0.1883743892 0.1220545647
C -0.9437695587 -0.9184942561 0.0333885714
C -0.9257433269 -2.3014914625 -0.1057391847
C 0.2886320448 -2.9831042223 -0.1811916367
C 1.4868855569 -2.2716533341 -0.1164579009
C 1.4685654368 -0.8905212369 0.0328088017
C 0.2518495249 1.26514305 0.2931506821
C -0.8242718764 2.0182728099 0.8461228372
C -0.8528654262 3.2370622089 0.1199832153
C -0.1855920137 2.9362576316 -1.0200605112
H -1.8896033913 -0.3891871412 0.056866295
H -1.8592800051 -2.8494871743 -0.1695346108
H 0.3013396838 -4.0607784603 -0.299180444
H 2.4336291196 -2.7963870267 -0.1801884742
H 2.4018827233 -0.3395926155 0.0884126318
```

```
H 1.2325352918 1.7250971543 0.3232160047
H -1.5814514859 1.6261471212 1.5173173281
H -1.3004528073 4.1836449999 0.4140653823
H 0.1548936271 3.4819623474 -1.8953307458
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    578.3689
         WellDepth[kcal/mol]         25.1
         WellDepth[kcal/mol]         33.7
       End
      Rotor     Hindered     ! CHCHCHCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  3.451302745  5.929965625 2.773592388     0.  3.38227669 5.917415434
2.7547671
     End
       Frequencies[1/cm]     49
 106.0198
 159.9342    306.4226    383.7378
 395.4791    418.3011    535.4840
 566.3003    633.0789    657.1537
 695.3808    707.3808    732.7821
 761.6850    793.2495    854.3851
 882.1229    892.2711    922.6019
 933.8947    981.3618   1003.1170
1015.0059   1047.3046   1058.7066
1098.9877   1154.1667   1182.1974
1199.5164   1222.5976   1252.6843
1316.3438   1350.4139   1363.3074
1438.7362   1474.2289   1503.1867
1526.7009   1617.4667   1639.3598
3124.2065   3157.3521   3160.3576
3162.9093   3164.9203   3167.6531
3174.2147   3182.1827   3190.4928
!69.1787
        ZeroEnergy[kcal/mol]          -12.4
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B19  W11   W12   #  ts [11]-[12]
     RRHO
       Geometry[angstrom]     19        #
C -0.1913379926 0.1029915695 0.3757791356
C -1.4889995464 -0.3214673719 0.7009253083
C -1.8314794856 -1.6701278951 0.6814042207
C -0.8786080151 -2.6307290753 0.3526529178
C 0.4222782659 -2.2245189846 0.0503073879
C 0.7643227054 -0.8787719215 0.0638709009
C 0.1296604869 1.5466799138 0.4634372965
C 0.2722327407 1.8861505711 -1.7290130427
```

```
C 1.5320218597 2.058122736 -1.2729258145
C 1.3603183995 2.1752901834 0.1356987511
H -2.2378606646 0.418961407 0.9634563559
H -2.8436843419 -1.9701007746 0.9297929033
H -1.1399337788 -3.6826653544 0.3434482445
H 1.1784178711 -2.9649271112 -0.1877322794
H 1.7809659068 -0.5785445776 -0.1593911215
H -0.5023630273 2.0509803514 1.1992256677
H -0.1977935239 1.6711424082 -2.684758716
H 2.4525220397 2.1250587207 -1.8496574781
H 1.8667993586 2.8844715941 0.784697179
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    655.4431
         WellDepth[kcal/mol]         41.6
         WellDepth[kcal/mol]         33.7
       End
      Rotor     Hindered     ! CHCHCHCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0. 2.61671499 5.15812883 3.344626115 0.03137548    2.152357894
5.114203159 2.993220744
     End
       Frequencies[1/cm]     49
 120.5620
 178.2063               236.9857               350.4093
 413.2794               425.3503               500.1730
 547.7664               634.4196               645.3588
 706.1006               736.2651               751.8153
 767.2074               823.0104               847.3115
 876.2254               894.2108               914.2567
 948.5510               975.1014               995.1491
1013.2287              1047.9356              1058.1973
1097.7580              1108.0863              1180.3021
1200.4220              1225.1293              1238.4969
1319.4387              1352.3097              1411.6410
1425.7759              1478.4009              1499.5431
1521.7293              1615.6116              1637.2069
3069.5350              3115.8891              3145.3074
3154.4096              3160.8205              3161.9371
3172.1130              3183.7774              3190.6199
!56.7786
        ZeroEnergy[kcal/mol]          -4.5
        ElectronicLevels[1/cm]        1
           0   2
   End
  Barrier      B20  W12  W13   #  [12]-[13] (A4b-A5)
     RRHO
       Geometry[angstrom]     19        #
C       -0.063117       -0.706617       0.30381
```

```
C       -1.146712       -1.372336       -0.274066
C       -2.346335       -0.715125       -0.509607
C       -2.493227       0.627777        -0.143905
C       -1.456321       1.294442        0.477825
C       -0.219941       0.650312        0.6924
C       1.242760        -1.338999       0.408889
C       2.393124        -0.705837       0.09983
C       2.473462        0.633789        -0.476949
C       1.508832        1.536650        -0.463133
H       -1.03304        -2.40933        -0.565635
H       -3.16824        -1.242066       -0.975427
H       -3.433654       1.133586        -0.319944
H       -1.58945        2.313554        0.816654
H       0.449881        1.051979        1.439301
H       1.277902        -2.395499       0.65146
H       3.320334        -1.262845       0.154525
H       3.398996        0.857819        -1.01087
H       1.422122        2.528462        -0.880638
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    377.
         WellDepth[kcal/mol]         3.6
         WellDepth[kcal/mol]         34.3
       End
       Frequencies[1/cm]     50
105. 151. 231. 293. 396. 415. 437. 516. 539. 617.
646. 701. 735. 753. 772. 819. 841. 870. 901. 940. 968.
984. 998. 1002. 1023. 1040. 1090. 1179. 1191. 1195.
1227. 1266. 1329. 1337. 1429. 1457. 1515. 1555. 1590.
1609. 1647. 3047. 3137. 3154. 3159. 3165. 3166. 3176.
3186. 3210.
        ZeroEnergy[kcal/mol]          -29.9
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B21  W13  P1    #  [13] (A5) - naphthalene
     RRHO
       Geometry[angstrom]     19        #
H       -1.638390       1.099432        0.000000
C       0.000000        0.720451        0.000000
C       -0.170994       -0.717961       0.000000
C       -0.271992       -1.385551       1.239785
C       -0.271992       -1.385551       -1.239785
C       -0.092674       -0.714184       2.422547
C       -0.092674       -0.714184       -2.422547
C       0.228794        0.665811        2.422888
C       0.228794        0.665811        -2.422888
C       0.301120        1.360293        1.252283
C       0.301120        1.360293        -1.252283
H       -0.470723       -2.450237       1.241968
H       -0.470723       -2.450237       -1.241968
H       -0.161745       -1.245028       3.362555
```

```
H       -0.161745       -1.245028       -3.362555
H       0.429415        1.164772        3.361827
H       0.429415        1.164772        -3.361827
H       0.543738        2.415097        1.246068
H       0.543738        2.415097        -1.246068
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1047.
         WellDepth[kcal/mol]         13.5
         WellDepth[kcal/mol]         12.2
       End
       Frequencies[1/cm]     50
167. 171. 348. 377. 458. 472. 493. 519. 550. 564.
622. 636. 727. 746. 785. 801. 812. 843. 910. 931. 967.
987. 1000. 1004. 1027. 1036. 1145. 1160. 1178. 1183.
1218. 1264. 1277. 1378. 1383. 1415. 1479. 1488. 1531.
1585. 1635. 1652. 3155. 3157. 3161. 3164. 3175. 3176.
3187. 3188.
        ZeroEnergy[kcal/mol]          -51.1
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B22  W9   P4    #  [9] - 4-phenyl-vinylacetylene
     RRHO
       Geometry[angstrom]     19        #
C -0.2096185303 -0.4398623724 -0.1363806309
C -0.3298262083 -1.2425431245 1.0147706906
C -0.7756738929 -2.5536613709 0.9124229295
C -1.1094896018 -3.0887327037 -0.3317758424
C -0.9948417813 -2.3028372642 -1.4784373821
C -0.5490259959 -0.9908174882 -1.3875595687
C 0.2453398978 0.8989017093 -0.0390994474
C 0.5447871911 2.0801676141 0.0203320784
C 1.1941265356 3.3462173611 0.127588572
C 1.9499824394 3.7163822744 1.1671654924
H -0.0716036013 -0.8230510064 1.9794603965
H -0.8647912841 -3.1610563046 1.8059475612
H -1.4575481306 -4.112511195 -0.4072695676
H -1.2547424996 -2.7148218863 -2.4469255723
H -0.4589076824 -0.3772218118 -2.2755269774
H -1.2649031554 2.8643716208 -0.372410373
H 1.0430529532 4.0328475985 -0.70039936
H 2.109512687 3.0626958215 2.0162674056
H 2.425370393 4.6894593532 1.186695139
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    586.5899
         WellDepth[kcal/mol]         41.0
         WellDepth[kcal/mol]         4.8
       End
```

```
      Rotor     Hindered     ! CHCHCH2
        Group                  9 10 16 17 18 19
        Axis                   1 8
        Symmetry                2
        Potential[kcal/mol]     4
0.  0.741442741  0.747060835 0.553475381      0.00261797 0.807847061
0.584479375 0.766457156
      End
       Frequencies[1/cm]     49
  68.7074
  89.5819     98.2314    217.4899
 252.5985    346.0750    410.3332
 422.2703    443.7053    508.4312
 550.0668    593.7245    638.2484
 692.7322    703.1959    717.3921
 774.7557    852.7241    933.0330
 944.0905    945.7508    982.5737
1004.2456   1008.9302   1013.3493
1047.4548   1098.3838   1101.9818
1183.1230   1199.7145   1296.6297
1310.6951   1321.0878   1351.8539
1444.3476   1472.4940   1521.7705
1604.9578   1635.5309   1663.1266
2227.3489   3143.0807   3150.9179
3165.7819   3174.3595   3185.6003
3193.5933   3197.4585   3235.8619
!42.8318
        ZeroEnergy[kcal/mol]          -5.3
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B23  W10  P3    #  [10]-trans-1-phenyl-vinylacetylene
(TS23)
     RRHO
       Geometry[angstrom]     19        #
C                 -0.425126   -0.178420   -0.0
C                 -1.289655   -1.285683   -0.0
C                 -2.670931   -1.121545   -0.0
C                 -3.220797    0.157502    0.0
C                 -2.376569    1.269591    0.0
C                 -0.998374    1.106023    0.0
C                  1.018333   -0.418236   -0.0
C                  1.995336    0.510160   -0.0
C                  3.380190    0.163610   -0.0
C                  4.433465   -0.449229    0.0
H                 -0.866810   -2.284879   -0.0
H                 -3.317050   -1.992140   -0.0
H                 -4.296621    0.290110    0.0
H                 -2.797795    2.268660    0.0
H                 -0.363219    1.983847    0.0
H                  1.316233   -1.463077   -0.0
H                  1.759674    1.567509   -0.0
H                  5.422151   -0.839476    0.0
H                  4.068207    1.946804   -0.0
```

```
      Core                                          MultiRotor
        SymmetryFactor          1
        InterpolationEnergyMax[kcal/mol]        100
        PotentialEnergySurface[kcal/mol]        c10h9_TS23.dat
!        QuantumLevelEnergyMax[kcal/mol]         5
        InternalRotation
                Group                           8 9 10 16 17 18 19
                Axis                            1 7
                Symmetry                        1
                MassExpansionSize               11
!               PotentialExpansionSize          11
!               HamiltonSizeMin                 13
!               HamiltonSizeMax                 101
                GridSize                        100
        End
        InternalRotation
                Group                           10 18 19
                Axis                            8 9
                Symmetry                        1
                MassExpansionSize               11
!               PotentialExpansionSize          11
!               HamiltonSizeMin                 13
!               HamiltonSizeMax                 101
                GridSize                        100
        End
      End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    718.3654
         WellDepth[kcal/mol]         35.0
         WellDepth[kcal/mol]         7.0
       End
       Frequencies[1/cm]     48
  98.2624               115.1594               252.8117
 254.7093               387.0064               409.6301
 434.8420               502.8817               535.7112
 544.9195               614.7725               631.4016
 636.9914               678.6516               702.8847
 767.2571               845.5012               860.3838
 873.9177               927.5396               977.5458
 993.3401              1006.1931              1014.0416
1023.4468              1051.2526              1106.7087
1183.7191              1204.7924              1234.1318
1297.5464              1330.8807              1350.4893
1363.3091              1480.2156              1527.3296
1614.6068              1640.7359              1660.6920
2094.9881              3150.7398              3161.0759
3166.4409              3174.7848              3178.3598
3185.5248              3192.9210              3464.0034
!30.8676                49.7706
        ZeroEnergy[kcal/mol]          -1.9
        ElectronicLevels[1/cm]        1
           0   2
   End
```

```
   Barrier      B24  W12  P2    #  [12]-cis-1-phenyl-vinylacetylene
(TS24)
     RRHO
       Geometry[angstrom]     19        #
C                  -0.334531    0.567235    0.056176
C                  -1.577154    1.223012   -0.019406
C                  -2.768809    0.510215   -0.064230
C                  -2.747891   -0.882588   -0.026279
C                  -1.526614   -1.549890    0.059546
C                  -0.332957   -0.838961    0.101341
C                   0.870134    1.395720    0.092195
C                   2.175743    1.067029    0.024177
C                   2.773805   -0.225925   -0.102741
C                   3.496828   -1.185638    0.110177
H                  -1.599346    2.307580   -0.047330
H                  -3.712739    1.039916   -0.126437
H                  -3.675035   -1.443583   -0.058970
H                  -1.503762   -2.633299    0.096997
H                   0.602316   -1.374231    0.180384
H                   0.668445    2.459713    0.182215
H                   2.897571    1.877921    0.069333
H                   4.059490   -2.087802    0.126460
H                   2.091742   -0.627472   -1.808386
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! CHCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  1.912830581 3.287504544 0.550407487
      End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    810.8493
         WellDepth[kcal/mol]         38.0
         WellDepth[kcal/mol]         7.5
       End
       Frequencies[1/cm]     49
 101.7526
 155.6757              178.7709              251.5379
 339.2533              389.1019              415.7034
 443.5299              472.7161              522.2708
 583.3551              629.3502              633.9998
 675.6758              705.9953              734.2292
 744.7180              796.3043              806.8454
 854.1682              934.9623              965.4064
 980.3677              992.5863             1006.5433
1016.0909             1052.3231             1111.9252
1184.1653             1206.9666             1212.3730
1269.5837             1344.5698             1365.0965
1436.9403             1480.5883             1528.0339
1612.4213             1641.6116             1662.0593
2078.2249             3135.4606             3154.0866
```

```
3159.3227              3166.9269              3177.3961
3189.2895              3221.4913              3457.3971
!28.8218
        ZeroEnergy[kcal/mol]          -0.2
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B25  R1    W14   #  ts 0-[14]
     RRHO
       Geometry[angstrom]     19        #
C -0.1733916419 -0.2942906459 0.0482834165
C 1.0313899327 -0.6658597429 -0.5055224166
C 1.4667462459 -1.9777274442 -0.2791096791
C 0.6930667472 -2.8525490842 0.4833039875
C -0.5191552672 -2.4302132175 1.0280357929
C -0.9678676591 -1.1216420139 0.8115587035
C -1.0339193141 1.8343386189 -0.3846318584
C -1.6081289221 2.2324463782 0.7888533047
C 0.1614872289 2.4328313688 -0.8890217062
C 1.1546437563 2.9410449637 -1.3416468226
H 1.623539699 0.0282536011 -1.0916639624
H 2.4107732524 -2.3103908864 -0.6986124409
H 1.0370347303 -3.866213152 0.6552798397
H -1.1166822956 -3.1131000165 1.6233405131
H -1.9049727914 -0.7801125986 1.2381403255
H -1.6396032937 1.3075328165 -1.1152785226
H -1.0794808129 2.8705837959 1.4853145716
H -2.5867641763 1.8697128641 1.0765515848
H 2.0269290481 3.4034584906 -1.7336882418
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    303.5296
         WellDepth[kcal/mol]         2.6
         WellDepth[kcal/mol]         35.6
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  0.181977781  0.552208439 0.213353261     0. 0.213353261 0.558483535
0.200803069
     End
       Frequencies[1/cm]     49
  76.7523
  93.5891    143.7615    220.4930
 233.7264    382.7460    402.7843
 441.4698    533.0371    555.7426
 611.0624    632.7470    646.1352
 682.2828    687.4444    728.7048
 830.3282    848.7906    873.3939
 901.5276    922.4916    966.2489
```

```
 992.7159    994.3618   1020.4091
1052.7385   1078.6883   1103.4276
1176.2365   1180.7711   1271.9980
1313.0682   1325.0460   1421.7814
1464.7926   1476.7712   1545.7803
1581.1926   1629.3898   2206.2559
3147.7873   3151.4778   3152.2406
3158.2368   3168.9692   3174.5395
3185.0968   3245.4844   3476.7255
!15.6941
        ZeroEnergy[kcal/mol]          2.6
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B26  W14   W15   #  ts [14]-[15]
     RRHO
       Geometry[angstrom]     19        #
C  0.025089073 -0.1896603848 0.2908565754
C -0.5533587761 -0.689725977 -0.8754446223
C -0.0726097599 -1.8648608946 -1.4525014547
C 0.9888707433 -2.5498953465 -0.868066664
C 1.5717316063 -2.0540873723 0.2982552324
C 1.0931609303 -0.8809820058 0.8726372538
C -0.4878444751 1.0661287842 0.9600036812
C 0.3998364291 2.2778813017 1.0055688958
C -1.2243158828 2.0445753992 0.1869129929
C -2.0152232627 2.7005777871 -0.5090117689
H -1.3772694101 -0.1531930715 -1.3315784072
H -0.5290763975 -2.2428881888 -2.3605868869
H 1.3626978533 -3.4628845711 -1.31772355
H 2.4002050682 -2.5811906783 0.7584401882
H 1.551884046 -0.4933194348 1.7766887464
H -0.9606149018 0.8478853119 1.9212846112
H 1.1855341779 2.3855497259 0.2717673346
H 0.3537327047 2.958102801 1.8437781803
H -2.3391128932 3.5822303588 -1.0173309456
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    664.9541
         WellDepth[kcal/mol]         17.7
         WellDepth[kcal/mol]         8.1
       End
!      Rotor     Hindered     ! H2CCHCCH
!        Group                  8 9 10 16 17 18 19
!        Axis                   1 7
!        Symmetry                1
!        Potential[kcal/mol]     8
!
!     End
       Frequencies[1/cm]     50
  22.3126    116.8340
 134.3862    275.0487    296.8815
```

```
 329.5760    414.0589    436.6953
 500.4396    537.6799    540.9899
 634.0829    663.7942    705.6823
 713.7710    718.7209    757.6371
 789.8215    859.4721    926.3822
 944.1183    982.1210   1001.4635
1006.5514   1018.3353   1051.2748
1094.7966   1106.1412   1181.1833
1195.8070   1201.7294   1217.9871
1319.1268   1339.2681   1355.9694
1439.5680   1479.8906   1527.5602
1625.3053   1645.9118   1940.6448
3049.1328   3155.3619   3156.6936
3164.5663   3173.9862   3183.4594
3190.6747   3275.5187   3386.9917
!
        ZeroEnergy[kcal/mol]          -15.3
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B27  W15   W16   #  ts [15]-[16]
     RRHO
       Geometry[angstrom]     19        #
C 0.2835706761 0.0871381067 -0.5770245951
C -0.5845169843 -0.5836020314 -1.4593122416
C -0.3528073535 -1.9053399019 -1.8191625838
C 0.7473895939 -2.5966886128 -1.3116429884
C 1.6145178765 -1.9486957263 -0.432375063
C 1.3842452155 -0.6282200751 -0.0679694273
C 0.0884755157 1.4726120201 -0.166207745
C -0.9047168691 2.4267347891 -0.7729447582
C -1.4458613785 1.9505953203 0.4827708649
C -2.1775657445 1.7426251594 1.4795513774
H -1.4543966179 -0.0741240296 -1.8572270528
H -1.036136889 -2.4010344521 -2.4999947403
H 0.924655837 -3.6273979604 -1.5961658779
H 2.4732173946 -2.4746911958 -0.0298361431
H 2.064801276 -0.1322373067 0.6164063824
H 0.8827102435 1.9236782254 0.4162091226
H -1.4125015986 2.1084778039 -1.6812967266
H -0.6043372659 3.4725477733 -0.8085572212
H -2.3049849276 1.2137890937 2.4029844171
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    597.1453
         WellDepth[kcal/mol]         3.6
         WellDepth[kcal/mol]         24.1
       End
      Rotor     Hindered     ! HCCH2CCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
```

```
        Potential[kcal/mol]     8
0.  2.083331839  6.256270612 3.043421512     0.  2.164908086
      6.287646092 3.131272854
     End
       Frequencies[1/cm]     49
  84.5334
 203.3800    216.4178    310.8203
 380.3253    410.9501    413.2070
 524.3381    554.1593    617.4088
 634.0867    683.8793    702.3323
 761.1566    779.7096    828.0218
 842.8273    896.5425    914.5508
 970.6720    993.0733    996.7352
1013.4417   1045.9022   1065.3057
1091.0529   1135.1664   1149.1054
1181.1709   1203.4521   1236.1597
1324.6091   1355.0912   1399.1252
1464.5620   1485.8089   1523.6426
1609.3138   1632.0251   1885.5390
3073.6687   3140.6997   3156.4306
3162.9845   3172.5389   3175.4872
3180.9224   3190.4698   3336.8069
!48.8902
        ZeroEnergy[kcal/mol]          -19.8
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B28  W16   P3    #  ts [16]-trans-phenyl-vinylacetylene
p3
     RRHO
       Geometry[angstrom]     19        #
C 0.0225191469 -0.458514189 -0.0274751468
C -1.3672625074 -0.4461302742 0.1965079922
C -2.0992003388 -1.6250459175 0.1853862471
C -1.4667983834 -2.8479458069 -0.0473882312
C -0.0912319975 -2.8803733774 -0.2645737462
C 0.6435252482 -1.7004483602 -0.2514386693
C 0.8432886324 0.7445445834 -0.033749985
C 0.4108592136 2.0292574683 0.0793063922
C 1.279796418 3.14921644 -0.0164477611
C 1.9932515521 4.1152550788 -0.1132470148
H -1.876593784 0.4900938101 0.3912142703
H -3.1683252539 -1.5941092396 0.3629266687
H -2.0427114914 -3.7662155258 -0.0545052943
H 0.4095751553 -3.8253234247 -0.4423257632
H 1.7148910166 -1.7309889884 -0.4198655294
H 1.9137491958 0.5848277076 -0.1238689069
H -0.6511644899 2.2526063503 0.0819336119
H 2.6280673281 4.9631279442 -0.1926473606
H 0.0600304189 2.1470874946 2.1558578405
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
```

```
         ImaginaryFrequency[1/cm]    523.9013
         WellDepth[kcal/mol]         39.2
         WellDepth[kcal/mol]         3.6
       End
      Rotor     Hindered     ! HCCH2CCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  2.579064415  5.848389379 1.568773975     0.  2.585339511
     5.810738803 1.556223783
     End
       Frequencies[1/cm]     49
  83.4110
 105.3004    225.8616    235.0835
 283.1682    331.5982    382.0387
 411.0510    437.2005    492.6538
 527.9877    626.3058    631.2262
 635.9377    684.7202    701.3249
 767.2293    844.1835    858.1073
 872.3300    926.9444    976.6448
 978.6898   1003.9089   1013.3978
1027.9609   1050.8504   1106.8602
1183.7466   1203.9655   1232.8016
1295.4415   1313.0541   1349.5026
1361.6406   1479.1373   1525.8150
1602.2292   1622.8947   1641.3656
2200.4534   3149.9511   3159.2575
3162.2959   3168.3538   3177.2185
3185.9076   3193.5618   3476.7398
!59.0161
        ZeroEnergy[kcal/mol]          -4.8
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B29  W16   P2    #  ts [16]-cis-phenyl-vinylacetylene p2
     RRHO
       Geometry[angstrom]     19        #
C -0.5160369283 -0.3758927618 0.0283926333
C 0.8856243876 -0.2372445359 0.0611535915
C 1.7075183983 -1.3563799256 0.0288994529
C 1.1614691274 -2.6384796362 -0.0378654957
C -0.2231776489 -2.7955796062 -0.0676133615
C -1.0482961778 -1.6793599145 -0.0315071943
C -1.4548048236 0.7353878943 0.0609396744
C -1.2519341197 2.0847323824 0.0654115432
C -0.0311758384 2.7900279732 -0.1136206505
C 0.9563655986 3.4591563031 -0.2859928638
H 1.3261497605 0.7478436194 0.1166710504
H 2.7839070397 -1.2286186721 0.0575124731
H 1.8099457554 -3.5068643017 -0.0637303573
H -0.6583873036 -3.7873521846 -0.1160262905
H -2.1256488554 -1.8072565337 -0.0509927038
H -2.4966714826 0.4325781022 0.1164390425
```

```
H -1.4496867031 2.4838050803 2.0969103319
H -2.1383023935 2.7107928055 0.0288977194
H 1.8353823328 4.0368630474 -0.4348652432
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    560.8863
         WellDepth[kcal/mol]         40.6
         WellDepth[kcal/mol]         4.3
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0. 2.196283565 5.490708912 1.725651372 0. 2.334335675 5.446783241
1.618974742
     End
       Frequencies[1/cm]     49
  120.7091
  143.9858               221.4601               263.9448
  277.7980               349.2655               381.2658
  413.4692               461.3818               518.8287
  581.5457               632.2179               636.5178
  679.1085               702.5619               737.4815
  757.2928               798.0744               823.5565
  852.2943               934.3448               964.9012
  978.2968               987.3985              1005.8130
 1014.9412              1051.3991              1111.9678
 1184.0241              1202.5775              1211.9227
 1267.4860              1344.4548              1364.8603
 1442.6542              1477.9250              1525.7703
 1585.2918              1617.8816              1640.2809
 2194.5600              3140.5609              3156.5410
 3160.4518              3167.4776              3177.8508
 3189.9086              3222.1222              3475.0076
!36.1061
        ZeroEnergy[kcal/mol]          -3.4
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B30  W2    W19   #  ts [2]-[19]
     RRHO
       Geometry[angstrom]     19        #
 C 0.300069472 0.513297684 -0.8845886339
 C -0.4936983924 -0.6454439171 -1.2297456509
 C 0.0904938804 -1.8827656956 -1.3859418294
 C 1.4679398476 -2.0662951066 -1.1719661704
 C 2.2540404115 -0.9717910262 -0.7708272521
 C 1.6997321162 0.2781278401 -0.6061592725
 C -0.3520075885 1.8191055556 -0.5243831863
 C -0.0757165089 2.0065289633 -1.7742539022
 C -0.9306910364 2.3759962485 0.6873176804
```

```
 C -1.4682523974 3.5957856176 0.7729031993
 H -1.5575822913 -0.5112432563 -1.3907052872
 H -0.5246423077 -2.7303009049 -1.6703021126
 H 1.9162426524 -3.0438673558 -1.3010107359
 H 3.3125809865 -1.1146039572 -0.5793466563
 H 2.3099782176 1.1172482076 -0.2911198749
 H -0.0549660167 2.5767970105 -2.6875724306
 H -0.9062491747 1.7289527199 1.5592197056
 H -1.5046178174 4.2606873187 -0.0835991613
 H -1.8869205277 3.9630947609 1.7021523082
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    552.9334
         WellDepth[kcal/mol]         24.3
         WellDepth[kcal/mol]         0.4
       End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   7 9
        Symmetry                1
        Potential[kcal/mol]     8
2.102157126 3.143823046     6.206069845 3.049696607     0.  3.049696607
      6.206069845 3.150098142
     End
       Frequencies[1/cm]     49
  92.0752
 107.0933              221.3497              248.8774
 324.6450              412.0884              425.4523
 459.1622              561.3245              596.5257
 617.4287              663.9908              688.3522
 734.1351              745.9915              764.6842
 798.5166              840.3203              881.4608
 955.0237              964.1155              974.5975
1000.7395             1018.5430             1027.1619
1091.4153             1093.3610             1160.6195
1181.8314             1215.0154             1289.1263
1324.4477             1334.7221             1439.8477
1444.3773             1469.5381             1543.4769
1583.7590             1671.5400             1784.3903
3136.9367             3155.1122             3156.5020
3158.7730             3176.6364             3177.6846
3191.8007             3225.2970             3262.7049
!55.8848
        ZeroEnergy[kcal/mol]          -14.0
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B31  W3    W19   #  ts [3]-[19]
     RRHO
       Geometry[angstrom]     19        #
C 0.3957380341 0.8687503473 -1.4258175907
C -0.5360961472 -0.2222963258 -1.7111929324
```

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C -0.1578061219 -1.5328348248 -1.5760029471
C 1.1577726477 -1.8802797171 -1.197387407
C 2.1020308536 -0.8600910983 -0.9702106154
C 1.7597419021 0.4651829892 -1.0894102263
C -0.2147607181 2.1999951093 -0.6559440438
C 0.1166536687 2.2773366716 -1.8979711111
C -0.684708969 2.6084663332 0.6305454788
C -1.8314444546 3.2684262287 0.8462843121
H -1.54595084 0.0365093417 -2.010293354
H -0.8794765936 -2.3188540725 -1.7741590153
H 1.4408336397 -2.9207424361 -1.0968661076
H 3.1198811997 -1.1255612382 -0.7028490237
H 2.4949848546 1.244988728 -0.9216450064
H 0.2772369996 2.9145282188 -2.7564602844
H -0.0756210625 2.2951611856 1.4751067527
H -2.4760559012 3.5707871191 0.0292584153
H -2.1548049158 3.5079425793 1.852171433
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    213.0432
         WellDepth[kcal/mol]         35.6
         WellDepth[kcal/mol]         0.3
       End
       Frequencies[1/cm]     50
  81.8891                85.3105
 127.5444               217.9523               310.8547
 342.5324               409.3304               443.4457
 478.1862               544.7083               611.0225
 652.2376               669.0403               709.9261
 732.0860               755.2823               783.9705
 815.8884               850.9018               927.9587
 963.3462               970.8378               977.9802
1001.5252              1006.0818              1021.3211
1089.4207              1097.2350              1135.1941
1151.1888              1199.6880              1278.7273
1314.4175              1329.9901              1422.2640
1435.4165              1462.5717              1536.1776
1583.7465              1636.7541              1868.7285
3136.1283              3143.6678              3152.6968
3155.5873              3172.6842              3175.1974
3192.6090              3199.1768              3231.1071
        ZeroEnergy[kcal/mol]          -14.1
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B32  W1    W14   #  ts [1]-[14]
     RRHO
       Geometry[angstrom]     19        #
C 0.0484198639 -0.3294056596 -0.0179414019
 C 1.1019214413 -1.0711945961 0.6194745982
 C 2.3122207528 -0.4741066169 0.9000737019
 C 2.5312999491 0.8820224562 0.6129436494
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 C 1.4877761775 1.6435429088 0.0636416755
 C 0.2662117855 1.0747157651 -0.2273993409
 C -0.6444399948 -1.1903471924 -1.5010807504
 C -1.3197425894 -0.9645681993 -0.1944710676
 C -2.4977974911 -0.1250128058 -0.1489972832
 C -3.4780561746 0.5694085167 -0.116590293
 H 0.9362933866 -2.1154750819 0.8635259714
 H 3.097857843 -1.0590762477 1.3663582255
 H 3.4848688918 1.3425635932 0.8402707553
 H 1.6346452297 2.7030693066 -0.1171836499
 H -0.5447764759 1.6781143604 -0.6173028144
 H -0.155856082 -2.1327874639 -1.6996360356
 H -0.8217159935 -0.5065798932 -2.3177374046
 H -1.4383778573 -1.8618008875 0.4122245321
 H -4.3469302246 1.1796663484 -0.0825345648
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    572.4825
         WellDepth[kcal/mol]         28.0
         WellDepth[kcal/mol]         16.2
       End
       Frequencies[1/cm]     50
  98.8853               111.6657
 168.0140               246.3052               302.1355
 399.1125               409.9380               421.2865
 523.0368               599.2171               618.6175
 652.9020               663.1991               669.7288
 683.4590               698.7739               771.2101
 781.6582               800.1509               847.9123
 851.7239               962.7540               976.2952
 990.6631              1025.0965              1041.9950
1080.0480              1109.5326              1160.2383
1171.0435              1183.7311              1212.4293
1317.3497              1345.7142              1376.9000
1446.9462              1466.0049              1480.8047
1554.8522              1593.6294              2222.1616
3090.2469              3154.3135              3159.9028
3162.1032              3171.9957              3185.8717
3193.6750              3280.3752              3476.4513
        ZeroEnergy[kcal/mol]          -16.8
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B33  W14   P6    #  ts [14]-p6 (2-phenyl-vinylacetylene)
     RRHO
       Geometry[angstrom]     19        #
C -0.5299497664 -0.4570234627 0.0045938778
C -0.2854976261 -1.1730425591 1.1830595035
C 0.2582655039 -2.451788758 1.1379588241
C 0.5622092395 -3.042715651 -0.0873311428
C 0.3099288314 -2.3454258024 -1.2658921839
C -0.2361142709 -1.0652429183 -1.2209376094
```

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C -1.1190209711 0.9246255063 0.061126005
C -1.0171209053 1.8106161144 -0.9744389533
C -2.1057219291 1.1633076071 1.0825754496
C -2.9449288771 1.344307315 1.9250610803
H -0.5171352663 -0.7167167874 2.1380989107
H 0.446144778 -2.9876462213 2.0615603886
H 0.9838263386 -4.0408066593 -0.1229147975
H 0.5261714376 -2.8018194228 -2.2253184964
H -0.4576300631 -0.5489626105 -2.1469915443
H 0.2587299754 1.6063240377 1.117851749
H -1.561455422 2.7447865963 -0.9567656929
H -0.3272093898 1.6415993777 -1.7904758727
H -3.6867615421 1.5095808161 2.6673136247
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    952.5978
         WellDepth[kcal/mol]         33.9
         WellDepth[kcal/mol]         8.45
       End
      Rotor     Hindered     ! H2CCHCCH
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.225903452 0.012550192     0.947539481 2.026855976     0.225903452 0.
1.123242166 2.133532606
     End
       Frequencies[1/cm]     49
 113.1977
 173.1142              257.1290              279.5939
 399.6391              409.3529              414.6186
 431.9119              497.0043              511.6169
 614.2250              632.3266              637.3657
 651.3170              666.6051              688.2284
 711.1035              741.0075              788.1252
 853.8173              886.8420              906.9086
 936.9345              981.5960             1003.1965
1018.1065             1049.9433             1103.6215
1123.4168             1183.4847             1207.6392
1280.0912             1330.9984             1355.7118
1403.7881             1477.9093             1525.5883
1559.0053             1623.4663             1642.9635
2208.2070             3159.8123             3163.4746
3172.1730             3182.6722             3189.6068
3194.4166             3256.3242             3476.6074
!40.2436
        ZeroEnergy[kcal/mol]          0.9
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B34  W7    W9    #  ts [7]-[9]
     RRHO
```

```
       Geometry[angstrom]     19        #
C -0.5498932182 0.2135512537 0.
C -1.0784486557 -1.0738276208 0.
C -2.4314474378 -1.3508685338 0.
C -3.2739035911 -0.2275508365 0.
C -2.7622561949 1.0774716163 0.
C -1.3890664085 1.3297841699 0.
C 0.8532569386 -0.1403278474 0.
C 2.0875764415 0.3653066913 0.
C 3.3095431168 -0.4164699101 0.
C 4.5417700466 0.1072693512 0.
H 0.2993059966 -1.4573306121 0.
H -2.8344947594 -2.3561070582 0.
H -4.3493040421 -0.3722626356 0.
H -3.4566524672 1.910365772 0.
H -1.0093068369 2.3450142584 0.
H 2.1945712991 1.4532112513 0.
H 3.1855583926 -1.4963712702 0.
H 4.7031766878 1.1805508899 0.
H 5.4236546922 -0.5213389295 0.
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    2270.5512
         WellDepth[kcal/mol]         30.0
         WellDepth[kcal/mol]         32.4
       End
      Rotor     Hindered     ! vinyl
        Group                  10 17 18 19
        Axis                   8 9
        Symmetry                1
        Potential[kcal/mol]     8
0. 4.04116176 7.850144971 4.229414637 3.281875156 4.229414637 7.850144971
4.04116176
     End
       Frequencies[1/cm]     49
  62.1489               95.0242
 177.5227              293.8730
 332.8633              347.1176              394.0095
 486.0947              518.2292              620.0969
 637.2403              654.5350              707.3383
 763.5584              838.9699              854.7559
 872.1638              924.6421              945.5477
 953.6349              991.1569              991.6238
1008.6311             1022.4026             1030.1849
1115.0283             1166.9751             1182.3523
1201.9986             1263.1728             1281.1761
1316.4472             1331.9873             1451.2568
1456.6734             1478.3866             1582.4069
1621.2088             1668.9422             1705.1344
1844.9666             3066.9265             3133.8353
3144.7323             3158.8241             3172.6886
3186.0051             3192.2211             3222.7787
```

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!137.0698
        ZeroEnergy[kcal/mol]          -11.3
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B35  W18   W20   #  ts [18]-[20]
     RRHO
       Geometry[angstrom]     19        #
C                   0.380120    0.696917   -0.0
C                   1.685995    1.213577    0.0
C                   2.780959    0.351854    0.0
C                   2.598182   -1.030501    0.0
C                   1.302540   -1.566873   -0.0
C                   0.238396   -0.691889   -0.0
C                  -0.811117    1.548718   -0.0
C                  -2.066157    1.047846    0.0
C                  -2.305284   -0.372632    0.0
C                  -3.424380   -1.088323    0.0
H                   1.838367    2.288576    0.0
H                   3.785000    0.761026    0.0
H                   3.457257   -1.692889    0.0
H                   1.153190   -2.641275   -0.0
H                  -0.657445    2.622889   -0.0
H                  -2.922336    1.720675    0.0
H                  -1.109763   -0.928152   -0.0
H                  -3.415483   -2.172934    0.0
H                  -4.404311   -0.610075    0.0
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1664.2371
         WellDepth[kcal/mol]         9.6
         WellDepth[kcal/mol]         24.8
       End
       Frequencies[1/cm]     50
  81.0980              157.6413
 206.3645              224.0501              325.4351
 396.8768              420.1933              425.8116
 496.9030              515.5954              596.9663
 651.1166              718.6258              719.9859
 761.4451              810.4439              827.1550
 871.9000              906.1191              935.1404
 944.2553              976.2342              990.1205
1007.8508             1043.5599             1091.2683
1103.2879             1143.5217             1178.8007
1201.9104             1238.4426             1275.8575
1329.7696             1391.0367             1443.2651
1465.1479             1466.5315             1584.4229
1600.1903             1605.5753             1645.2506
1695.9701             3082.6389             3114.8913
3153.4359             3159.8779             3169.6643
3171.9591             3183.8705             3185.0317
        ZeroEnergy[kcal/mol]          -28.6
```

```
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B36  W20  P2    #  ts [20]-P2
     RRHO
       Geometry[angstrom]     19        #
C 0.8015086613 -0.656778364 0.0506919024
C 2.0326063906 -1.3261527205 -0.0807562555
C 3.2277159294 -0.6264751651 -0.1926933069
C 3.2217246046 0.7666370113 -0.1773900938
C 2.0110748861 1.4477031498 -0.0499339987
C 0.8146572912 0.7504997522 0.0629717606
C -0.4046253257 -1.474345474 0.1634087403
C -1.70450847 -1.1357398533 0.3236651793
C -2.2788051686 0.1504127359 0.4367359363
C -2.8558127962 1.2108860099 0.5129926552
H 2.0432849999 -2.4111934726 -0.0937167969
H 4.1623259237 -1.1668387752 -0.2923518209
H 4.151211416 1.3177443256 -0.265010529
H 1.9994762948 2.5319256493 -0.0395313807
H -0.1134056849 1.2957097779 0.1586990792
H -0.2136345605 -2.5427652965 0.1091225366
H -2.4212618108 -1.9508346419 0.3800954205
H -3.3342789701 2.1449988714 0.676650677
H -3.3576196109 1.7010774797 -1.7731937049
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! CHCHCCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  1.529549606  4.528941279 1.551622255
     End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    203.9629
         WellDepth[kcal/mol]         47.1
         WellDepth[kcal/mol]         1.4
       End
       Frequencies[1/cm]     49
  51.0165
 123.4476              144.6758              184.0508
 234.3717              317.1704              381.7155
 413.2780              438.6976              518.2988
 583.8385              632.9027              659.7409
 669.7023              704.2187              739.9080
 749.1595              802.1497              806.8434
 853.2709              934.7559              974.2079
 979.6212              993.3719             1006.8055
1016.3205             1052.2769             1111.7542
1184.1038             1206.0415             1212.9783
1272.6603             1345.1707             1365.2873
1445.5570             1481.6453             1527.9009
```

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1610.2794              1638.6899              1651.5823
2162.5744              3133.0312              3152.1874
3159.1562              3166.7586              3177.3407
3189.2985              3221.0225              3474.3093
!28.5256
        ZeroEnergy[kcal/mol]          -6.3
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B37  W20  P5    #  ts [20]-P5
     RRHO
       Geometry[angstrom]     19        #
C 0.9427388379 -0.5307518098 0.1242147582
C 2.0693645985 -1.3476746516 0.3253558968
C 3.3541208353 -0.8432891889 0.1613746918
C 3.5398045165 0.486607403 -0.211485601
C 2.4296221086 1.3087199748 -0.4190993869
C 1.1460606314 0.8092621648 -0.2544146148
C -0.3869739552 -1.0909076635 0.316362329
C -1.5488448565 -0.4447834956 0.1520950342
C -2.6379056642 0.189941168 0.267311687
C -3.769184209 0.8486089044 0.3963743274
H 1.9273735611 -2.3839681976 0.6139494519
H 4.2110327515 -1.4876412467 0.3223006767
H 4.5409997761 0.8811547674 -0.3418681993
H 2.5703377517 2.3430775764 -0.7122713233
H 0.2858155743 1.4476030699 -0.4190416984
H -0.4312177115 -2.1487649867 0.5694813014
H -1.7450554377 -0.7099535299 -1.8850713578
H -3.817405209 1.9229643416 0.2520674109
H -4.6915259 0.3377374001 0.6529696162
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! CHCHCCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0.  3.143823046  7.894070642 3.394826882 0.  3.106172471  7.134784038
     2.986945648
     End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    619.4285
         WellDepth[kcal/mol]         56.1
         WellDepth[kcal/mol]         4.9
       End
       Frequencies[1/cm]     49
  46.0098
 103.9074              198.8695              253.6469
 264.8307              339.2867              377.1169
 414.0783              419.8885              444.4728
 536.9103              596.4036              628.5405
 633.1717              704.1772              771.0579
```

```
 825.2980               847.7753               858.7604
 865.5187               934.3263               943.4898
 982.5127              1004.3636              1014.0283
1025.7362              1047.9574              1106.2867
1182.2818              1197.5124              1230.2759
1301.4437              1349.3550              1360.9717
1438.6521              1485.6836              1521.9096
1609.6509              1628.0015              1641.7005
2149.5483              3119.9052              3122.6061
3159.8318              3166.7089              3176.2754
3185.2359              3192.5310              3199.2077
!57.3773
        ZeroEnergy[kcal/mol]          2.7
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B38  W9   W18   #  ts [9]-[18]
     RRHO
       Geometry[angstrom]     19        #
C                   0.423082   -0.118154    0.0
C                   0.878571    1.202282   -0.0
C                   2.262747    1.386632   -0.0
C                   3.152455    0.303912   -0.0
C                   2.697348   -1.024266    0.0
C                   1.324923   -1.178936    0.0
C                  -0.800273   -0.896524   -0.0
C                  -2.133508   -0.828830   -0.0
C                  -2.898861    0.410490    0.0
C                  -4.236556    0.464435   -0.0
H                   0.207186    2.052950   -0.0
H                   2.665238    2.393539   -0.0
H                   4.219996    0.498306   -0.0
H                   3.390630   -1.856356   -0.0
H                   0.137516   -1.969080   -0.0
H                  -2.702746   -1.755305   -0.0
H                  -2.331665    1.337433    0.0
H                  -4.765457    1.409736    0.0
H                  -4.840264   -0.437466   -0.0
       Core     RigidRotor
         SymmetryFactor    1
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    2272.9631
         WellDepth[kcal/mol]         55.0
         WellDepth[kcal/mol]         46.9
       End
       Frequencies[1/cm]     50
  53.0627                88.3526
 121.9304               155.9981               295.2807
 350.6640               362.6440               407.3843
 500.8941               525.7519               614.4272
 648.0342               704.5775               712.9376
 765.4202               772.5000               863.6287
 873.9838               925.6335               943.7640
```

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 949.5002               991.1964               992.5865
1010.4204              1021.1530              1021.7444
1115.1686              1147.7842              1179.9829
1191.2316              1262.0544              1309.7031
1319.4295              1343.8384              1450.0187
1455.1124              1478.2112              1583.3436
1621.0863              1662.3477              1689.4172
1855.4066              3130.6183              3135.8902
3148.2765              3158.7676              3172.8011
3186.1943              3191.9749              3222.0726
        ZeroEnergy[kcal/mol]          8.7
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B39  W3   W20   #  ts [3]-[20]
     RRHO
       Geometry[angstrom]     19        #
C 0.4352214575 -0.6053249068 -0.0073767488
C 1.6624555036 -1.2989050924 0.0298828839
C 2.8712063311 -0.6160779316 0.0491889215
C 2.8924652683 0.7786996289 0.037711431
C 1.6862689653 1.4814200983 0.0027493296
C 0.4749763409 0.804783363 -0.0184540628
C -0.8077795293 -1.3555738287 -0.0318560697
C -2.0437922364 -0.8084903938 0.1255537638
C -2.9778657231 0.1003524302 -0.07510788
C -3.9256401878 1.028273741 0.08103906
H 1.6546194479 -2.3839734166 0.0411154517
H 3.8017223445 -1.1726781368 0.073526729
H 3.8358696215 1.3120222797 0.0547636494
H 1.6929996286 2.565906754 -0.0107451838
H -0.451836465 1.3655288279 -0.0546486161
H -0.727774967 -2.4362525192 -0.0934477781
H -3.1383259556 -1.0870617873 -0.5709739515
H -3.8249499729 1.7695703677 0.8666019682
H -4.776496872 1.0982495223 -0.5820368973
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! CHCHCCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  3.074796991  7.693267573 3.601905047
     End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1509.8231
         WellDepth[kcal/mol]         53.0
         WellDepth[kcal/mol]         56.7
       End
       Frequencies[1/cm]     49
  65.2785
 166.1855              232.0478               255.3776
```

```
 355.6614              381.3842              413.8747
 483.0445              511.9830              535.9530
 631.0490              634.5622              698.3391
 701.5651              750.2862              784.8101
 805.3493              844.5997              895.2093
 907.7770              913.1562              973.8750
 994.7358             1008.6808             1046.4411
1049.8053             1107.0611             1180.4003
1197.4939             1228.5234             1301.9912
1341.3453             1355.9381             1408.4355
1474.6969             1507.8082             1517.6676
1604.9084             1627.8524             1844.4424
2206.8385             3132.3139             3147.6027
3156.5422             3163.1843             3173.1207
3182.2814             3190.5353             3228.0424
!53.5350
        ZeroEnergy[kcal/mol]          3.3
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B40  W12 W20   #  ts [12]-[20]
     RRHO
       Geometry[angstrom]     19        #
  C                                                  0.368682560862     -
0.655368593825      0.012559495142
  C                                                  1.634785369496     -
1.277146432500     -0.030541253905
  C                                                  2.807988725456     -
0.535695379557     -0.051202121840
  C                                                  2.756036429484
0.857668530346     -0.024559509551
  C                                                  1.515030684678
1.492997530035      0.022233244443
  C                                                  0.338528133930
0.754480747810      0.037772881009
  C                                                 -0.806615064352     -
1.509281276806      0.038491821166
  C                                                 -2.145068031012     -
1.211439834511      0.066078628444
  C                                                 -2.793071426006
0.031352930300      0.133534355952
  C                                                 -3.329186461628
1.192466582703     -0.070775284913
  H                                                  1.685686625178     -
2.361123636958     -0.046842352719
  H                                                  3.765273845279     -
1.044081989549     -0.086553972531
  H                                                  3.669730333366
1.440767495616     -0.040303882610
  H                                                  1.463400852594
2.576181689076      0.044851968311
  H                                                 -0.608176118089
1.274088269752      0.076468764811
```

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  H                                                  -0.582413193494     -
2.571875201236      0.040396983947
  H                                                  -2.826424958129     -
2.056566313973      0.119616560091
  H                                                  -3.673049461633
0.353489678637      0.943637566215
  H                                                  -3.656195845994
1.774731204644     -0.936412891465
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! CHCHCCH2
        Group                  8 9 10 16 17 18 19
        Axis                   1 7
        Symmetry                1
        Potential[kcal/mol]     8
0. 2.014305784   5.070277487 1.298944851 0.  1.857428386  5.076552583
      1.39307129
     End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1828.6142
         WellDepth[kcal/mol]         58.9
         WellDepth[kcal/mol]         44.1
       End
       Frequencies[1/cm]     49
 101.1202
 141.9551               172.0304               238.2874
 281.1057               386.1224               399.7575
 413.9915               503.2365               538.5702
 589.0525               632.6119               701.2938
 726.5536               749.8414               789.1726
 795.6944               846.0140               864.6329
 917.1262               929.9458               944.2469
 975.6910               997.3765              1012.2004
1050.0331              1111.1135              1181.6317
1195.5343              1208.4023              1262.1193
1340.3669              1361.7677              1434.7862
1467.6880              1522.4705              1542.7916
1610.1386              1635.3207              1882.8379
2319.5121              3028.1066              3133.3726
3152.6219              3156.8764              3163.8787
3173.7988              3187.5213              3220.3623
!31.5063
        ZeroEnergy[kcal/mol]          5.9
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B41  W20 W21   #  ts [20]-[21]
     RRHO
       Geometry[angstrom]     19        #
C 0.2760357893 -0.7446514879 0.1254281533
C 1.550880749 -1.3774993228 0.1838863513
C 2.7194954709 -0.641853724 0.1131060636
C 2.673324034 0.7510556544 -0.0195133201
```

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C 1.433526061 1.3965869511 -0.0783568028
C 0.2561871839 0.6723402804 -0.0069206611
C -0.9041036163 -1.5179227689 0.1960086349
H 1.593268685 -2.4568158656 0.286769035
H 3.6774758921 -1.1480812096 0.1608364979
H 3.5911264238 1.3247656589 -0.0749016329
H 1.3931950397 2.4757198318 -0.1799919566
H -0.6994478293 1.1809339903 -0.0472983766
H -0.8023845047 -2.5964682387 0.2838317967
C -2.279023249 -0.9735658417 0.1000109686
C -2.996023181 -0.6038543027 1.1283096817
C -3.7116018773 -0.2392458744 2.1537474679
H -2.7297682106 -0.8973594177 -0.8932520262
H -4.3508247103 -0.9443795792 2.6765443788
H -3.6912271502 0.7812412663 2.5241057464
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! CHCHCCH2
        Group                  13 14 15 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  5.346381707  13.42243013 5.208329597
     End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    124.1074
         WellDepth[kcal/mol]         6.9
         WellDepth[kcal/mol]         8.3
       End
       Frequencies[1/cm]     49
 143.9683
 166.2218               243.1417               314.1109
 372.9293               409.7463               463.7325
 491.9838               556.4702               625.2135
 640.2570               686.4023               700.4408
 771.9387               833.5253               834.0664
 870.3528               876.6709               902.4555
 974.2060               983.7801               991.4250
1007.0760              1016.2602              1037.7122
1103.9103              1143.2348              1174.8631
1183.4915              1229.1751              1317.5505
1333.7209              1348.6795              1405.0858
1469.0230              1480.9123              1499.5517
1578.7464              1600.6983              2048.1510
3054.7524              3115.9085              3137.6221
3157.1881              3163.8883              3173.9028
3185.2962              3187.7649              3191.9978
!67.0840
        ZeroEnergy[kcal/mol]          -46.5
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B42  W21 P3    #  ts [21]-P3
```

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     RRHO
       Geometry[angstrom]     19        #
C                                                  0.395711664508     -
0.665141863679      0.579496158597
C                                                  1.626885328759     -
1.330480038074      0.454744566772
C                                                  2.821324767314     -
0.624252543921      0.359334204109
C                                                  2.812294355683
0.767774799500      0.386801283896
C                                                  1.598035955970
1.445833432050      0.510425384327
C                                                  0.406105469339
0.741307130437      0.605438177308
C                                                 -0.824986808000     -
1.464526456005      0.676034555738
H                                                  1.640060068043     -
2.415166001644      0.433241861324
H                                                  3.758474961291     -
1.160922219689      0.263835800915
H                                                  3.740855217079
1.322105507634      0.312957248553
H                                                  1.583441833433
2.529747287022      0.532780439396
H                                                 -0.523785175594
1.289251270556      0.701321557514
H                                                 -0.680028803976     -
2.540930512665      0.646927550285
C                                                 -2.089507827462     -
1.010169067924      0.795751362484
C                                                 -3.219632427072     -
1.855518931720      0.882526682288
C                                                 -4.204082702437     -
2.549092461160      0.982722923875
H                                                 -2.293203773524
0.056380561738      0.829784670536
H                                                 -5.069303931997     -
3.164861499773      0.992611372630
H                                                 -4.350174172563     -
2.852171393195      3.434090198732
       Core     RigidRotor
         SymmetryFactor    1
       End
      Rotor     Hindered     ! CHCHCCH2
        Group                  13 14 15 16 17 18 19
        Axis                   1 7
        Symmetry                2
        Potential[kcal/mol]     4
0.  1.581324167  5.013801624 1.506023016
     End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    133.0289
         WellDepth[kcal/mol]         47.4
         WellDepth[kcal/mol]         1.2
```

```
       End
       Frequencies[1/cm]     49
  59.7882
  80.3592               106.6141               154.7928
 237.7857               251.1357               378.3230
 408.9829               424.7893               493.0303
 534.5041               632.4628               637.1407
 644.6380               676.8770               702.7781
 767.5589               845.3708               858.9206
 870.6972               927.0064               977.6302
 988.7143              1004.9231              1014.3861
1035.3456              1052.3500              1106.9249
1183.7843              1204.8977              1233.8619
1296.4457              1327.8315              1351.1398
1363.9879              1480.6001              1527.4704
1614.7022              1640.3807              1663.1865
2175.5663              3143.0454              3153.3255
3161.2904              3167.2099              3176.1991
3184.0949              3192.7481              3476.8941
!36.4205
        ZeroEnergy[kcal/mol]          -7.4
        ElectronicLevels[1/cm]        1
           0   2
   End
   Barrier      B43  W1  W16   #  ts [1]-[16]
     RRHO
       Geometry[angstrom]     19        #
C 0.3422039155 -0.1964594664 -0.0207900371
C 1.3232287055 -1.1346083665 -0.4148376197
C 2.6738666547 -0.8318952824 -0.3465955242
C 3.0966797888 0.4148674037 0.1225751855
C 2.1431275128 1.3553654285 0.5108469641
C 0.7867951964 1.0622390007 0.4380778795
C -1.0546790819 -0.5652343366 -0.1000469402
C -2.2000580573 0.2733034011 0.3567786859
C -3.5172418944 0.0567982866 -0.0779898795
C -4.6565323186 -0.1507260413 -0.4300439752
H 1.0060888925 -2.1075124279 -0.7762104494
H 3.4046857038 -1.5696164697 -0.6593468824
H 4.1530337948 0.6500046277 0.1785792286
H 2.4587739301 2.3311371881 0.8638644563
H 0.0686068639 1.8225695263 0.7211074821
H -1.6825907476 -0.7145971508 1.0416246631
H -1.3268261589 -1.4361423658 -0.6842328473
H -1.9755799348 1.1827891584 0.8995006683
H -5.6544777653 -0.3178381135 -0.7521530584
       Core     RigidRotor
         SymmetryFactor    0.5
       End
       Tunneling      Eckart
         ImaginaryFrequency[1/cm]    1807.8345
         WellDepth[kcal/mol]         39.0
         WellDepth[kcal/mol]         38.2
       End
```

```
      Frequencies[1/cm]     50
  72.2803                74.2178
 132.9156               212.7155               245.3039
 366.0180               388.1152               415.2779
 488.8174               495.6305               514.4667
 612.5347               632.9953               690.9585
 697.7560               730.6351               765.6888
 801.4509               831.8871               858.2499
 900.4507               968.9674               991.2337
 998.4781              1011.9865              1046.7834
1103.6330              1151.6403              1179.9802
1192.2273              1208.9642              1252.4699
1314.5627              1336.7155              1357.9638
1447.4330              1484.0759              1526.0011
1597.9333              1626.3391              2110.8896
2145.5332              3156.0630              3162.8275
3172.8854              3177.7063              3182.4650
3190.0801              3192.4390              3475.0371
       ZeroEnergy[kcal/mol]          -5.8
       ElectronicLevels[1/cm]        1
          0   2
  End
End
```