SUPPORTING INFORMATION

Biomimetic 7-endo Radical Cyclizations Catalyzed by Titanocene(III). Straightforward Synthesis of Terpenoids with Seven-Membered Carbocycles

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Model procedure for the synthesis of alkenynes 52-54. Ethynylmagnesium bromide (0.5 M in THF, 2.0 mmol, method A) or sodium acetylide (18 % weight, 4.0 mmol, method B) was added to a solution of ketone (**49-51**)¹ (1.0 mmol) in THF (25 mL) at 0 °C and the mixture was stirred for 30 min. Acetic anhydride (8.0 mmol) was then added and the reaction stirred for another 30 min before being quenched with ice-water, extracted with *t*-BuOMe, dried with anhyd Na₂SO₄ and the solvent removed. Flash chromatography (hexane/EtOAc 9:1) of the residue gave the corresponding alkenynes at the following yields: **52** (method A, 85 %; method B, 67 %), **53** (method A, 53 %), **54** (method A, 80 %; method B, 75 %).

Model procedure for the synthesis of epoxy-derivatives 11-13 and 55-57. Powdered NBS (6.0 mmol) was gradually added to a solution of the corresponding substrate (nerolidol, geranyl linalyl acetate, geranyl linalool, **52-54**) (6.0 mmol) in a mixture of DME:water (200 mL, 3:1) at 0°C. The reaction was stirred for 30 min, diluted with *t*-BuOMe, washed with water, dried with anhyd Na₂SO₄ and the solvent removed. The residue was dissolved in 0.5 M methanolic K₂CO₃ (20 mL) and stirred for 10 min.² The methanolic solution was then diluted with *t*-BuOMe, washed with water, dried with anhyd Na₂SO₄ and the solvent removed, giving a residue which was submitted to flash chromatography (hexane/EtOAc 4:1) to give the corresponding

¹ Farnesylacetone (**51**) was bought from Fluka in the form of a mixture of four stereoisomers containing 31% of the all-*trans* isomer (GC-MS analysis with an authentic sample as standard). This mixture was used as received because it was easier to isolate cyclic product **64** and **65** than the stereoisomers of the starting material.

² Substantial amounts of products deriving from acetate hydrolysis were obtained using longer reaction times.

epoxides at the following yields: **11** (51 %), **12** (56 %), **13** (50 %), **55** (87 %), **56** (51 %), **57** (35 %).

Epoxyalkene 12. Colorless oil; ^1H NMR (300 MHz, CDCl_3) (mixture of stereoisomers $3S^*,14S^*$ and $3R^*,14S^*$ in a ratio of roughly 1:1) δ 5.95 (dd, $J = 17.4$, 10.9 Hz, 1H), 5.15-5.10 (m, 2H), 5.14 (d, $J = 17.4$ Hz, 1H), 5.10 (d, $J = 10.9$ Hz, 1H), 2.68 (t, $J = 6.3$ Hz, 1H), 2.20-1.50 (m, 12H), 1.99 (s, 3H), 1.70 (s, 3H), 1.67 (s, 3H), 1.52 (s, 3H), 1.29 (s, 3H), 1.23 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 169.85 (C), 141.85 (CH), 135.24 (C), 134.07 (C), 124.81 (CH), 123.80 (CH), 113.08 (CH_2), 82.87 (C), 64.13 (CH), 58.81 (C), 39.74 (CH_2), 39.59 (CH_2), 36.31 (CH_2), 27.49 (CH_2), 26.56 (CH_2), 24.90 (CH_3), 23.62 (CH_3), 22.27 (CH_2), 22.15 (CH_3), 18.76 (CH_3), 16.00 (CH_3), 15.90 (CH_3); FABHRMS calcd for $\text{C}_{22}\text{H}_{36}\text{O}_3\text{Na}$ m/z 371.2562, found m/z 371.2561.

Epoxyalkene 13. Colorless oil; ^1H NMR (300 MHz, CDCl_3) (mixture of stereoisomers $3S^*,14S^*$ and $3R^*,14S^*$ in a ratio of roughly 1:1) δ 5.85 (dd, $J = 17.3$, 10.7 Hz, 1H), 5.15 (d, $J = 17.3$ Hz, 1H), 5.10-4.02 (m, 2H), 4.97 (d, $J = 10.7$ Hz, 1H), 2.64 (t, $J = 6.2$ Hz, 1H), 2.15-1.90 (m, 12H), 1.55 (s, 3H), 1.54 (s, 3H), 1.23 (s, 3H), 1.19 (s, 3H), 1.13 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 145.12 (CH), 135.20 (C), 134.05 (C), 124.77 (CH), 124.42 (CH), 111.58 (CH_2), 73.27 (C), 64.13 (CH), 58.30 (C), 42.13 (CH_2), 39.59 (CH_2), 36.28 (CH_2), 27.80 (CH_3), 27.44 (CH_2), 26.94 (CH_3), 26.50 (CH_2), 24.87 (CH_3), 22.68 (CH_2), 18.72 (CH_3), 15.97 (CH_3).

Cyclohexanol 14. Vitreous solid (8:1, *E:Z* mixture); ^1H NMR (300 MHz, CDCl_3) δ (*E* stereoisomer) 5.10 (q, $J = 6.7$ Hz, 1H), 3.43 (dd, $J = 9.5$, 3.9 Hz, 1H), 2.45 (dt, $J = 13.6$, 4.9 Hz, 1H), 1.90-1.70 (m, 4H), 1.56 (d, $J = 6.8$ Hz, 3H), 1.50-1.40 (m, 1H), 0.93 (s, 3H), 0.78 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 135.84 (C), 117.74 (CH), 76.94 (CH), 47.83 (CH_2), 36.82 (C), 30.53 (CH_2), 27.53 (CH_3), 24.83 (CH_2), 19.79 (CH_3), 12.79 (CH_3). ^1H NMR (300 MHz, CDCl_3) δ (*Z* stereoisomer, only distinctive signals) 5.30 (q, $J = 6.6$ Hz, 1H), 0.99 (s, 3H), 0.80 (s, 3H); we were unable to obtain a good quality HRMS.

Cyclohexanol 15. Colorless oil; ^1H NMR (300 MHz, CDCl_3) δ (5.5:4:1 mixture of three stereoisomers) 3.54 (dd, $J = 11.3$, 3.4 Hz, 1H, one stereoisomer), 3.41 (m, 1H, one

stereoisomer), 3.22 (dd, $J = 11.5, 3.9$ Hz, 1H, one stereoisomer), 1.90-1.10 (m, 6H), 0.98 (s, 3H, one stereoisomer), 0.96 (s, 3H, one stereoisomer), 0.93 (s, 3H, one stereoisomer), 0.85-0.80 (m, 6H), 0.77 (s, 3H, one stereoisomer), 0.74 (s, 3H, one stereoisomer), 0.70 (s, 3H, one stereoisomer); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 78.29 (CH), 77.12 (CH), 73.25 (CH), 46.84 (CH), 45.46 (CH), 40.96 (CH), 40.06 (C), 39.10 (C), 38.70 (C), 33.88 (CH_2), 33.68 (CH_2), 33.67 (CH), 33.41 (CH), 30.78 (CH_2), 29.41 (CH_2), 28.77 (CH_2), 28.59 (CH_2), 26.63 (CH_3), 26.58 (CH_3), 25.91 (CH_3), 20.77 (CH_3), 20.13 (CH_3), 19.92 (CH_3), 12.64 (CH_3); EIHRMS calcd for $\text{C}_{10}\text{H}_{20}\text{O} - \text{H}_2\text{O}$ m/z 138.1408, found m/z 138.1406.

Tricyclic alcohol 20. White solid; mp 119-121 °C; ^1H NMR (300 MHz, CDCl_3) δ 5.36 (bt, $J = 5.2$ Hz, 1H), 3.22 (dd, $J = 11.5, 4.8$ Hz, 1H), 2.07 (bt, $J = 11.7$, 1H), 2.00 (dd, $J = 12.3, 7.1$ Hz, 1H), 1.91-1.80 (m, 1H), 1.83 (dt, $J = 13.1, 3.6$ Hz, 1H), 1.74 (s, 3H), 1.70-1.40 (m, 10H), 1.30-1.10 (m, 2H), 0.99 (s, 3H), 0.83 (s, 3H), 0.79 (s, 3H), 0.78 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 141.35 (C), 122.71 (CH), 78.91 (CH), 64.57 (CH), 55.63 (CH), 46.44 (CH_2), 44.54 (CH_2), 39.08 (C), 38.51 (C), 38.34 (CH_2), 35.93 (C), 34.68 (CH_2), 28.15 (CH_3), 27.52 (CH_2), 25.43 (CH_3), 20.58 (CH_2), 20.46 (CH_3), 18.82 (CH_2), 16.11 (CH_3), 15.46 (CH_3); EIMS m/z 290 $[\text{M}]^+$ (10), 243 (5), 207 (100), 191 (25), 135 (40), 67 (35); FABHRMS calcd for $\text{C}_{20}\text{H}_{34}\text{ONa}$ m/z 313.2507, found m/z 313.2515.

Alkenyne 54. Colorless oil; ^1H NMR (300 MHz, CDCl_3) (mixture of *E/Z* stereoisomers) δ 5.30-5.10 (m, 3H), 2.57 (s, 1H, one stereoisomer), 2.55 (s, 1H, one stereoisomer), 2.20-1.90 (m, 12H), 2.00 (s, 3H, one stereoisomer), 1.99 (s, 3H, one stereoisomer), 1.98 (s, 3H, one stereoisomer), 1.70 (s, 9H), 1.62 (s, 3H, one stereoisomer), 1.60 (s, 3H, one stereoisomer).

Epoxyalkenyne 56. Colorless oil; ^1H NMR (300 MHz, CDCl_3) (mixture of stereoisomers 3*S**,10*S** and 3*R**,10*S** in a ratio of roughly 1:1) δ 5.15 (t, $J = 6.8$ Hz, 1H), 2.66 (t, $J = 6.2$ Hz, 1H), 2.53 (s, 1H), 2.25-1.70 (m, 8H), 1.99 (s, 3H), 1.65 (s, 3H),

1.61 (s, 3H), 1.27 (s, 3H), 1.22 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 169.75 (C), 135.05 (C), 123.63 (CH), 83.73 (C), 74.67 (C), 73.34 (CH), 64.09 (CH), 58.26 (C), 41.24 (CH_2), 36.26 (CH_2), 27.39 (CH_2), 26.38 (CH_3), 24.87 (CH_3), 22.79 (CH_2), 21.86 (CH_3), 18.74 (CH_3), 15.93 (CH_3).

Epoxyalkenyne 57. Colorless oil; ^1H NMR (300 MHz, CDCl_3) (stereoisomers mixture) δ 5.20-5.00 (m, 2H), 2.61 (t, $J = 6.2$ Hz, 1H), 2.49 (s, 1H), 2.20-1.70 (m, 12H), 1.94 (s, 3H), 1.60 (s, 6H), 1.54 (s, 3H), 1.22 (s, 3H), 1.17 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 169.77 (C), 135.71 (C), 135.59 (C), 135.54 (C), 134.20 (C), 133.96 (C), 125.48 (CH), 124.63 (CH), 124.56 (CH), 123.99 (CH), 123.86 (CH), 123.09 (CH), 123.02 (CH), 83.63 (C), 74.57 (C), 73.26 (CH), 63.97 (CH), 58.11 (C), 41.51 (CH_2), 41.19 (CH_2), 39.71 (CH_2), 39.44 (CH_2), 36.21 (CH_2), 31.68 (CH_2), 28.42 (CH_2), 27.34 (CH_2), 26.30 (CH_3), 24.78 (CH_3), 23.25 (CH_3), 22.66 (CH_2), 21.73 (CH_3), 18.64 (CH_3), 15.85 (CH_3).

Cycloheptenol 58. Colorless oil; (2:1 mixture of stereoisomers) (Only the major diastereoisomer was isolated as a pure sample); Major isomer: ^1H NMR (300 MHz, CDCl_3) δ 5.76 (d, $J = 12.6$ Hz, 1H), 5.29 (d, $J = 12.6$ Hz, 1H), 3.60 (dd, $J = 7.6, 2.0$ Hz, 1H), 2.30-2.20 (m, 1H), 2.00-1.60 (m, 3H), 1.97 (s, 3H), 1.53 (s, 3H), 1.09 (s, 6H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 169.89 (C), 138.33 (CH), 133.41 (CH), 81.31 (C), 76.23 (CH), 41.57 (C), 33.44 (CH_2), 28.22 (CH_3), 28.03 (CH_3), 27.90 (CH_2), 26.08 (CH_3), 22.24 (CH_3); Minor isomer: ^1H NMR (300 MHz, CDCl_3) δ 5.60 (d, $J = 12.2$ Hz, 1H), 5.25 (d, $J = 12.2$ Hz, 1H), 3.45 (dd, $J = 7.6, 2.1$ Hz, 1H), 2.30-1.50 (m, 4H), 1.96 (s, 3H), 1.49 (s, 3H), 1.08 (s, 3H), 1.06 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 170.00 (C), 137.20 (CH), 133.06 (CH), 81.31 (C), 76.58 (CH), 41.51 (C), 34.57 (CH_2), 28.73 (CH_3), 28.03 (CH_3), 27.96 (CH_2), 24.11 (CH_3), 22.24 (CH_3); FABHRMS calcd for $\text{C}_{12}\text{H}_{20}\text{O}_3\text{Na}$ m/z 235.1310, found m/z 235.1313.

Methylcyclohexanol 59. Colorless oil; (2:1 mixture of stereoisomers) (Only the major diastereoisomer was isolated as a pure sample); Major isomer: ^1H NMR (300 MHz, CDCl_3) δ 5.24 (s, 1H), 5.19 (s, 1H), 3.28 (dd, $J = 9.8, 3.9$ Hz, 1H) 2.25 (ddd, $J =$

14.3, 5.8, 4.4 Hz, 1H), 1.94 (s, 3H), 1.90-1.65 (m, 2H), 1.60 (s, 3H), 1.39 (ddd, $J = 14.3$, 10.8, 4.5 Hz, 1H), 1.16 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 170.06 (C), 152.67 (C), 112.92 (CH_2), 80.99 (C), 76.89 (CH), 42.08 (C), 35.82 (CH_2), 27.62 (CH_3), 26.93 (CH_3), 26.20 (CH_2), 22.63 (CH_3), 21.67 (CH_3); EIHRMS calcd for $\text{C}_{12}\text{H}_{20}\text{O}_3$ - AcOH m/z 152.1201, found m/z 152.1202. Minor isomer; ^1H NMR (300 MHz, CDCl_3) δ 5.41 (s, 1H), 5.21 (s, 1H), 3.55 (m, 1H), 2.20 (m, 1H), 2.00-1.50 (m, 3H), 1.94 (s, 3H), 1.68 (s, 3H), 1.16 (s, 3H), 1.15 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 170.03 (C), 149.78 (C), 114.92 (CH_2), 81.85 (C), 76.27 (CH), 41.60 (C), 34.25 (CH_2), 27.06 (CH_3), 26.84 (CH_3), 25.23 (CH_2), 25.19 (CH_3), 21.79 (CH_3).

Bicyclic acetate 60. Colorless oil; ^1H NMR (300 MHz, CDCl_3) δ 5.49 (d, $J = 12.6$ Hz, 1H), 5.14 (d, $J = 12.6$ Hz, 1H), 3.20 (dd, $J = 7.0$, 6.8 Hz, 1H), 2.25-2.10 (m, 1H), 1.95-1.50 (m, 8H), 1.95 (s, 3H), 1.46 (s, 3H), 1.01 (s, 3H), 1.00 (s, 3H), 0.81 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 170.26 (C), 143.17 (CH), 130.30 (CH), 82.24 (C), 78.39 (CH), 50.74 (CH), 40.16 (CH_2), 40.04 (C), 39.67 (C), 37.97 (CH_2), 28.15 (CH_3), 27.41 (CH_2), 22.33 (CH_3), 21.29 (CH_2), 19.83 (CH_3), 15.36 (CH_3), 14.97 (CH_3); EIHRMS calcd for $\text{C}_{17}\text{H}_{28}\text{O}_3$ - AcOH m/z 220.1827, found m/z 220.1821.

Conjugated diene 61. Colorless oil; ^1H NMR (300 MHz, CDCl_3) δ 5.71 (br d, $J = 8.1$ Hz, 1H), 5.43 (d, $J = 12.3$ Hz, 1H), 5.25 (d, $J = 12.3$ Hz, 1H), 3.22 (dd, $J = 7.9$, 5.6 Hz, 1H), 2.19 (dd, $J = 17.0$, 8.5 Hz, 1H), 2.10-1.95 (m, 1H), 1.70-1.20 (m, 5H), 1.75 (s, 3H), 1.02 (s, 3H), 1.01 (s, 3H), 0.79 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 144.02 (CH), 130.82 (C), 129.04 (CH), 124.09 (CH), 78.86 (CH), 50.71 (CH), 41.70 (C), 39.92 (C), 38.17 (CH_2), 28.10 (CH_3), 27.40 (CH_2), 26.71 (CH_2), 25.10 (CH_3), 23.33 (CH_3), 15.28 (CH_3); EIMS m/z 220 (8), 202 (5), 187 (10), 105 (100); EIHRMS calcd for $\text{C}_{15}\text{H}_{24}\text{O}$ - H m/z 219.1748, found m/z 219.1756.

Drimane 62. Colorless oil; ^1H NMR (300 MHz, CDCl_3) δ 5.25 (s, 1H), 5.06 (s, 1H), 3.20 (dd, $J = 10.5, 6.6$ Hz, 1H), 2.24 (dt, $J = 13.9, 3.1$ Hz, 1H), 1.94 (s, 3H), 1.80-1.40 (m, 7H), 1.63 (s, 3H), 1.30 (td, $J = 12.9, 4.5$ Hz, 1H), 1.05 (s, 3H), 0.96 (s, 3H), 0.82 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 170.30 (C), 155.33 (C), 110.42 (CH_2), 81.66 (C), 78.63 (CH), 53.53 (CH), 41.89 (CH_2), 40.05 (C), 39.35 (C), 36.68 (CH_2), 28.15 (CH_3), 27.63 (CH_2), 25.04 (CH_3), 22.81 (CH_3), 20.20 (CH_3), 17.93 (CH_2), 15.43 (CH_3); FABHRMS calcd for $\text{C}_{17}\text{H}_{28}\text{O}_3\text{Na}$ m/z 303.1936, found m/z 303.1930.

Drimane 63. Colorless oil; ^1H NMR (300 MHz, CDCl_3) δ 5.67 (m, 1H), 4.81 (m, 2H), 3.24 (dd, $J = 10.6, 4.6$ Hz, 1H), 2.10-1.00 (m, 7H), 1.79 (s, 3H), 0.97 (s, 3H), 0.96 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 159.01 (C), 134.28 (C), 126.45 (CH), 104.29 (CH_2), 78.87 (CH), 48.03 (CH), 39.99 (C), 37.70 (C), 35.80 (CH_2), 29.71 (CH_2), 27.70 (CH_3), 23.86 (CH_2), 21.24 (CH_3), 20.41 (CH_3), 15.40 (CH_3); ESIHRMS calcd for $\text{C}_{15}\text{H}_{24}\text{OH} - \text{H}_2\text{O}$ m/z 203.1794, found 203.1787.

Tricyclic alcohol 64. Colorless oil; ^1H NMR (300 MHz, CDCl_3) δ 5.69 (br d, $J = 4.5$ Hz, 1H), 5.43 (d, $J = 12.2$ Hz, 1H), 5.23 (d, $J = 12.2$ Hz, 1H), 3.17 (dd, $J = 10.9, 5.4$ Hz, 1H), 2.10 (dd, $J = 16.3, 8.5$ Hz, 1H), 1.95-1.85 (m, 1H), 1.90 (dt, $J = 13.1, 2.2$ Hz, 1H), 1.74 (s, 3H), 1.70-0.80 (m, 9H), 1.01 (s, 3H), 0.95 (s, 3H), 0.81 (s, 3H), 0.76 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 144.89 (CH), 131.23 (C), 129.45 (CH), 123.68 (CH), 78.97 (CH), 57.03 (CH), 55.12 (CH), 42.85 (C), 41.51 (CH_2), 38.96 (C), 38.41 (C), 38.02 (CH_2), 28.19 (CH_3), 27.36 (CH_2), 25.87 (CH_2), 24.96 (CH_3), 24.86 (CH_3), 18.50 (CH_2), 16.39 (CH_3), 15.42 (CH_3); EIHRMS calcd for $\text{C}_{20}\text{H}_{32}\text{O}$ m/z 288.2453, found m/z 288.2454.

Tricyclic alcohol 65. Colorless oil; ^1H NMR (300 MHz, CDCl_3) δ 5.62 (m, 1H), 4.80 (br s, 1H), 4.78 (br s, 1H), 3.17 (dd, $J = 10.4, 5.7$ Hz, 1H), 2.10-1.50 (m, 12H), 1.77 (s, 3H), 0.98 (s, 3H), 0.94 (s, 3H), 0.92 (s, 3H), 0.78 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ;

DEPT) δ 158.33 (C), 131.11 (C), 126.37 (CH), 104.12 (CH₂), 78.96 (CH), 55.25 (CH), 53.36 (CH), 41.43 (C), 39.46 (CH₂), 38.85 (C), 38.17 (CH₂), 37.38 (C), 28.17 (CH₃), 27.30 (CH₂), 23.21 (CH₂), 22.42 (CH₃), 20.58 (CH₃), 18.77 (CH₂), 16.18 (CH₃), 15.68 (CH₃); EIHRMS calcd for C₂₀H₃₂O m/z 288.2453, found m/z 288.2458.

Ketone 76. Vitreous solid; ¹H NMR (300 MHz, CDCl₃) δ 5.30 (bt, J = 5.2 Hz, 1H), 2.40 (m, 2H), 2.15-1.75 (m, 4H), 1.67 (s, 3H), 1.65-1.30 (m, 7H), 1.45 (s, 3H), 1.25-1.10 (m, 3H), 1.02 (s, 3H), 0.96 (s, 3H), 0.79 (s, 3H); ¹³C NMR (75 MHz, CDCl₃; DEPT) δ 218.24 (C), 141.30 (C), 122.65 (CH), 63.85 (CH), 55.04 (CH), 47.36 (C), 46.35 (CH₂), 43.64 (CH₂), 39.39 (CH₂), 38.19 (C), 35.99 (C), 34.78 (CH₂), 34.10 (CH₂), 27.13 (CH₃), 25.45 (CH₃), 21.38 (CH₂), 20.96 (CH₃), 20.13 (CH₂), 19.93 (CH₃), 16.30 (CH₃); FABHRMS calcd for C₂₀H₃₂ONa m/z 311.2350, found m/z 311.2357.

Tosylhydrazone 77. White solid: mp 89-91 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.82 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 5.30 (bt, J = 4.4 Hz, 1H), 2.40-1.10 (m, 16H), 2.39 (s, 3H), 1.69 (s, 3H), 1.02 (s, 3H), 0.89 (s, 3H), 0.77 (s, 3H), 0.61 (s, 3H); ¹³C NMR (75 MHz, CDCl₃; DEPT) δ 177.32 (C), 143.77 (C), 141.25 (C), 135.55 (C), 129.33 (CH), 128.39 (CH), 122.63 (CH), 63.81 (CH), 54.85 (CH), 46.39 (CH₂), 43.73 (CH₂), 41.89 (C), 38.17 (CH₂), 35.98 (C), 34.76 (CH₂), 28.56 (CH₃), 25.47 (CH₃), 23.03 (CH₃), 21.67 (CH₃), 21.35 (CH₂), 20.16 (CH₃), 20.01 (CH₂), 19.82 (CH₂), 15.87 (CH₃), (One carbon signal was not observed); EIMS m/z 456 [M]⁺ (1), 353 (1), 288 (25), 273 (10), 205 (100), 163 (20), 121 (18), 107 (20); FABHRMS calcd for C₂₇H₄₀N₂O₂SNa m/z 479.2714, found m/z 479.2713.

Tricyclic alkene 78. White solid: mp 99-101 °C; ¹H NMR (300 MHz, CDCl₃) δ 5.30 (bt, J = 5.3 Hz, 1H), 2.10-1.00 (m, 18H), 1.71 (s, 3H), 0.84 (s, 3H), 0.80 (s, 3H), 0.78 (s, 3H), 0.76 (s, 3H); ¹³C NMR (75 MHz, CDCl₃; DEPT) δ 141.37 (C), 122.78 (CH), 64.83 (CH), 56.76 (CH), 46.74 (CH₂), 44.58 (CH₂), 42.11 (CH₂), 40.00 (CH₂), 39.52 (C),

36.20 (C), 34.85 (CH₂), 33.62 (CH₃), 25.45 (CH₃), 21.70 (CH₃), 20.58 (CH₃), 20.46 (CH₂), 19.22 (CH₂), 18.92 (CH₂), 16.12 (CH₃), (One carbon signal was not observed); EIMS m/z 274 [M]⁺ (3), 252 (3), 205 (8), 191 (90), 123 (50), 95 (89), 81 (100); EIHRMS calcd for C₂₀H₃₄ m/z 274.2661, found m/z 274.2666.

Tricyclic diene 79. White solid: mp 95-96 °C; ¹H NMR (300 MHz, CDCl₃) δ 5.50-5.30 (m, 3H), 2.20-1.95 (m, 4H), 1.87 (bd, J = 14.5 Hz, 1H), 1.70-1.00 (m, 9H), 1.72 (s, 3H), 0.94 (s, 3H), 0.87 (s, 3H), 0.83 (s, 3H), 0.79 (s, 3H); ¹³C NMR (75 MHz, CDCl₃; DEPT) δ 141.42 (C), 138.07 (CH), 122.85 (CH), 121.56 (CH), 63.43 (CH), 52.18 (CH), 46.59 (CH₂), 43.75 (CH₂), 41.06 (CH₂), 37.81 (C), 36.22 (C), 35.18 (C), 34.94 (CH₂), 31.98 (CH₃), 25.49 (CH₃), 22.85 (CH₃), 21.09 (CH₂), 20.00 (CH₂), 19.87 (CH₃), 16.39 (CH₃); EIMS m/z 272 [M]⁺ (10), 257 (20), 203 (14), 189 (100), 121 (95), 107 (90), 67 (60); EIHRMS calcd for C₂₀H₃₂ m/z 272.2504, found m/z 272.2502.

Epoxide 80. White solid: mp 111-115 °C; ¹H NMR (300 MHz, CDCl₃) δ 5.36 (m, 2H), 2.71 (t, J = 7.2 Hz, 1H), 2.07-2.00 (m, 2H), 1.84 (dd, J = 14.1, 6.6 Hz, 1H), 1.70-1.10 (m, 11H), 1.32 (s, 3H), 1.02 (s, 3H), 0.93 (s, 3H), 0.86 (s, 3H), 0.84 (s, 3H); NOE-dif. experiment: proton irradiated δ 2.71 (H-14), NOEs observed δ 1.32 (H₃-16), 1.02 (H₃-17); ¹³C NMR (75 MHz, CDCl₃; DEPT) δ 138.11 (CH), 121.41 (CH), 63.39 (CH), 60.90 (CH), 60.90 (C), 52.37 (CH), 47.46 (CH₂), 42.42 (CH₂), 41.46 (CH₂), 37.97 (C), 37.88 (C), 36.37 (CH₂), 35.20 (C), 32.03 (CH₃), 22.91 (CH₃), 22.79 (CH₃), 20.86 (CH₂), 19.47 (CH₂), 19.26 (CH₃), 16.44 (CH₃); EIMS m/z 288 [M]⁺ (20), 255 (17), 215 (12), 187 (30), 145 (40), 119 (100), 107 (90); FABHRMS calcd for C₂₀H₃₂ONa m/z 311.2350, found m/z 311.2358.

NMR data for synthetic laukarlaol (81). ¹H NMR (300 MHz, CDCl₃) δ 5.37 (m, 2H), 5.02 (br s, 1H), 4.89 (br s, 1H), 4.27 (dd, J = 10.7, 4.5 Hz, 1H), 2.44 (m, 1H), 2.19 (td, J = 11.7, 2.9 Hz, 1H), 2.04 (dd, J = 16.3, 5.0 Hz, 1H), 1.85-1.74 (m, 1H), 1.69 (dd, J

= 13.6, 4.5 Hz, 1H), 1.60-1.00 (m, 9H), 0.95 (s, 3H), 0.93 (s, 3H), 0.86 (s, 3H), 0.81 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 155.04 (C), 138.03 (CH), 121.23 (CH), 111.13 (CH_2), 71.05 (CH), 59.47 (CH), 54.70 (CH_2), 52.30 (CH), 44.37 (CH_2), 40.87 (CH_2), 37.57 (C), 36.00 (C), 34.96 (C), 33.21 (CH_2), 31.90 (CH_3), 25.02 (CH_2), 22.69 (CH_3), 19.46 (CH_3), 19.29 (CH_2), 16.07 (CH_3);

Table: ^{13}C NMR data for natural laukarlaol⁴³ and synthetic 81

C	laukarlaol	81
1	40.8	40.9
2	121.2	121.2
3	138.0	138.0
4	34.9	35.0
5	52.3	52.3
6	19.4	19.5
7	25.0	25.0
8	36.0	36.0
9	59.4	59.5
10	37.5	37.6
11	44.3	44.4
12	33.2	33.2
13	155.0	155.0
14	71.0	71.1
15	54.7	54.7
16	111.0	111.1
17	19.4	19.3
18	16.1	16.1
19	22.7	22.7
20	31.8	31.9

5-hydroxy-1,4,4-trimethylcycloheptyl acetate. Colorless oil (4:1 mixture of stereoisomers); (major stereoisomer) ^1H NMR (300 MHz, CDCl_3) δ 3.35 (dd, $J = 9.1$, 2.0 Hz, 1H), 2.20-1.40 (m, 8H), 1.96 (s, 3H), 1.47 (s, 3H), 0.97 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3 ; DEPT) δ 171.06 (C), 85.68 (C), 79.79 (CH), 36.36 (C), 34.32 (CH_2), 33.76 (CH_2), 33.12 (CH_2), 28.84 (CH_3), 27.94 (CH_2), 26.61 (CH_3), 22.67 (CH_3), 21.77 (CH_3); (minor stereoisomer) ^1H NMR (300 MHz, CDCl_3) δ (only distinctive signals) 3.30 (br d, $J = 9.0$ Hz, 1H), 1.98 (s, 3H), 0.89 (s, 3H). EIHRMS calcd for $\text{C}_{12}\text{H}_{22}\text{O}_3\text{-AcOH}$ m/z 154.1357, found m/z 154.1355.

Reference 55 (full author list): Frisch, M. J.; Trucks, G. W. ;Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam,, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision B.03, Gaussian, Inc., Pittsburgh PA, **2003**.

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Computational methods

UB3LYP/6-31G(d) E+ZPE (kcal mol⁻¹)

Reaction profile including different conformers for the reagents

Connections determined by IRC studies

UB3LYP/6-31G(d) E+ZPE (kcal mol⁻¹)

Reaction profile including different conformers for the reagents

Connections determined by IRC studies

Atomic coordinates and energy values for the stationary points

DFT UB3LYP/6-31G(d)

All stationary points are doublets in the ground state

I

Zero-point correction= 0.311948 (Hartree/Particle)
 Thermal correction to Energy= 0.331110
 Thermal correction to Enthalpy= 0.332054
 Thermal correction to Gibbs Free Energy= 0.262379
 Sum of electronic and zero-point Energies= -695.202465
 Sum of electronic and thermal Energies= -695.183304
 Sum of electronic and thermal Enthalpies= -695.182360
 Sum of electronic and thermal Free Energies= -695.252035

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.375431	-0.761558	-0.606908
2	6	0	2.736236	-0.074049	-0.835713
3	6	0	3.201764	0.796582	0.301257
4	6	0	-1.194813	-0.986102	1.157044
5	6	0	-1.178070	-0.406282	-0.240599
6	6	0	0.206800	0.225038	-0.532445
7	6	0	-1.227930	-2.275874	1.488623
8	8	0	-2.043942	0.790353	-0.264644
9	6	0	-3.365755	0.699700	0.012698
10	6	0	-1.613048	-1.374262	-1.342391
11	8	0	-3.957925	-0.322604	0.278026
12	8	0	3.651437	-1.158800	-1.074287
13	6	0	3.128905	2.288847	0.211917
14	6	0	3.518733	0.163211	1.621875
15	6	0	-4.003147	2.072648	-0.059798
16	1	0	1.432967	-1.357948	0.310470
17	1	0	1.236828	-1.467087	-1.434707
18	1	0	2.658163	0.547604	-1.744710
19	1	0	-1.116104	-0.232746	1.941852
20	1	0	0.120251	0.779864	-1.475947
21	1	0	0.396085	0.972420	0.248387
22	1	0	-1.309979	-3.068247	0.750463
23	1	0	-1.188047	-2.587619	2.528566
24	1	0	-1.618915	-0.854201	-2.306310
25	1	0	-0.915807	-2.213628	-1.418014
26	1	0	-2.611756	-1.763397	-1.140715
27	1	0	4.540114	-0.771256	-1.124575
28	1	0	2.266669	2.700662	0.766753

29	1	0	3.036687	2.635548	-0.824068
30	1	0	4.018995	2.763817	0.651329
31	1	0	2.679974	0.249170	2.335593
32	1	0	4.378379	0.648516	2.105433
33	1	0	3.745082	-0.901244	1.504950
34	1	0	-3.519358	2.752943	0.648916
35	1	0	-5.066006	1.990187	0.170689
36	1	0	-3.871413	2.497643	-1.060479

I'

Zero-point correction=	0.311739 (Hartree/Particle)
Thermal correction to Energy=	0.331078
Thermal correction to Enthalpy=	0.332022
Thermal correction to Gibbs Free Energy=	0.261714
Sum of electronic and zero-point Energies=	-695.198733
Sum of electronic and thermal Energies=	-695.179393
Sum of electronic and thermal Enthalpies=	-695.178449
Sum of electronic and thermal Free Energies=	-695.248758

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.239166	-0.565624	-0.106955
2	6	0	-1.342371	-0.871546	1.379030
3	6	0	-0.577580	-0.355632	2.342431
4	6	0	3.079931	0.798858	0.092397
5	6	0	2.658552	-0.303421	-0.841162
6	6	0	1.315521	-0.965055	-0.447573
7	6	0	0.126568	-0.001449	-0.544385
8	6	0	3.687643	0.442671	1.413944
9	8	0	3.702742	-1.290532	-0.848807
10	6	0	-1.647985	-1.784500	-0.943262
11	8	0	-2.138895	0.566264	-0.449318
12	6	0	-3.453433	0.531328	-0.149540
13	8	0	-4.026531	-0.388892	0.395417
14	6	0	-4.121258	1.818634	-0.587967
15	6	0	3.215413	2.202856	-0.409487
16	1	0	-2.138958	-1.559635	1.647157
17	1	0	-0.737749	-0.625824	3.382904
18	1	0	0.226592	0.349158	2.149815
19	1	0	2.541861	0.118515	-1.854588
20	1	0	1.407006	-1.370625	0.565966
21	1	0	1.153381	-1.821445	-1.118933
22	1	0	0.333863	0.899184	0.044173
23	1	0	0.012260	0.336879	-1.582246
24	1	0	3.453280	1.195038	2.179680

25	1	0	4.788110	0.392329	1.349044
26	1	0	3.355959	-0.536878	1.772887
27	1	0	3.370090	-2.065785	-1.329208
28	1	0	-0.979845	-2.626935	-0.737057
29	1	0	-1.589687	-1.550661	-2.012087
30	1	0	-2.667702	-2.089755	-0.701614
31	1	0	-3.697177	2.664830	-0.036696
32	1	0	-5.192899	1.754038	-0.395620
33	1	0	-3.940676	1.999427	-1.652431
34	1	0	4.240781	2.412797	-0.767170
35	1	0	3.011224	2.937298	0.381310
36	1	0	2.540751	2.410634	-1.248443

TS_{I-II}

-407.4105 cm⁻¹

Zero-point correction= 0.312620 (Hartree/Particle)
Thermal correction to Energy= 0.329927
Thermal correction to Enthalpy= 0.330871
Thermal correction to Gibbs Free Energy= 0.268429
Sum of electronic and zero-point Energies= -695.180956
Sum of electronic and thermal Energies= -695.163649
Sum of electronic and thermal Enthalpies= -695.162705
Sum of electronic and thermal Free Energies= -695.225147

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.480086	-1.804830	0.225255
2	6	0	2.345688	-0.788280	-0.515337
3	6	0	2.073132	0.662243	-0.162951
4	6	0	-0.180003	0.807893	-0.396570
5	6	0	-0.751806	-0.444871	0.270648
6	6	0	0.000492	-1.721759	-0.158139
7	6	0	-0.489548	2.081964	0.020768
8	8	0	-2.072442	-0.704194	-0.365550
9	6	0	-3.170387	0.050856	-0.145514
10	6	0	-0.905137	-0.374670	1.791920
11	8	0	-3.259196	0.978498	0.629640
12	8	0	3.710987	-1.146281	-0.218738
13	6	0	2.498709	1.661766	-1.215429
14	6	0	2.407715	1.097384	1.243577
15	6	0	-4.305632	-0.434617	-1.026150
16	1	0	1.620854	-1.698586	1.306785
17	1	0	1.856875	-2.801491	-0.032707
18	1	0	2.165580	-0.920311	-1.596408

19	1	0	-0.018946	0.663931	-1.465038
20	1	0	-0.537463	-2.576494	0.267943
21	1	0	-0.096805	-1.812453	-1.248329
22	1	0	-0.877268	2.292137	1.009991
23	1	0	-0.292858	2.938275	-0.617580
24	1	0	-1.390207	-1.289591	2.149530
25	1	0	0.074775	-0.302016	2.269482
26	1	0	-1.513050	0.473802	2.100789
27	1	0	4.288079	-0.544050	-0.714249
28	1	0	2.115754	2.663789	-0.993265
29	1	0	2.159208	1.379086	-2.219370
30	1	0	3.598092	1.752753	-1.257027
31	1	0	1.892050	2.032392	1.492748
32	1	0	3.488234	1.281629	1.343511
33	1	0	2.146383	0.350468	1.997935
34	1	0	-4.062021	-0.254541	-2.079119
35	1	0	-5.219570	0.101046	-0.765923
36	1	0	-4.452345	-1.512419	-0.904971

TS_{I-III}

-291.3044 cm⁻¹

Zero-point correction= 0.312607 (Hartree/Particle)
Thermal correction to Energy= 0.330146
Thermal correction to Enthalpy= 0.331090
Thermal correction to Gibbs Free Energy= 0.267519
Sum of electronic and zero-point Energies= -695.184482
Sum of electronic and thermal Energies= -695.166944
Sum of electronic and thermal Enthalpies= -695.166000
Sum of electronic and thermal Free Energies= -695.229570

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.080471	0.521640	0.302967
2	6	0	0.526670	-0.853713	0.583657
3	6	0	-0.266130	-1.538569	-0.279339
4	6	0	-2.474641	-0.740150	0.001845
5	6	0	-2.372771	0.637325	-0.622109
6	6	0	-1.291684	1.601495	-0.083253
7	6	0	0.151446	1.376969	-0.586008
8	6	0	-2.676173	-0.812055	1.490528
9	8	0	-3.678249	1.224886	-0.430112
10	6	0	1.447614	1.257887	1.596677
11	8	0	2.300540	0.441401	-0.548527
12	6	0	3.338130	-0.330584	-0.168352

13	8	0	3.393197	-0.974027	0.858787
14	6	0	4.432516	-0.292911	-1.216091
15	6	0	-3.232407	-1.749226	-0.819689
16	1	0	0.736999	-1.269937	1.564217
17	1	0	-0.575666	-2.553286	-0.047044
18	1	0	-0.359581	-1.250517	-1.322510
19	1	0	-2.194836	0.510325	-1.704470
20	1	0	-1.337662	1.636518	1.010346
21	1	0	-1.596447	2.603235	-0.417456
22	1	0	0.128769	0.932586	-1.588588
23	1	0	0.645525	2.348053	-0.707987
24	1	0	-2.655151	-1.850211	1.842008
25	1	0	-3.652532	-0.386101	1.768378
26	1	0	-1.909332	-0.258029	2.042201
27	1	0	-3.686985	2.081678	-0.887354
28	1	0	0.550077	1.450790	2.193807
29	1	0	1.918239	2.219673	1.365380
30	1	0	2.137055	0.659763	2.195488
31	1	0	4.068646	-0.736340	-2.149496
32	1	0	5.296742	-0.853284	-0.857111
33	1	0	4.718558	0.740618	-1.435487
34	1	0	-4.304320	-1.494850	-0.849653
35	1	0	-3.147848	-2.759269	-0.401424
36	1	0	-2.882413	-1.778142	-1.859417

II

Zero-point correction=	0.314774 (Hartree/Particle)
Thermal correction to Energy=	0.332082
Thermal correction to Enthalpy=	0.333026
Thermal correction to Gibbs Free Energy=	0.270924
Sum of electronic and zero-point Energies=	-695.210853
Sum of electronic and thermal Energies=	-695.193545
Sum of electronic and thermal Enthalpies=	-695.192601
Sum of electronic and thermal Free Energies=	-695.254704

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.552584	-1.866204	0.141076
2	6	0	2.245675	-0.705627	-0.563518
3	6	0	1.692414	0.685391	-0.133976
4	6	0	0.124184	0.696385	-0.345895
5	6	0	-0.639223	-0.538078	0.274024
6	6	0	0.051181	-1.848819	-0.152010
7	6	0	-0.482836	2.014573	0.017842
8	8	0	-1.926963	-0.646220	-0.441792

9	6	0	-3.027447	0.078890	-0.147529
10	6	0	-0.868383	-0.519636	1.789969
11	8	0	-3.120520	0.921702	0.718495
12	8	0	3.644245	-0.848597	-0.321023
13	6	0	2.288283	1.755078	-1.077443
14	6	0	2.130850	1.032648	1.302771
15	6	0	-4.159676	-0.319254	-1.074631
16	1	0	1.755483	-1.819231	1.217551
17	1	0	1.992306	-2.804851	-0.214362
18	1	0	2.050585	-0.810034	-1.646362
19	1	0	-0.018371	0.552970	-1.426543
20	1	0	-0.452525	-2.690819	0.337921
21	1	0	-0.108438	-1.973977	-1.230472
22	1	0	-0.421378	2.400764	1.029008
23	1	0	-1.133813	2.541834	-0.669639
24	1	0	-1.629438	-1.265152	2.044584
25	1	0	0.048231	-0.800348	2.314927
26	1	0	-1.209283	0.448024	2.153951
27	1	0	4.112134	-0.201277	-0.870241
28	1	0	1.886670	2.746832	-0.846310
29	1	0	2.057288	1.537284	-2.128273
30	1	0	3.379339	1.815543	-0.972788
31	1	0	1.825513	2.049711	1.568606
32	1	0	3.220697	0.975222	1.376284
33	1	0	1.721488	0.355639	2.055370
34	1	0	-3.881427	-0.121618	-2.115386
35	1	0	-5.054661	0.248592	-0.817327
36	1	0	-4.360141	-1.392273	-0.990030

III

Zero-point correction=	0.315948 (Hartree/Particle)
Thermal correction to Energy=	0.332985
Thermal correction to Enthalpy=	0.333929
Thermal correction to Gibbs Free Energy=	0.271801
Sum of electronic and zero-point Energies=	-695.223620
Sum of electronic and thermal Energies=	-695.206584
Sum of electronic and thermal Enthalpies=	-695.205639
Sum of electronic and thermal Free Energies=	-695.267768

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.045412	0.649722	0.279506
2	6	0	0.372921	-0.610851	0.713682
3	6	0	-0.642850	-1.329765	-0.111932
4	6	0	-2.118812	-0.820273	0.020436

5	6	0	-2.263444	0.565192	-0.661877
6	6	0	-1.291568	1.677292	-0.218641
7	6	0	0.167868	1.489495	-0.671217
8	6	0	-2.534508	-0.763487	1.502190
9	8	0	-3.613077	0.986119	-0.444657
10	6	0	1.532557	1.480817	1.472037
11	8	0	2.229522	0.354823	-0.598723
12	6	0	3.219170	-0.445039	-0.155846
13	8	0	3.257783	-0.980635	0.932554
14	6	0	4.293161	-0.586500	-1.216980
15	6	0	-3.032905	-1.816727	-0.720783
16	1	0	0.670443	-1.031674	1.667710
17	1	0	-0.644104	-2.389048	0.175348
18	1	0	-0.367494	-1.299927	-1.177648
19	1	0	-2.099977	0.405929	-1.743617
20	1	0	-1.361798	1.826670	0.865269
21	1	0	-1.663273	2.608500	-0.670832
22	1	0	0.184321	1.018585	-1.661646
23	1	0	0.649640	2.466300	-0.794879
24	1	0	-2.437939	-1.755726	1.960036
25	1	0	-3.574257	-0.440147	1.598625
26	1	0	-1.907903	-0.074560	2.078548
27	1	0	-3.743550	1.820962	-0.919972
28	1	0	0.676837	1.873692	2.032133
29	1	0	2.129755	2.329824	1.121301
30	1	0	2.140475	0.874243	2.145945
31	1	0	3.861384	-0.981532	-2.142398
32	1	0	5.073951	-1.256406	-0.854602
33	1	0	4.723722	0.393054	-1.450629
34	1	0	-4.070638	-1.472191	-0.708003
35	1	0	-2.989852	-2.805778	-0.249234
36	1	0	-2.725582	-1.932474	-1.768300

IV

Zero-point correction=	0.312047 (Hartree/Particle)
Thermal correction to Energy=	0.331130
Thermal correction to Enthalpy=	0.332074
Thermal correction to Gibbs Free Energy=	0.262867
Sum of electronic and zero-point Energies=	-695.205030
Sum of electronic and thermal Energies=	-695.185948
Sum of electronic and thermal Enthalpies=	-695.185004
Sum of electronic and thermal Free Energies=	-695.254211

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	0.771868	0.100729	0.134004
2	6	0	0.801410	-0.293960	1.623247
3	6	0	1.145626	0.855922	2.533594
4	6	0	1.964079	-0.329902	-2.671954
5	6	0	0.564132	-0.773716	-2.301487
6	6	0	0.479508	-1.090320	-0.788736
7	6	0	2.320472	0.827885	-3.226132
8	8	0	-0.301848	0.354239	-2.645978
9	6	0	-1.644954	0.291396	-2.504727
10	6	0	0.197166	-2.007281	-3.146576
11	8	0	-2.267243	-0.665681	-2.098179
12	8	0	-0.490441	-0.842668	1.917016
13	6	0	2.577814	1.121265	2.878211
14	6	0	0.131156	1.931197	2.777081
15	6	0	-2.269962	1.604085	-2.930351
16	1	0	1.737346	0.552259	-0.124676
17	1	0	0.009259	0.876526	-0.001948
18	1	0	1.572207	-1.076725	1.747046
19	1	0	2.724265	-1.080046	-2.451964
20	1	0	-0.508862	-1.495027	-0.564249
21	1	0	1.206885	-1.890595	-0.589854
22	1	0	1.591398	1.596242	-3.459372
23	1	0	3.359679	1.037537	-3.464312
24	1	0	0.198685	-1.746121	-4.209930
25	1	0	0.943079	-2.794386	-2.989999
26	1	0	-0.785546	-2.392171	-2.870360
27	1	0	-0.503032	-1.047679	2.865589
28	1	0	3.051637	1.830165	2.174464
29	1	0	3.181805	0.205517	2.860835
30	1	0	2.675381	1.574790	3.874517
31	1	0	0.302015	2.813579	2.134200
32	1	0	0.174362	2.299437	3.812119
33	1	0	-0.882003	1.568385	2.579604
34	1	0	-1.900947	2.419255	-2.298781
35	1	0	-3.354691	1.532274	-2.842890
36	1	0	-1.992704	1.839594	-3.963068

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Zero-point correction=	0.312058 (Hartree/Particle)
Thermal correction to Energy=	0.331142
Thermal correction to Enthalpy=	0.332086
Thermal correction to Gibbs Free Energy=	0.263010
Sum of electronic and zero-point Energies=	-695.204571
Sum of electronic and thermal Energies=	-695.185487
Sum of electronic and thermal Enthalpies=	-695.184543
Sum of electronic and thermal Free Energies=	-695.253620

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.758135	-0.337859	-0.567111
2	6	0	-2.096070	-1.035065	-0.256625
3	6	0	-3.181087	-0.121827	0.249797
4	6	0	1.101636	2.133785	-0.487454
5	6	0	1.286757	0.926439	0.407742
6	6	0	-0.076767	0.243517	0.675757
7	6	0	1.668428	2.349315	-1.673337
8	8	0	2.189340	0.037809	-0.322766
9	6	0	2.583464	-1.151498	0.182763
10	6	0	1.947594	1.375182	1.723584
11	8	0	2.250534	-1.604613	1.257371
12	8	0	-2.475157	-1.660265	-1.496938
13	6	0	-3.558464	-0.098080	1.698073
14	6	0	-3.732579	0.933377	-0.660323
15	6	0	3.504470	-1.849209	-0.795957
16	1	0	-0.931896	0.443811	-1.315524
17	1	0	-0.110080	-1.084186	-1.041111
18	1	0	-1.907710	-1.811903	0.504185
19	1	0	0.431748	2.882975	-0.064573
20	1	0	0.074025	-0.540147	1.423870
21	1	0	-0.723800	1.003656	1.134042
22	1	0	2.339167	1.627138	-2.125936
23	1	0	1.472745	3.262866	-2.227962
24	1	0	2.930636	1.810887	1.518142
25	1	0	1.330679	2.141775	2.205537
26	1	0	2.061363	0.532956	2.408473
27	1	0	-3.357651	-2.041380	-1.361324
28	1	0	-3.133266	0.772993	2.228679
29	1	0	-3.214627	-0.994043	2.228090
30	1	0	-4.648440	-0.021986	1.830422
31	1	0	-3.289949	1.926297	-0.463322
32	1	0	-4.816909	1.055131	-0.525247
33	1	0	-3.542157	0.687872	-1.709721
34	1	0	2.971024	-2.055675	-1.730046
35	1	0	3.855723	-2.784374	-0.358314
36	1	0	4.356168	-1.206556	-1.041150

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Zero-point correction=	0.312248 (Hartree/Particle)
Thermal correction to Energy=	0.331135
Thermal correction to Enthalpy=	0.332079
Thermal correction to Gibbs Free Energy=	0.264595
Sum of electronic and zero-point Energies=	-695.193048
Sum of electronic and thermal Energies=	-695.174161

Sum of electronic and thermal Enthalpies= -695.173217
Sum of electronic and thermal Free Energies= -695.240701

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.092648	1.040215	0.082275
2	6	0	0.154698	1.768492	-0.869005
3	6	0	-0.412686	2.953788	-0.637293
4	6	0	-2.073640	-0.387215	-0.578481
5	6	0	-1.974764	-0.226135	0.914938
6	6	0	-0.579103	-0.431638	1.541771
7	6	0	0.444319	0.714855	1.450988
8	6	0	-1.683926	-1.691813	-1.204811
9	8	0	-2.892330	-1.200148	1.467825
10	6	0	2.370821	1.876178	0.279660
11	8	0	1.429417	-0.180732	-0.667463
12	6	0	2.284489	-1.101429	-0.172866
13	8	0	2.795749	-1.066481	0.926856
14	6	0	2.526331	-2.190808	-1.197011
15	6	0	-3.065893	0.461924	-1.312657
16	1	0	0.006727	1.272822	-1.824676
17	1	0	-1.039214	3.430567	-1.385285
18	1	0	-0.282817	3.496787	0.296587
19	1	0	-2.321941	0.786353	1.179178
20	1	0	-0.141461	-1.366625	1.178254
21	1	0	-0.744344	-0.591188	2.617994
22	1	0	-0.020338	1.644761	1.804729
23	1	0	1.252312	0.479003	2.148271
24	1	0	-1.400791	-1.559243	-2.257427
25	1	0	-2.527259	-2.403133	-1.188551
26	1	0	-0.851902	-2.178593	-0.687568
27	1	0	-2.859066	-1.118644	2.435316
28	1	0	2.114299	2.825325	0.760904
29	1	0	2.826619	2.103937	-0.689254
30	1	0	3.092194	1.345522	0.903830
31	1	0	1.577607	-2.604372	-1.552358
32	1	0	3.136475	-2.977158	-0.750959
33	1	0	3.045330	-1.772695	-2.066669
34	1	0	-4.092021	0.073043	-1.184720
35	1	0	-2.867085	0.478389	-2.392064
36	1	0	-3.065774	1.495545	-0.948318

TS_{IV-V} Ts de 6 confi (tsjm6_1ciclo_confi)

-393.3398

Zero-point correction= 0.312453 (Hartree/Particle)
 Thermal correction to Energy= 0.329869
 Thermal correction to Enthalpy= 0.330813
 Thermal correction to Gibbs Free Energy= 0.267901
 Sum of electronic and zero-point Energies= -695.185840
 Sum of electronic and thermal Energies= -695.168423
 Sum of electronic and thermal Enthalpies= -695.167479
 Sum of electronic and thermal Free Energies= -695.230391

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.624754	-1.515993	-0.955373
2	6	0	1.981348	-0.892703	-0.638596
3	6	0	1.964417	0.186165	0.426679
4	6	0	0.309956	1.573581	-0.351406
5	6	0	-0.831058	0.645105	-0.770830
6	6	0	-0.354777	-0.547158	-1.623677
7	6	0	0.149645	2.510677	0.637396
8	8	0	-1.429590	0.189188	0.490348
9	6	0	-2.530408	-0.594885	0.519120
10	6	0	-1.858342	1.479615	-1.561324
11	8	0	-3.120162	-1.018727	-0.451935
12	8	0	2.833485	-1.990648	-0.244996
13	6	0	3.145162	1.128621	0.400315
14	6	0	1.528498	-0.219393	1.812092
15	6	0	-2.925150	-0.881614	1.953245
16	1	0	0.190360	-1.942700	-0.044575
17	1	0	0.805122	-2.359408	-1.632028
18	1	0	2.376176	-0.452160	-1.571041
19	1	0	0.979438	1.814538	-1.176217
20	1	0	-1.237372	-1.097627	-1.956697
21	1	0	0.111486	-0.124927	-2.525660
22	1	0	-0.628144	2.412730	1.387528
23	1	0	0.859074	3.322758	0.762743
24	1	0	-2.270439	2.265851	-0.921819
25	1	0	-1.361886	1.964347	-2.409236
26	1	0	-2.669078	0.853243	-1.938413
27	1	0	3.720692	-1.631964	-0.085348
28	1	0	2.969277	2.006109	1.032384
29	1	0	3.376869	1.476064	-0.614424
30	1	0	4.055775	0.642700	0.792850
31	1	0	1.381871	0.664230	2.443246
32	1	0	2.295995	-0.848350	2.288784
33	1	0	0.593921	-0.784488	1.808059
34	1	0	-2.128565	-1.437448	2.459635
35	1	0	-3.844803	-1.467842	1.963785
36	1	0	-3.069896	0.053721	2.503262

TS_{IV-VI} Ts de 7 confi (tsjm7_1ciclo_confi)
-323.3329

Zero-point correction= 0.312615 (Hartree/Particle)
Thermal correction to Energy= 0.330115
Thermal correction to Enthalpy= 0.331059
Thermal correction to Gibbs Free Energy= 0.267419
Sum of electronic and zero-point Energies= -695.185018
Sum of electronic and thermal Energies= -695.167518
Sum of electronic and thermal Enthalpies= -695.166574
Sum of electronic and thermal Free Energies= -695.230214

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.103007	0.999079	-0.231982
2	6	0	-0.094197	1.638001	0.690597
3	6	0	1.175817	1.971915	0.346988
4	6	0	2.427540	-0.003537	0.439590
5	6	0	1.973092	-0.666826	-0.846152
6	6	0	0.466761	-0.958390	-1.023731
7	6	0	-0.457915	0.221639	-1.397830
8	6	0	2.000856	-0.640205	1.733825
9	8	0	2.707270	-1.910092	-0.896031
10	6	0	-2.096038	2.057098	-0.744926
11	8	0	-1.811406	0.064365	0.674681
12	6	0	-2.845625	-0.698012	0.258923
13	8	0	-3.296395	-0.726871	-0.867466
14	6	0	-3.370338	-1.531009	1.410875
15	6	0	3.827019	0.551466	0.396703
16	1	0	-0.428858	1.757071	1.718640
17	1	0	1.807019	2.498372	1.056939
18	1	0	1.494312	2.033979	-0.689055
19	1	0	2.294762	-0.031640	-1.690970
20	1	0	0.083673	-1.483015	-0.142522
21	1	0	0.402211	-1.682378	-1.848579
22	1	0	0.087933	0.943217	-2.019961
23	1	0	-1.274430	-0.156942	-2.016178
24	1	0	2.353747	-0.059338	2.594075
25	1	0	2.422615	-1.653443	1.821484
26	1	0	0.912024	-0.727425	1.813846
27	1	0	2.485752	-2.350697	-1.732675
28	1	0	-1.552459	2.808203	-1.327483
29	1	0	-2.572756	2.566598	0.099373
30	1	0	-2.868543	1.606750	-1.371659
31	1	0	-2.581815	-2.189707	1.790053
32	1	0	-4.217649	-2.127097	1.069696

33	1	0	-3.678097	-0.882661	2.237738
34	1	0	4.565955	-0.264892	0.357401
35	1	0	4.051446	1.154249	1.284820
36	1	0	3.993620	1.174260	-0.491741

V tsjm6_1ciclo_confi_ircr_min2

Zero-point correction= 0.315217 (Hartree/Particle)
Thermal correction to Energy= 0.332341
Thermal correction to Enthalpy= 0.333285
Thermal correction to Gibbs Free Energy= 0.271733
Sum of electronic and zero-point Energies= -695.217830
Sum of electronic and thermal Energies= -695.200706
Sum of electronic and thermal Enthalpies= -695.199762
Sum of electronic and thermal Free Energies= -695.261314

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.630338	-1.736360	-0.756845
2	6	0	1.925512	-0.976075	-0.497538
3	6	0	1.711491	0.326434	0.329908
4	6	0	0.614928	1.213130	-0.401743
5	6	0	-0.690524	0.460274	-0.815963
6	6	0	-0.360796	-0.863249	-1.527362
7	6	0	0.313820	2.478026	0.339754
8	8	0	-1.395720	0.203611	0.452055
9	6	0	-2.598539	-0.411154	0.500022
10	6	0	-1.557184	1.359653	-1.708029
11	8	0	-3.218969	-0.825604	-0.456232
12	8	0	2.825276	-1.888860	0.129956
13	6	0	3.033600	1.125160	0.333007
14	6	0	1.347201	-0.002240	1.790901
15	6	0	-3.068388	-0.520848	1.936099
16	1	0	0.200555	-2.070569	0.194392
17	1	0	0.863816	-2.640709	-1.330022
18	1	0	2.338225	-0.675151	-1.478538
19	1	0	1.076328	1.488784	-1.362918
20	1	0	-1.289569	-1.401730	-1.727567
21	1	0	0.071127	-0.602655	-2.504052
22	1	0	-0.454124	2.498501	1.104380
23	1	0	0.906132	3.373992	0.189919
24	1	0	-1.855413	2.264731	-1.169964
25	1	0	-0.983960	1.665107	-2.590435
26	1	0	-2.451950	0.829374	-2.037710

27	1	0	3.694932	-1.464517	0.184994
28	1	0	2.928052	2.064923	0.884118
29	1	0	3.363225	1.366064	-0.686239
30	1	0	3.836527	0.560908	0.824640
31	1	0	1.267030	0.917031	2.380983
32	1	0	2.126315	-0.630128	2.233359
33	1	0	0.396439	-0.530367	1.874263
34	1	0	-2.379345	-1.150071	2.510081
35	1	0	-4.067099	-0.958751	1.956346
36	1	0	-3.080690	0.465543	2.410467

VI tsjm7_1ciclo_conf_iircr_min

Zero-point correction= 0.315743 (Hartree/Particle)
Thermal correction to Energy= 0.332827
Thermal correction to Enthalpy= 0.333771
Thermal correction to Gibbs Free Energy= 0.271206
Sum of electronic and zero-point Energies= -695.223042
Sum of electronic and thermal Energies= -695.205959
Sum of electronic and thermal Enthalpies= -695.205015
Sum of electronic and thermal Free Energies= -695.267580

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.039102	0.940052	-0.230112
2	6	0	0.032231	1.455718	0.683382
3	6	0	1.483993	1.538481	0.347185
4	6	0	2.290007	0.194457	0.395233
5	6	0	1.931345	-0.677619	-0.835990
6	6	0	0.447493	-1.033617	-1.038374
7	6	0	-0.482516	0.133168	-1.416354
8	6	0	2.013520	-0.551749	1.713200
9	8	0	2.704119	-1.876553	-0.723529
10	6	0	-1.933558	2.099823	-0.709510
11	8	0	-1.833574	0.053960	0.663787
12	6	0	-2.947936	-0.583233	0.245949
13	8	0	-3.413511	-0.538556	-0.874321
14	6	0	-3.545128	-1.382852	1.386636
15	6	0	3.790033	0.543585	0.312717
16	1	0	-0.303348	1.766335	1.669418
17	1	0	1.962279	2.226190	1.055384
18	1	0	1.633096	1.980667	-0.651712
19	1	0	2.259699	-0.115321	-1.730044
20	1	0	0.065388	-1.557706	-0.155548
21	1	0	0.414281	-1.763526	-1.860944
22	1	0	0.047878	0.831404	-2.078516

23	1	0	-1.335182	-0.244318	-1.984348
24	1	0	2.311781	0.067314	2.568423
25	1	0	2.581075	-1.485472	1.749797
26	1	0	0.951001	-0.787830	1.833654
27	1	0	2.494987	-2.435049	-1.487914
28	1	0	-1.325800	2.821071	-1.266749
29	1	0	-2.369362	2.618760	0.150802
30	1	0	-2.738129	1.739226	-1.354249
31	1	0	-2.826520	-2.129783	1.740287
32	1	0	-4.454960	-1.877662	1.044472
33	1	0	-3.772147	-0.724810	2.231720
34	1	0	4.396729	-0.365122	0.278307
35	1	0	4.098031	1.134759	1.183548
36	1	0	4.010660	1.132792	-0.587043

VII

Zero-point correction=	0.434631 (Hartree/Particle)
Thermal correction to Energy=	0.458100
Thermal correction to Enthalpy=	0.459044
Thermal correction to Gibbs Free Energy=	0.380623
Sum of electronic and zero-point Energies=	-890.426013
Sum of electronic and thermal Energies=	-890.402544
Sum of electronic and thermal Enthalpies=	-890.401600
Sum of electronic and thermal Free Energies=	-890.480020

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.547557	-1.503770	0.707656
2	6	0	-3.473311	0.020781	0.684114
3	6	0	-2.536010	0.585229	-0.431867
4	6	0	-1.102164	-0.041353	-0.186090
5	6	0	-1.195454	-1.552776	-0.187361
6	6	0	-2.141217	-2.128143	0.827463
7	6	0	0.007901	0.548191	-1.101843
8	6	0	0.932696	1.599015	-0.451038
9	6	0	2.135735	1.067081	0.372914
10	6	0	3.006067	2.247564	0.819023
11	6	0	-0.406379	-2.443494	-1.098169
12	6	0	1.691204	0.174266	1.513311
13	8	0	-4.819029	0.486161	0.566440
14	6	0	-2.488357	2.119207	-0.285081
15	6	0	-3.085525	0.232811	-1.826750
16	6	0	1.591099	0.523199	2.795995
17	8	0	2.875371	0.259011	-0.612432

18	6	0	3.996985	-0.410815	-0.256351
19	8	0	4.488800	-0.407104	0.849954
20	6	0	4.548197	-1.168290	-1.446586
21	1	0	-4.039378	-1.852622	-0.207849
22	1	0	-4.183194	-1.810633	1.546836
23	1	0	-3.054902	0.356102	1.650862
24	1	0	-0.855274	0.253788	0.849099
25	1	0	-2.208475	-3.218535	0.735247
26	1	0	-1.768344	-1.928704	1.850064
27	1	0	-0.449420	1.009682	-1.984230
28	1	0	0.643258	-0.247577	-1.496516
29	1	0	0.360722	2.265141	0.204562
30	1	0	1.360683	2.225761	-1.243953
31	1	0	3.851981	1.904591	1.416180
32	1	0	2.413610	2.951944	1.412208
33	1	0	3.379879	2.782146	-0.060353
34	1	0	-0.756604	-3.479289	-1.027591
35	1	0	-0.478173	-2.143141	-2.154433
36	1	0	0.673334	-2.457507	-0.865165
37	1	0	1.387636	-0.826389	1.209542
38	1	0	-4.820930	1.441180	0.729714
39	1	0	-1.817888	2.577968	-1.018708
40	1	0	-2.147606	2.418799	0.714977
41	1	0	-3.478097	2.561707	-0.455249
42	1	0	-2.542390	0.763654	-2.616971
43	1	0	-4.140655	0.516235	-1.894793
44	1	0	-3.010559	-0.839119	-2.036349
45	1	0	1.218823	-0.177989	3.537508
46	1	0	1.881765	1.503108	3.163705
47	1	0	3.808892	-1.890039	-1.810105
48	1	0	5.460374	-1.689143	-1.153050
49	1	0	4.760664	-0.477858	-2.269449

VII'

Zero-point correction=	0.434620 (Hartree/Particle)
Thermal correction to Energy=	0.458005
Thermal correction to Enthalpy=	0.458950
Thermal correction to Gibbs Free Energy=	0.381508
Sum of electronic and zero-point Energies=	-890.424658
Sum of electronic and thermal Energies=	-890.401273
Sum of electronic and thermal Enthalpies=	-890.400329
Sum of electronic and thermal Free Energies=	-890.477770

Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	3.593745	-2.074861	0.892701
2	6	0	2.895624	-2.633972	-0.344762
3	6	0	1.982517	-1.592825	-1.070698
4	6	0	0.918567	-1.096981	-0.008203
5	6	0	1.641876	-0.513515	1.187836
6	6	0	2.581045	-1.458763	1.879325
7	6	0	-0.198602	-0.192794	-0.595372
8	6	0	-1.469049	-0.926211	-1.085976
9	6	0	-2.658864	-0.966118	-0.089023
10	6	0	-3.845933	-1.678741	-0.761953
11	6	0	1.365362	0.841795	1.761219
12	6	0	-2.269358	-1.670288	1.192349
13	8	0	3.928498	-3.150407	-1.186014
14	6	0	1.303492	-2.301680	-2.259215
15	6	0	2.827822	-0.426008	-1.616711
16	6	0	-2.055190	-1.123249	2.387376
17	8	0	-2.955415	0.446346	0.141090
18	6	0	-4.064811	0.862052	0.801935
19	8	0	-4.909734	0.143534	1.284929
20	6	0	-4.091894	2.376493	0.845316
21	1	0	4.321484	-1.317721	0.578259
22	1	0	4.162018	-2.882434	1.369445
23	1	0	2.238974	-3.463065	-0.022429
24	1	0	0.422931	-2.019377	0.349444
25	1	0	3.115296	-0.959826	2.696699
26	1	0	2.011554	-2.285546	2.346358
27	1	0	0.205022	0.401282	-1.423287
28	1	0	-0.512715	0.537083	0.153573
29	1	0	-1.242817	-1.962001	-1.359452
30	1	0	-1.847902	-0.443356	-1.995420
31	1	0	-4.696313	-1.758975	-0.085687
32	1	0	-3.538891	-2.684133	-1.071077
33	1	0	-4.153164	-1.128411	-1.658059
34	1	0	2.157936	1.137071	2.458778
35	1	0	1.295041	1.623000	0.991850
36	1	0	0.416344	0.883424	2.325622
37	1	0	-2.144056	-2.746546	1.069929
38	1	0	3.511968	-3.675962	-1.885162
39	1	0	0.626173	-1.632381	-2.798540
40	1	0	0.726609	-3.178682	-1.936441
41	1	0	2.049954	-2.637174	-2.990234
42	1	0	2.242698	0.209962	-2.290934
43	1	0	3.681611	-0.816753	-2.179526
44	1	0	3.213583	0.209593	-0.813191
45	1	0	-1.765567	-1.731964	3.239010
46	1	0	-2.170800	-0.059270	2.568887
47	1	0	-3.203114	2.757371	1.359585
48	1	0	-4.991050	2.706854	1.366698

49	1	0	-4.078505	2.784135	-0.170847
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TS_{VII-VIII}

-370.8689 cm⁻¹

Zero-point correction=	0.435249 (Hartree/Particle)
Thermal correction to Energy=	0.457270
Thermal correction to Enthalpy=	0.458214
Thermal correction to Gibbs Free Energy=	0.385534
Sum of electronic and zero-point Energies=	-890.413146
Sum of electronic and thermal Energies=	-890.391125
Sum of electronic and thermal Enthalpies=	-890.390181
Sum of electronic and thermal Free Energies=	-890.462861

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
<hr/>					
1	6	0	-3.403633	1.495533	0.536084
2	6	0	-3.678287	0.192116	-0.209675
3	6	0	-2.559450	-0.890614	-0.046282
4	6	0	-1.174675	-0.213395	-0.434494
5	6	0	-0.941877	1.096032	0.314381
6	6	0	-2.052092	2.096513	0.099448
7	6	0	0.023052	-1.197321	-0.414039
8	6	0	1.163235	-0.921503	-1.425230
9	6	0	2.329490	-0.011316	-0.982110
10	6	0	3.412346	0.014421	-2.074776
11	6	0	-0.293524	1.122047	1.675735
12	6	0	1.907031	1.380354	-0.582572
13	8	0	-4.956889	-0.261527	0.237012
14	6	0	-2.882260	-2.028557	-1.042670
15	6	0	-2.569448	-1.478729	1.377118
16	6	0	0.742925	1.974299	-0.971134
17	8	0	2.856068	-0.733088	0.205312
18	6	0	3.946114	-0.312882	0.879899
19	8	0	4.598721	0.677353	0.622541
20	6	0	4.242658	-1.257085	2.027898
21	1	0	-3.411067	1.308538	1.616657
22	1	0	-4.225462	2.192290	0.331880
23	1	0	-3.732007	0.432849	-1.287227
24	1	0	-1.325690	0.068159	-1.491327
25	1	0	-1.857278	3.025602	0.649016
26	1	0	-2.121439	2.365731	-0.966442
27	1	0	-0.351928	-2.196796	-0.650794
28	1	0	0.447508	-1.279589	0.590517
29	1	0	0.748600	-0.519174	-2.358005

30	1	0	1.620868	-1.882073	-1.691062
31	1	0	4.249101	0.648993	-1.780516
32	1	0	2.980802	0.409800	-3.000491
33	1	0	3.784368	-0.998495	-2.270906
34	1	0	-0.006153	2.148003	1.936796
35	1	0	-0.967314	0.771225	2.472259
36	1	0	0.611397	0.509541	1.721773
37	1	0	2.572866	1.893095	0.103254
38	1	0	-5.253316	-0.967486	-0.356509
39	1	0	-2.210476	-2.884887	-0.933218
40	1	0	-2.822196	-1.683443	-2.082916
41	1	0	-3.894316	-2.418199	-0.874236
42	1	0	-1.778955	-2.227971	1.496969
43	1	0	-3.530231	-1.963204	1.576298
44	1	0	-2.427637	-0.718711	2.149505
45	1	0	0.562757	3.012413	-0.703104
46	1	0	0.172843	1.615498	-1.822430
47	1	0	3.423347	-1.230954	2.754754
48	1	0	5.171662	-0.955346	2.513324
49	1	0	4.324058	-2.286622	1.665311

TS_{VII-IX}

-401.9046 cm⁻¹

Zero-point correction=	0.435356 (Hartree/Particle)
Thermal correction to Energy=	0.457043
Thermal correction to Enthalpy=	0.457987
Thermal correction to Gibbs Free Energy=	0.386973
Sum of electronic and zero-point Energies=	-890.411541
Sum of electronic and thermal Energies=	-890.389854
Sum of electronic and thermal Enthalpies=	-890.388910
Sum of electronic and thermal Free Energies=	-890.459924

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.787141	0.575189	-1.072212
2	6	0	-3.024653	-0.842789	-0.553227
3	6	0	-2.080206	-1.261359	0.622690
4	6	0	-0.597857	-0.981396	0.147947
5	6	0	-0.395647	0.441506	-0.358458
6	6	0	-1.320331	0.764943	-1.511413
7	6	0	0.499596	-1.423526	1.135256
8	6	0	1.870661	-1.614215	0.468250
9	6	0	2.501065	-0.373404	-0.192109
10	6	0	3.909754	-0.726641	-0.704463

11	6	0	-0.208996	1.600508	0.597252
12	6	0	1.637322	0.215432	-1.316447
13	8	0	-4.408195	-0.915915	-0.206466
14	6	0	-2.270570	-2.777974	0.853466
15	6	0	-2.457545	-0.528419	1.923403
16	6	0	1.445554	-0.502472	-2.475282
17	8	0	2.645066	0.567438	0.932593
18	6	0	3.229702	1.776187	0.785784
19	8	0	3.624037	2.245830	-0.260889
20	6	0	3.310053	2.482717	2.123437
21	1	0	-3.059967	1.297137	-0.292739
22	1	0	-3.467991	0.753988	-1.912938
23	1	0	-2.819566	-1.538870	-1.386871
24	1	0	-0.482540	-1.620055	-0.743712
25	1	0	-1.164542	1.790350	-1.871091
26	1	0	-1.116289	0.093737	-2.355832
27	1	0	0.230459	-2.383736	1.588004
28	1	0	0.592715	-0.714261	1.963937
29	1	0	1.791558	-2.393162	-0.301074
30	1	0	2.583096	-1.987048	1.214755
31	1	0	4.371369	0.128690	-1.199019
32	1	0	3.846796	-1.550703	-1.420888
33	1	0	4.543068	-1.042858	0.132968
34	1	0	0.367107	2.404411	0.119976
35	1	0	-1.176402	2.048373	0.871970
36	1	0	0.301165	1.325787	1.521374
37	1	0	1.688350	1.295117	-1.408505
38	1	0	-4.630420	-1.845241	-0.045809
39	1	0	-1.703985	-3.139422	1.716904
40	1	0	-1.960682	-3.361362	-0.023003
41	1	0	-3.322258	-3.014395	1.061670
42	1	0	-1.805136	-0.836366	2.748382
43	1	0	-3.489504	-0.764408	2.200755
44	1	0	-2.389697	0.557974	1.832772
45	1	0	1.056707	-0.024951	-3.368863
46	1	0	1.601223	-1.576413	-2.534122
47	1	0	2.302713	2.742207	2.467886
48	1	0	3.900327	3.393613	2.015106
49	1	0	3.756656	1.829223	2.878900

TS_{VII-X}

-392.1589 cm⁻¹

Zero-point correction=	0.435403 (Hartree/Particle)
Thermal correction to Energy=	0.457099
Thermal correction to Enthalpy=	0.458043
Thermal correction to Gibbs Free Energy=	0.386907

Sum of electronic and zero-point Energies= -890.409472
Sum of electronic and thermal Energies= -890.387775
Sum of electronic and thermal Enthalpies= -890.386831
Sum of electronic and thermal Free Energies= -890.457968

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.649043	-0.364441	-2.276032
2	6	0	-2.807489	-1.742067	-1.631721
3	6	0	-2.243372	-1.839751	-0.174155
4	6	0	-0.755741	-1.305057	-0.222411
5	6	0	-0.650673	0.079695	-0.846556
6	6	0	-1.176446	0.095240	-2.265215
7	6	0	0.037990	-1.424345	1.091377
8	6	0	1.558676	-1.398403	0.869961
9	6	0	2.167513	-0.118724	0.257204
10	6	0	3.694858	-0.299269	0.177039
11	6	0	-0.968657	1.334977	-0.068151
12	6	0	1.599978	0.179534	-1.135672
13	8	0	-4.196877	-2.062350	-1.711526
14	6	0	-2.247052	-3.331877	0.226860
15	6	0	-3.135266	-1.073209	0.819205
16	6	0	1.857219	1.334338	-1.832353
17	8	0	1.807780	0.910750	1.249572
18	6	0	2.419940	2.103562	1.401356
19	8	0	3.291247	2.561049	0.692932
20	6	0	1.843860	2.819916	2.607108
21	1	0	-3.282727	0.356830	-1.745638
22	1	0	-3.031228	-0.417438	-3.302460
23	1	0	-2.231441	-2.461827	-2.241691
24	1	0	-0.263173	-1.989818	-0.936038
25	1	0	-1.089468	1.093920	-2.708973
26	1	0	-0.591568	-0.587904	-2.899735
27	1	0	-0.195148	-2.371907	1.588879
28	1	0	-0.244114	-0.634369	1.794613
29	1	0	1.840367	-2.238212	0.220072
30	1	0	2.060694	-1.567395	1.830441
31	1	0	4.178874	0.582961	-0.238026
32	1	0	3.917871	-1.159569	-0.463728
33	1	0	4.108444	-0.501729	1.172426
34	1	0	-0.381388	2.173071	-0.464763
35	1	0	-2.026769	1.619128	-0.174570
36	1	0	-0.753878	1.250630	0.998618
37	1	0	1.469230	-0.729350	-1.722532
38	1	0	-4.304375	-2.999809	-1.491754
39	1	0	-1.943245	-3.480152	1.267415
40	1	0	-1.575914	-3.922999	-0.409438
41	1	0	-3.255053	-3.758343	0.142108

42	1	0	-2.749710	-1.164639	1.841256
43	1	0	-4.150429	-1.481431	0.801468
44	1	0	-3.210463	-0.008873	0.586235
45	1	0	1.629741	1.392554	-2.893017
46	1	0	2.224950	2.233074	-1.353231
47	1	0	0.780584	3.027358	2.444679
48	1	0	2.380445	3.756912	2.761133
49	1	0	1.921444	2.190760	3.499427

VIII

Zero-point correction=	0.438270 (Hartree/Particle)
Thermal correction to Energy=	0.460021
Thermal correction to Enthalpy=	0.460965
Thermal correction to Gibbs Free Energy=	0.388914
Sum of electronic and zero-point Energies=	-890.447307
Sum of electronic and thermal Energies=	-890.425557
Sum of electronic and thermal Enthalpies=	-890.424613
Sum of electronic and thermal Free Energies=	-890.496663

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.206396	-3.292002	1.713676
2	6	0	2.640109	-3.482409	0.266464
3	6	0	2.262406	-2.284984	-0.663770
4	6	0	0.721999	-1.973855	-0.487609
5	6	0	0.198032	-1.853741	0.989780
6	6	0	0.695447	-3.077019	1.796887
7	6	0	0.250276	-0.819061	-1.404407
8	6	0	-1.249586	-0.800390	-1.762041
9	6	0	-2.196380	-0.124377	-0.757265
10	6	0	-3.633118	-0.118310	-1.309610
11	6	0	0.596059	-0.560049	1.732352
12	6	0	-2.137336	-0.714427	0.616027
13	8	0	4.042940	-3.748372	0.293649
14	6	0	2.518051	-2.757940	-2.117370
15	6	0	3.185638	-1.076618	-0.403331
16	6	0	-1.373026	-1.943343	0.987674
17	8	0	-1.692886	1.286616	-0.740174
18	6	0	-2.275576	2.239166	0.014685
19	8	0	-3.237925	2.080084	0.737392
20	6	0	-1.547703	3.558216	-0.155621
21	1	0	2.755254	-2.451901	2.155352
22	1	0	2.498891	-4.182763	2.282030
23	1	0	2.108566	-4.369893	-0.123025

24	1	0	0.228333	-2.883802	-0.869628
25	1	0	0.387462	-2.967003	2.845082
26	1	0	0.188884	-3.979353	1.421533
27	1	0	0.790045	-0.890806	-2.352731
28	1	0	0.525577	0.153308	-0.985071
29	1	0	-1.607731	-1.824182	-1.933401
30	1	0	-1.373890	-0.268952	-2.713161
31	1	0	-4.316837	0.369070	-0.613519
32	1	0	-3.967847	-1.149345	-1.468714
33	1	0	-3.669004	0.406674	-2.271800
34	1	0	0.055064	-0.506759	2.685403
35	1	0	1.662053	-0.516798	1.965619
36	1	0	0.338431	0.339690	1.166761
37	1	0	-2.727283	-0.210908	1.373337
38	1	0	4.311185	-4.055964	-0.584985
39	1	0	2.405237	-1.952857	-2.849133
40	1	0	1.839577	-3.571844	-2.402760
41	1	0	3.546935	-3.122409	-2.231878
42	1	0	2.924044	-0.237147	-1.056517
43	1	0	4.224761	-1.352317	-0.605672
44	1	0	3.146183	-0.720484	0.627836
45	1	0	-1.679093	-2.228193	2.002181
46	1	0	-1.652498	-2.791386	0.340005
47	1	0	-0.535648	3.480543	0.257049
48	1	0	-2.094834	4.342905	0.368583
49	1	0	-1.449630	3.809691	-1.216166

IX

Zero-point correction= 0.437368 (Hartree/Particle)
 Thermal correction to Energy= 0.459218
 Thermal correction to Enthalpy= 0.460162
 Thermal correction to Gibbs Free Energy= 0.389127
 Sum of electronic and zero-point Energies= -890.439749
 Sum of electronic and thermal Energies= -890.417899
 Sum of electronic and thermal Enthalpies= -890.416955
 Sum of electronic and thermal Free Energies= -890.487991

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.828535	-1.152730	2.120920
2	6	0	2.666106	-1.185448	0.846373
3	6	0	2.143583	-0.229930	-0.273294
4	6	0	0.622642	-0.553394	-0.503795
5	6	0	-0.290698	-0.598401	0.770110
6	6	0	0.367729	-1.516470	1.831955

7	6	0	-0.048625	0.273404	-1.618982
8	6	0	-1.403385	-0.326804	-2.016502
9	6	0	-2.385022	-0.490846	-0.846136
10	6	0	-3.662640	-1.199697	-1.317081
11	6	0	-0.532767	0.778760	1.439543
12	6	0	-1.691326	-1.227484	0.360878
13	8	0	4.011039	-0.906475	1.237177
14	6	0	2.925783	-0.567688	-1.566523
15	6	0	2.443038	1.243593	0.070112
16	6	0	-1.617044	-2.697595	0.065349
17	8	0	-2.735841	0.902745	-0.509591
18	6	0	-3.644132	1.209430	0.439942
19	8	0	-4.215830	0.412505	1.155249
20	6	0	-3.839245	2.709897	0.509163
21	1	0	1.919402	-0.165371	2.588609
22	1	0	2.260255	-1.866008	2.832858
23	1	0	2.610231	-2.211611	0.439360
24	1	0	0.635998	-1.592234	-0.871471
25	1	0	-0.221265	-1.485339	2.758706
26	1	0	0.330591	-2.556810	1.482785
27	1	0	0.585805	0.300913	-2.511203
28	1	0	-0.184300	1.314477	-1.307330
29	1	0	-1.242878	-1.319303	-2.457010
30	1	0	-1.883924	0.287244	-2.787841
31	1	0	-4.356429	-1.361263	-0.490594
32	1	0	-3.417390	-2.167062	-1.765001
33	1	0	-4.158850	-0.586312	-2.078078
34	1	0	-1.399128	0.714952	2.108242
35	1	0	0.316159	1.081550	2.056200
36	1	0	-0.723651	1.580774	0.725473
37	1	0	-2.360452	-1.105979	1.217300
38	1	0	4.589346	-1.088816	0.481537
39	1	0	2.668005	0.102240	-2.392216
40	1	0	2.737672	-1.597755	-1.895668
41	1	0	4.006653	-0.455658	-1.411558
42	1	0	2.091545	1.909282	-0.726011
43	1	0	3.522607	1.385999	0.176575
44	1	0	1.983683	1.570659	1.003977
45	1	0	-2.310118	-3.390780	0.529820
46	1	0	-0.931101	-3.106978	-0.670112
47	1	0	-2.936013	3.180317	0.914409
48	1	0	-4.685092	2.934794	1.160250
49	1	0	-4.006258	3.125706	-0.488873

X

Zero-point correction= 0.437454 (Hartree/Particle)
Thermal correction to Energy= 0.459214

Thermal correction to Enthalpy= 0.460158
 Thermal correction to Gibbs Free Energy= 0.388997
 Sum of electronic and zero-point Energies= -890.439037
 Sum of electronic and thermal Energies= -890.417276
 Sum of electronic and thermal Enthalpies= -890.416332
 Sum of electronic and thermal Free Energies= -890.487493

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.197894	-1.727621	1.634420
2	6	0	2.916505	-1.742039	0.289839
3	6	0	2.520869	-0.552900	-0.641393
4	6	0	0.953021	-0.531128	-0.740951
5	6	0	0.155808	-0.539004	0.611078
6	6	0	0.674710	-1.726264	1.463326
7	6	0	0.388122	0.530166	-1.702156
8	6	0	-1.081388	0.244177	-2.026834
9	6	0	-1.990296	0.160178	-0.787312
10	6	0	-3.396300	-0.274497	-1.220891
11	6	0	0.270295	0.753134	1.455063
12	6	0	-1.372832	-0.822901	0.254213
13	8	0	4.313950	-1.788649	0.578369
14	6	0	3.106313	-0.854857	-2.042934
15	6	0	3.151109	0.768263	-0.156339
16	6	0	-2.230603	-1.046920	1.460196
17	8	0	-1.985654	1.558585	-0.307834
18	6	0	-2.922786	2.137345	0.470317
19	8	0	-3.875662	1.588940	0.983097
20	6	0	-2.605895	3.610755	0.635530
21	1	0	2.535036	-0.861103	2.215071
22	1	0	2.511153	-2.612357	2.201132
23	1	0	2.620703	-2.668970	-0.235137
24	1	0	0.707647	-1.506029	-1.198788
25	1	0	0.197254	-1.713370	2.449586
26	1	0	0.373661	-2.670928	0.984857
27	1	0	0.950436	0.539928	-2.641580
28	1	0	0.480497	1.534202	-1.275190
29	1	0	-1.152593	-0.713297	-2.560216
30	1	0	-1.485081	1.012282	-2.697333
31	1	0	-4.086447	-0.344477	-0.382156
32	1	0	-3.331204	-1.253082	-1.709477
33	1	0	-3.802400	0.438263	-1.947744
34	1	0	-0.546422	0.781638	2.185361
35	1	0	1.203592	0.786408	2.021429
36	1	0	0.211177	1.662930	0.855471
37	1	0	-1.339358	-1.780272	-0.295257
38	1	0	4.787683	-1.968415	-0.247476

39	1	0	2.968203	-0.021378	-2.738194
40	1	0	2.649505	-1.747424	-2.489068
41	1	0	4.189301	-1.024433	-1.985519
42	1	0	2.852005	1.602058	-0.801059
43	1	0	4.242269	0.692974	-0.187214
44	1	0	2.877381	1.024289	0.868094
45	1	0	-2.104872	-1.951021	2.046406
46	1	0	-2.983908	-0.335651	1.771083
47	1	0	-1.666696	3.727815	1.187700
48	1	0	-3.413854	4.095121	1.185356
49	1	0	-2.473005	4.087978	-0.340208

XI

Zero-point correction=	0.435012 (Hartree/Particle)
Thermal correction to Energy=	0.458392
Thermal correction to Enthalpy=	0.459336
Thermal correction to Gibbs Free Energy=	0.382048
Sum of electronic and zero-point Energies=	-890.425079
Sum of electronic and thermal Energies=	-890.401699
Sum of electronic and thermal Enthalpies=	-890.400754
Sum of electronic and thermal Free Energies=	-890.478043

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.912258	0.473183	0.968057
2	6	0	3.187284	-0.871899	0.918915
3	6	0	2.223940	-1.029565	-0.303401
4	6	0	1.208491	0.189133	-0.240164
5	6	0	1.970258	1.496634	-0.235803
6	6	0	2.908324	1.648803	0.928873
7	6	0	0.042132	0.107928	-1.264112
8	6	0	-1.302378	-0.415637	-0.707231
9	6	0	-2.230012	0.638814	-0.042358
10	6	0	-2.787985	1.664018	-1.045983
11	6	0	2.179906	2.383569	-1.426973
12	6	0	-1.530581	1.382170	1.076288
13	8	0	4.203900	-1.874977	0.955659
14	6	0	1.470994	-2.366790	-0.151612
15	6	0	3.021402	-1.059408	-1.619855
16	6	0	-1.835502	1.343907	2.373197
17	8	0	-3.336613	-0.070598	0.608433
18	6	0	-4.245532	-0.789002	-0.085094
19	8	0	-4.256903	-0.946309	-1.287752
20	6	0	-5.267843	-1.379319	0.864478
21	1	0	4.606572	0.538473	0.121612

22	1	0	4.521366	0.508565	1.879248
23	1	0	2.563100	-0.952263	1.827466
24	1	0	0.756093	0.103190	0.761493
25	1	0	3.450135	2.601514	0.886713
26	1	0	2.342026	1.648886	1.875240
27	1	0	0.328844	-0.533260	-2.105044
28	1	0	-0.126601	1.092356	-1.711481
29	1	0	-1.121534	-1.198864	0.037297
30	1	0	-1.875147	-0.871346	-1.519140
31	1	0	-3.264646	1.167190	-1.892382
32	1	0	-1.982933	2.306236	-1.417050
33	1	0	-3.520231	2.306062	-0.545715
34	1	0	2.050177	3.443922	-1.160438
35	1	0	3.207825	2.302486	-1.823152
36	1	0	1.502942	2.167989	-2.258521
37	1	0	-0.709676	2.011871	0.735590
38	1	0	3.776649	-2.730052	1.114363
39	1	0	0.758115	-2.527244	-0.966652
40	1	0	0.916257	-2.414386	0.794476
41	1	0	2.167664	-3.214583	-0.180720
42	1	0	2.373262	-1.282665	-2.474842
43	1	0	3.791599	-1.835434	-1.569891
44	1	0	3.522171	-0.108841	-1.824601
45	1	0	-2.647504	0.734313	2.754254
46	1	0	-1.273872	1.931334	3.094466
47	1	0	-4.772318	-2.008358	1.611289
48	1	0	-5.987680	-1.971497	0.298258
49	1	0	-5.786666	-0.579762	1.403815

XI'

Zero-point correction=	0.434774 (Hartree/Particle)
Thermal correction to Energy=	0.457459
Thermal correction to Enthalpy=	0.458404
Thermal correction to Gibbs Free Energy=	0.382091
Sum of electronic and zero-point Energies=	-890.423722
Sum of electronic and thermal Energies=	-890.401037
Sum of electronic and thermal Enthalpies=	-890.400093
Sum of electronic and thermal Free Energies=	-890.476405

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.046207	0.223913	-0.900131
2	6	0	-3.194272	-1.043707	-0.856633
3	6	0	-2.138804	-1.055992	0.299271
4	6	0	-1.240874	0.237573	0.109971
5	6	0	-2.121252	1.466535	0.114547
6	6	0	-3.161363	1.488174	-0.969562

7	6	0	-0.014200	0.319344	1.057382
8	6	0	1.285027	-0.344326	0.531294
9	6	0	2.343077	0.647434	-0.022482
10	6	0	2.980223	1.516959	1.064059
11	6	0	-2.206217	2.477513	1.217421
12	6	0	1.765144	1.443861	-1.174157
13	8	0	-4.109598	-2.137672	-0.783039
14	6	0	-1.302262	-2.344260	0.169713
15	6	0	-2.844658	-1.069748	1.668561
16	6	0	1.522320	2.753964	-1.201858
17	8	0	3.398801	-0.134104	-0.708200
18	6	0	4.186002	-1.017049	-0.056793
19	8	0	4.127709	-1.284108	1.125469
20	6	0	5.176202	-1.634112	-1.023714
21	1	0	-4.683984	0.257137	-0.008716
22	1	0	-4.716308	0.165617	-1.766387
23	1	0	-2.628249	-1.105325	-1.804462
24	1	0	-0.839574	0.153477	-0.916243
25	1	0	-3.787730	2.386318	-0.906182
26	1	0	-2.676409	1.515081	-1.961214
27	1	0	-0.265521	-0.112022	2.032648
28	1	0	0.193457	1.374823	1.254352
29	1	0	1.056206	-1.046958	-0.276521
30	1	0	1.766283	-0.923092	1.322937
31	1	0	3.434127	0.888042	1.830629
32	1	0	2.229384	2.155115	1.539752
33	1	0	3.748896	2.163140	0.628983
34	1	0	-1.954368	3.491546	0.862846
35	1	0	-3.230788	2.551049	1.618296
36	1	0	-1.545102	2.258047	2.060701
37	1	0	1.523153	0.835753	-2.045415
38	1	0	-3.612883	-2.955494	-0.935090
39	1	0	-0.523470	-2.401635	0.936385
40	1	0	-0.815175	-2.417593	-0.811580
41	1	0	-1.931788	-3.233611	0.302785
42	1	0	-2.133012	-1.244698	2.483343
43	1	0	-3.588249	-1.872527	1.692845
44	1	0	-3.362254	-0.128420	1.876967
45	1	0	1.078137	3.221283	-2.076323
46	1	0	1.749844	3.412245	-0.368401
47	1	0	4.648485	-2.105579	-1.859034
48	1	0	5.781289	-2.374206	-0.498558
49	1	0	5.822985	-0.856888	-1.444507

XI''

Zero-point correction=	0.434757 (Hartree/Particle)
Thermal correction to Energy=	0.458208
Thermal correction to Enthalpy=	0.459152

Thermal correction to Gibbs Free Energy= 0.381292
 Sum of electronic and zero-point Energies= -890.418060
 Sum of electronic and thermal Energies= -890.394610
 Sum of electronic and thermal Enthalpies= -890.393665
 Sum of electronic and thermal Free Energies= -890.471525

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.982592	0.977624	-0.534921
2	6	0	-3.629545	-0.481785	-0.811332
3	6	0	-2.498807	-1.055302	0.106867
4	6	0	-1.236139	-0.100099	-0.038789
5	6	0	-1.633584	1.330527	0.251744
6	6	0	-2.724896	1.868119	-0.626879
7	6	0	0.015995	-0.607529	0.732473
8	6	0	1.363584	-0.627146	-0.044496
9	6	0	2.366582	0.527425	0.180233
10	6	0	2.702438	0.755162	1.661901
11	6	0	-1.194928	2.085255	1.469647
12	6	0	2.008439	1.856487	-0.460964
13	8	0	-4.850585	-1.215779	-0.705950
14	6	0	-2.165087	-2.471350	-0.409561
15	6	0	-2.976750	-1.147955	1.566917
16	6	0	1.122388	2.069329	-1.432949
17	8	0	3.615616	0.183961	-0.555977
18	6	0	4.408254	-0.850704	-0.204709
19	8	0	4.205314	-1.626679	0.706610
20	6	0	5.609465	-0.913920	-1.127009
21	1	0	-4.434868	1.060591	0.460491
22	1	0	-4.743615	1.295182	-1.258093
23	1	0	-3.255046	-0.543330	-1.849790
24	1	0	-0.996507	-0.156223	-1.116595
25	1	0	-2.976793	2.902492	-0.366076
26	1	0	-2.396130	1.882144	-1.681494
27	1	0	-0.163188	-1.639229	1.044833
28	1	0	0.128958	-0.055663	1.669251
29	1	0	1.176350	-0.721500	-1.120985
30	1	0	1.902644	-1.529868	0.251156
31	1	0	2.941957	-0.181431	2.166131
32	1	0	1.860265	1.234167	2.170281
33	1	0	3.563680	1.427450	1.744441
34	1	0	-1.745075	3.028448	1.560115
35	1	0	-1.352348	1.526675	2.406283
36	1	0	-0.124313	2.340885	1.439535
37	1	0	2.591622	2.698723	-0.087778
38	1	0	-4.704091	-2.100245	-1.073000
39	1	0	-1.388488	-2.962194	0.184412
40	1	0	-1.821682	-2.446841	-1.452268

41	1	0	-3.044253	-3.125844	-0.356290
42	1	0	-2.230509	-1.646697	2.196100
43	1	0	-3.907311	-1.721311	1.622803
44	1	0	-3.169280	-0.160840	1.999036
45	1	0	0.965440	3.066159	-1.836277
46	1	0	0.526139	1.275794	-1.870093
47	1	0	5.282326	-1.015291	-2.166949
48	1	0	6.235307	-1.762792	-0.848575
49	1	0	6.187147	0.013734	-1.057104

TS_{XI-XII}

-330.9032 cm⁻¹

Zero-point correction=	0.435189 (Hartree/Particle)
Thermal correction to Energy=	0.457302
Thermal correction to Enthalpy=	0.458246
Thermal correction to Gibbs Free Energy=	0.385119
Sum of electronic and zero-point Energies=	-890.410288
Sum of electronic and thermal Energies=	-890.388175
Sum of electronic and thermal Enthalpies=	-890.387231
Sum of electronic and thermal Free Energies=	-890.460358

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.669684	1.175576	-0.707552
2	6	0	-3.571364	-0.340980	-0.861303
3	6	0	-2.535488	-1.021434	0.096435
4	6	0	-1.148657	-0.266080	-0.083811
5	6	0	-1.296548	1.243914	0.070183
6	6	0	-2.288369	1.833688	-0.903202
7	6	0	0.018436	-0.895836	0.722150
8	6	0	1.418442	-0.825482	0.056574
9	6	0	2.318317	0.378412	0.417848
10	6	0	2.794981	0.342156	1.876587
11	6	0	-1.238004	1.919183	1.417216
12	6	0	1.684150	1.715872	0.120112
13	8	0	-4.896314	-0.845518	-0.690702
14	6	0	-2.392858	-2.491382	-0.361308
15	6	0	-3.043772	-1.014716	1.549778
16	6	0	0.726647	1.927691	-0.823074
17	8	0	3.511690	0.349087	-0.479772
18	6	0	4.409658	-0.656172	-0.459956
19	8	0	4.360852	-1.645360	0.243461
20	6	0	5.517341	-0.377852	-1.457683
21	1	0	-4.073853	1.418504	0.282497
22	1	0	-4.390387	1.553157	-1.442701

23	1	0	-3.231594	-0.546594	-1.892984
24	1	0	-0.909951	-0.434959	-1.147870
25	1	0	-2.368159	2.920643	-0.778209
26	1	0	-1.960784	1.654033	-1.938987
27	1	0	-0.195159	-1.957990	0.866484
28	1	0	0.056380	-0.476129	1.732732
29	1	0	1.303353	-0.850604	-1.034421
30	1	0	1.981696	-1.723447	0.321510
31	1	0	3.279619	-0.605740	2.113559
32	1	0	1.945454	0.486709	2.552458
33	1	0	3.504275	1.157851	2.056326
34	1	0	-1.061789	2.995018	1.293847
35	1	0	-2.180090	1.819027	1.977688
36	1	0	-0.439987	1.529647	2.055122
37	1	0	1.975094	2.536403	0.773777
38	1	0	-4.907939	-1.770979	-0.977071
39	1	0	-1.759597	-3.079405	0.309202
40	1	0	-1.969343	-2.560389	-1.371443
41	1	0	-3.369070	-2.993020	-0.368259
42	1	0	-2.316593	-1.485507	2.221076
43	1	0	-3.982824	-1.571779	1.621142
44	1	0	-3.239671	-0.006966	1.924151
45	1	0	0.378106	2.938070	-1.020551
46	1	0	0.544402	1.210131	-1.617068
47	1	0	5.098346	-0.228682	-2.458031
48	1	0	6.216611	-1.215030	-1.466020
49	1	0	6.044256	0.543025	-1.185813

TS_{XI-XIII}

-360.3903 cm⁻¹

Zero-point correction=	0.435317 (Hartree/Particle)
Thermal correction to Energy=	0.457122
Thermal correction to Enthalpy=	0.458066
Thermal correction to Gibbs Free Energy=	0.386653
Sum of electronic and zero-point Energies=	-890.409126
Sum of electronic and thermal Energies=	-890.387321
Sum of electronic and thermal Enthalpies=	-890.386377
Sum of electronic and thermal Free Energies=	-890.457790

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.233059	1.460084	-0.635875
2	6	0	-3.436457	-0.029537	-0.919304
3	6	0	-2.609149	-0.981656	0.008647
4	6	0	-1.106497	-0.494688	-0.066747

5	6	0	-0.953701	0.982946	0.255902
6	6	0	-1.740796	1.850126	-0.702433
7	6	0	-0.074315	-1.366926	0.669694
8	6	0	1.344453	-1.198352	0.099419
9	6	0	1.998025	0.192470	0.242417
10	6	0	2.401082	0.516157	1.684184
11	6	0	-0.978559	1.489431	1.680262
12	6	0	1.187575	1.299333	-0.442480
13	8	0	-4.842971	-0.260156	-0.838398
14	6	0	-2.719565	-2.409945	-0.569901
15	6	0	-3.177982	-0.998506	1.439469
16	6	0	1.451820	2.632002	-0.243209
17	8	0	3.226891	0.182179	-0.605704
18	6	0	4.263567	-0.650015	-0.379105
19	8	0	4.342566	-1.469680	0.513540
20	6	0	5.345237	-0.416499	-1.415941
21	1	0	-3.651266	1.699631	0.349316
22	1	0	-3.815341	2.032905	-1.367342
23	1	0	-3.092745	-0.219601	-1.952501
24	1	0	-0.863719	-0.589897	-1.139200
25	1	0	-1.617819	2.914489	-0.469072
26	1	0	-1.385237	1.705395	-1.733171
27	1	0	-0.332092	-2.426054	0.565860
28	1	0	-0.082979	-1.165360	1.747399
29	1	0	1.314355	-1.433736	-0.973675
30	1	0	2.012327	-1.928341	0.562377
31	1	0	2.982149	-0.305620	2.104311
32	1	0	1.518383	0.681306	2.305129
33	1	0	3.014910	1.420808	1.720570
34	1	0	-0.332218	2.371155	1.778482
35	1	0	-1.988516	1.813287	1.972437
36	1	0	-0.657755	0.748710	2.417330
37	1	0	0.830424	1.009550	-1.429844
38	1	0	-5.026015	-1.143587	-1.191833
39	1	0	-2.228854	-3.152224	0.066834
40	1	0	-2.274500	-2.476050	-1.570914
41	1	0	-3.769548	-2.721557	-0.645197
42	1	0	-2.590938	-1.662921	2.084010
43	1	0	-4.209719	-1.362891	1.427850
44	1	0	-3.191613	-0.009927	1.903590
45	1	0	1.046200	3.384207	-0.913311
46	1	0	1.995600	2.999466	0.620812
47	1	0	4.951804	-0.608858	-2.419720
48	1	0	6.188310	-1.078938	-1.215250
49	1	0	5.674467	0.627341	-1.390763

TS_{XI-XIV}

-392.7936 cm⁻¹

Zero-point correction= 0.435022 (Hartree/Particle)
 Thermal correction to Energy= 0.456889
 Thermal correction to Enthalpy= 0.457833
 Thermal correction to Gibbs Free Energy= 0.386277
 Sum of electronic and zero-point Energies= -890.406854
 Sum of electronic and thermal Energies= -890.384987
 Sum of electronic and thermal Enthalpies= -890.384043
 Sum of electronic and thermal Free Energies= -890.455599

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.262454	1.556119	-0.200146
2	6	0	-3.445135	0.170495	-0.819790
3	6	0	-2.581349	-0.950124	-0.150009
4	6	0	-1.088421	-0.431882	-0.135070
5	6	0	-0.945991	0.943428	0.503417
6	6	0	-1.779656	1.982174	-0.215947
7	6	0	-0.041522	-1.434732	0.384863
8	6	0	1.378892	-1.131148	-0.120922
9	6	0	1.997823	0.206636	0.333651
10	6	0	2.332784	0.246784	1.828589
11	6	0	-0.967541	1.115715	2.009338
12	6	0	1.174380	1.434754	-0.091773
13	8	0	-4.845371	-0.105723	-0.773707
14	6	0	-2.682310	-2.209292	-1.040416
15	6	0	-3.122201	-1.306943	1.246962
16	6	0	1.139478	1.812139	-1.416164
17	8	0	3.273908	0.385328	-0.418162
18	6	0	4.317520	-0.460123	-0.301946
19	8	0	4.359931	-1.459541	0.387288
20	6	0	5.465388	0.021108	-1.168426
21	1	0	-3.658484	1.549549	0.822659
22	1	0	-3.873767	2.270391	-0.764372
23	1	0	-3.119155	0.233432	-1.873852
24	1	0	-0.851547	-0.276251	-1.200763
25	1	0	-1.667877	2.973235	0.243279
26	1	0	-1.450201	2.072047	-1.259011
27	1	0	-0.286580	-2.445539	0.042680
28	1	0	-0.052514	-1.484688	1.480305
29	1	0	1.365937	-1.134026	-1.219277
30	1	0	2.053962	-1.932686	0.188310
31	1	0	2.976803	-0.590907	2.099107
32	1	0	1.426765	0.202850	2.433616
33	1	0	2.851849	1.181714	2.067462
34	1	0	-0.322583	1.947804	2.322134
35	1	0	-1.976815	1.372915	2.362926
36	1	0	-0.656489	0.226099	2.562110

37	1	0	1.131317	2.231401	0.649183
38	1	0	-5.018316	-0.884256	-1.323932
39	1	0	-2.170748	-3.069935	-0.599123
40	1	0	-2.254021	-2.034574	-2.035619
41	1	0	-3.728749	-2.513655	-1.171879
42	1	0	-2.516567	-2.094177	1.710314
43	1	0	-4.150563	-1.672561	1.167960
44	1	0	-3.137654	-0.453353	1.928657
45	1	0	1.433757	1.139029	-2.215342
46	1	0	0.777291	2.791496	-1.712408
47	1	0	5.140348	0.121284	-2.209007
48	1	0	6.291510	-0.688052	-1.101385
49	1	0	5.797251	1.010266	-0.835346

XII

Zero-point correction=	0.438335 (Hartree/Particle)
Thermal correction to Energy=	0.460110
Thermal correction to Enthalpy=	0.461054
Thermal correction to Gibbs Free Energy=	0.389059
Sum of electronic and zero-point Energies=	-890.444810
Sum of electronic and thermal Energies=	-890.423034
Sum of electronic and thermal Enthalpies=	-890.422090
Sum of electronic and thermal Free Energies=	-890.494085

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.512339	1.278472	-0.691927
2	6	0	-3.516979	-0.233456	-0.880375
3	6	0	-2.507919	-0.988606	0.044213
4	6	0	-1.086307	-0.320831	-0.118793
5	6	0	-1.039179	1.244051	0.009608
6	6	0	-2.112586	1.850405	-0.924818
7	6	0	0.016216	-1.041942	0.700364
8	6	0	1.441896	-0.962034	0.105558
9	6	0	2.271976	0.262424	0.537659
10	6	0	2.836892	0.126110	1.958589
11	6	0	-1.237103	1.803745	1.435257
12	6	0	1.518644	1.548567	0.399230
13	8	0	-4.867790	-0.658100	-0.697004
14	6	0	-2.440970	-2.447505	-0.474985
15	6	0	-3.023962	-1.039484	1.497069
16	6	0	0.354918	1.755983	-0.511515
17	8	0	3.418356	0.430878	-0.416210
18	6	0	4.363071	-0.518403	-0.575250
19	8	0	4.397304	-1.591056	-0.007075
20	6	0	5.400990	-0.052896	-1.578307
21	1	0	-3.882362	1.523817	0.310414

22	1	0	-4.227457	1.716191	-1.398219
23	1	0	-3.207869	-0.436272	-1.921988
24	1	0	-0.835587	-0.504827	-1.176797
25	1	0	-2.126418	2.941730	-0.802667
26	1	0	-1.821366	1.661796	-1.969341
27	1	0	-0.233497	-2.104232	0.762136
28	1	0	0.018604	-0.688961	1.738435
29	1	0	1.375260	-0.962603	-0.989786
30	1	0	2.005821	-1.857280	0.376753
31	1	0	3.451678	-0.770651	2.050950
32	1	0	2.017726	0.069533	2.683575
33	1	0	3.445027	1.002655	2.207797
34	1	0	-1.007617	2.876831	1.439689
35	1	0	-2.262108	1.694433	1.793888
36	1	0	-0.575016	1.330640	2.166332
37	1	0	1.901482	2.397484	0.961009
38	1	0	-4.939118	-1.580400	-0.984890
39	1	0	-1.859782	-3.102696	0.180239
40	1	0	-2.002265	-2.499157	-1.479436
41	1	0	-3.444864	-2.888395	-0.523031
42	1	0	-2.298781	-1.534026	2.152726
43	1	0	-3.958864	-1.606067	1.540391
44	1	0	-3.232468	-0.052697	1.914351
45	1	0	0.250716	2.832654	-0.698942
46	1	0	0.544557	1.287384	-1.489558
47	1	0	4.922148	0.205619	-2.528251
48	1	0	6.136249	-0.843665	-1.733460
49	1	0	5.899668	0.849791	-1.209478

XIII

Zero-point correction= 0.437441 (Hartree/Particle)
 Thermal correction to Energy= 0.459352
 Thermal correction to Enthalpy= 0.460296
 Thermal correction to Gibbs Free Energy= 0.388790
 Sum of electronic and zero-point Energies= -890.439602
 Sum of electronic and thermal Energies= -890.417691
 Sum of electronic and thermal Enthalpies= -890.416746
 Sum of electronic and thermal Free Energies= -890.488253

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.008585	1.596246	-0.514543
2	6	0	-3.345339	0.162775	-0.909503
3	6	0	-2.578989	-0.908526	-0.071624
4	6	0	-1.050340	-0.558968	-0.145850
5	6	0	-0.638618	0.908132	0.234216

6	6	0	-1.504889	1.876073	-0.617916
7	6	0	-0.121696	-1.577270	0.539215
8	6	0	1.331658	-1.397769	0.080990
9	6	0	1.871069	0.018584	0.340941
10	6	0	2.298746	0.229850	1.797489
11	6	0	-0.826147	1.267816	1.730749
12	6	0	0.864592	1.093319	-0.206079
13	8	0	-4.764653	0.041803	-0.813425
14	6	0	-2.813224	-2.278154	-0.754473
15	6	0	-3.148001	-1.004698	1.358869
16	6	0	1.390719	2.479843	-0.010783
17	8	0	3.045951	0.260949	-0.527190
18	6	0	4.155700	-0.505050	-0.473778
19	8	0	4.322748	-1.462413	0.252786
20	6	0	5.185587	0.007137	-1.460886
21	1	0	-3.383184	1.787695	0.497782
22	1	0	-3.561399	2.274644	-1.174864
23	1	0	-3.037156	0.025367	-1.962050
24	1	0	-0.816970	-0.629389	-1.222470
25	1	0	-1.313603	2.915888	-0.328973
26	1	0	-1.200719	1.789313	-1.671395
27	1	0	-0.423901	-2.600697	0.295964
28	1	0	-0.189516	-1.497282	1.630881
29	1	0	1.382716	-1.582417	-1.000868
30	1	0	1.985222	-2.130919	0.559264
31	1	0	3.110125	-0.455792	2.047915
32	1	0	1.468190	0.037175	2.479882
33	1	0	2.634073	1.258909	1.957831
34	1	0	-0.154710	2.086136	2.010450
35	1	0	-1.843841	1.604629	1.941756
36	1	0	-0.622522	0.432491	2.404973
37	1	0	0.867350	0.893704	-1.294773
38	1	0	-5.025190	-0.799050	-1.218233
39	1	0	-2.399075	-3.107286	-0.173187
40	1	0	-2.368404	-2.311186	-1.757074
41	1	0	-3.886414	-2.485085	-0.854387
42	1	0	-2.594027	-1.742285	1.950382
43	1	0	-4.194567	-1.321628	1.320705
44	1	0	-3.120759	-0.056470	1.897705
45	1	0	0.739808	3.325276	0.176839
46	1	0	2.437109	2.684422	-0.205182
47	1	0	4.754787	0.067907	-2.465327
48	1	0	6.048177	-0.660421	-1.462624
49	1	0	5.502588	1.017595	-1.180492

XIV

Zero-point correction= 0.437173 (Hartree/Particle)
Thermal correction to Energy= 0.459179

Thermal correction to Enthalpy= 0.460123
 Thermal correction to Gibbs Free Energy= 0.388473
 Sum of electronic and zero-point Energies= -890.434498
 Sum of electronic and thermal Energies= -890.412491
 Sum of electronic and thermal Enthalpies= -890.411547
 Sum of electronic and thermal Free Energies= -890.483198

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.034374	-1.673911	0.013891
2	6	0	3.360357	-0.385498	-0.735798
3	6	0	2.561517	0.856815	-0.226362
4	6	0	1.036075	0.478947	-0.245442
5	6	0	0.639023	-0.854411	0.474852
6	6	0	1.538454	-1.997518	-0.063133
7	6	0	0.082861	1.618117	0.164938
8	6	0	-1.379474	1.306555	-0.198642
9	6	0	-1.877792	-0.017602	0.407341
10	6	0	-2.233195	0.109297	1.894598
11	6	0	0.796259	-0.835097	2.018227
12	6	0	-0.873555	-1.182187	0.083471
13	8	0	4.775462	-0.215626	-0.648349
14	6	0	2.803795	2.005305	-1.236214
15	6	0	3.087907	1.329793	1.143600
16	6	0	-1.019521	-1.608755	-1.349286
17	8	0	-3.108498	-0.470711	-0.278343
18	6	0	-4.219713	0.288622	-0.358914
19	8	0	-4.350572	1.409929	0.087824
20	6	0	-5.308636	-0.469484	-1.091781
21	1	0	3.384562	-1.587440	1.049261
22	1	0	3.616858	-2.487507	-0.434228
23	1	0	3.075252	-0.535054	-1.793084
24	1	0	0.827241	0.283940	-1.309715
25	1	0	1.322759	-2.926261	0.483468
26	1	0	1.279984	-2.190550	-1.112011
27	1	0	0.358464	2.548369	-0.342144
28	1	0	0.166343	1.828263	1.238153
29	1	0	-1.466359	1.240546	-1.290971
30	1	0	-2.035240	2.121157	0.116321
31	1	0	-3.073965	0.796590	2.008163
32	1	0	-1.401813	0.499249	2.481682
33	1	0	-2.515123	-0.865606	2.306880
34	1	0	0.121016	-1.566042	2.477292
35	1	0	1.808833	-1.113454	2.319548
36	1	0	0.590370	0.135270	2.473497
37	1	0	-1.168446	-2.038058	0.705673
38	1	0	5.032894	0.495749	-1.253699
39	1	0	2.345956	2.944445	-0.911132

40	1	0	2.405883	1.761351	-2.229456
41	1	0	3.876254	2.212325	-1.344707
42	1	0	2.534342	2.209052	1.491557
43	1	0	4.142856	1.607235	1.058872
44	1	0	3.019920	0.563893	1.917690
45	1	0	-1.085434	-0.891843	-2.160044
46	1	0	-1.149295	-2.654556	-1.604401
47	1	0	-4.940625	-0.828131	-2.058126
48	1	0	-6.170657	0.183275	-1.235343
49	1	0	-5.606392	-1.348871	-0.510126