Enhanced stereocontrol in Diels-Alder reactions of chiral dienols

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1. General Experimental Details

NMR spectra were recorded at 298K using a Varian Unity INOVA 500 MHz, Bruker DPX/DRX 400 MHz or a Varian Unity INOVA 300 MHz spectrometer. Residual protio-acetone (δ 2.04 ppm), -benzene (δ 7.15 ppm), -chloroform (δ 7.26 ppm), and -methanol (δ 3.31 ppm) were used as internal references for ¹H NMR spectra measured in these solvents. The ¹³C NMR resonances of acetone (δ 29.8 ppm , 206.8 ppm), benzene (δ 128.1 ppm), chloroform (δ 77.1 ppm) and methanol (δ 49.0 ppm) were used as internal references for ¹³C NMR spectra. Assignment of proton signals was assisted by ¹H-¹H COSY and NOESY experiments when necessary; assignment of carbon signals was assisted by DEPT experiments. IR spectra were recorded on a Perkin–Elmer 1600 F.T.I.R. or Perkin–Elmer Spectrum One spectrometer as neat films on NaCl plates for oils or as KBr pellets for solid products. Low resolution mass spectra were recorded on a Finnigan PolarisQ ion trap mass spectrometer using electron impact (EI) ionisation mode at 40 or 70 eV. High resolution mass spectra were recorded on a VG Autospec mass spectrometer operating at 70 eV. High resolution electrospray ionisation spectra were recorded on a Bruker BioApex FTICR with an Analytica ESI source, operating at 4.7 T. Microanalyses were performed at the Research School of Chemistry, Australian National University. Optical rotations were measured with an Optical Activity Polaar 2001 a Perkin Elmer 241 optical polarimeter. Melting points were measured on a Reichert melting point stage and are uncorrected. HPLC was performed using a Waters 510EF chromatograph pump and Waters U6K injector monitored by an Waters Lambda-Max 481 UV spectrophotometer at $\lambda =$ 254 nm and an Erma ERC-7512 refractive index detector or a Waters 510EF chromatograph pump and Waters U6K injector monitored by an ISCO 226 UV spectrophotometer at $\lambda = 254$ nm and a Waters R403 refractive index detector. GC measurements were recorded on an Agilent 6850 gas chromatograph with a split/splitless capillary inlet and FID detector or GC measurements were recorded on a Hewlett Packard 5890A gas chromatograph with a split/splitless capillary inlet and FID detector. GC data was processed using Hewlett Packard ChemStation software. Analytical TLC was performed with Merck silica gel plates, precoated with silica gel 60 F254 (0.2 mm). Flash chromatography employed Merck Kiesegel 60 (230–400 mesh) silica gel. Reactions were conducted under a positive pressure of dry argon or nitrogen. Diethyl ether, toluene and THF were dried over sodium wire and distilled from sodium benzophenone ketyl. Dichloromethane was distilled from calcium hydride. Commercially available chemicals were purified by standard procedures or used as purchased.

2. Synthetic Procedures

(±)-Methyl (1*S*,2*E*)-1-Methylpenta-2,4-dien-1-yl Maleate (18Z)



Triethylamine (1.707 g, 16.86 mmol, 1.6 equiv), maleic anhydride (2.326 g, 23.72 mmol, 2.25 equiv) and DMAP (128.8 mg, 1.054 mmol, 0.1 equiv) were added to a stirred solution of hexa-3,5-dien-2-ol (**28**)¹ (1.034 g, 10.54 mmol, 1.0 equiv) in dichloromethane (50 mL) at 0 °C. The mixture was stirred at this temperature for 10 min. The solution was allowed to warm to room temperature before being diluted with diethyl ether (200 mL). The mixture was

washed with 2M HCl (100 mL), sat. aq. NaHCO₃ (100 mL), brine (100 mL), dried (Na₂SO₄) and concentrated *in vacuo*. The crude material was diluted with toluene (5 mL) and cooled to -78 °C with stirring. An ethereal solution of diazomethane was added dropwise until TLC confirmed the reaction had gone to completion. Excess diazomethane was removed by bubbling N₂ gas through the solution. The solution was concentrated *in vacuo* and subjected to column chromatography on silica (hexanes/ethyl acetate 80:20) to give maleate **18Z** (1.257 g, 5.979 mmol, 57%) as a colourless oil. $R_f = 0.45$ (hexanes/ethyl acetate 80:20). ¹H NMR (400 MHz, CDCl₃): $\delta = 6.32$ -6.19 (3H, m), 5.67 (1H, dd, J = 14.2, 6.7 Hz), 5.47 (1H, m), 5.22 (1H, m), 5.10 (1H, m), 3.73 (3H, s), 1.35 (3H, d, J = 6.5 Hz). ¹³C NMR (50 MHz, CDCl₃): $\delta = 165.6$ (C), 164.3 (C), 135.9 (CH), 132.6 (CH), 132.0 (CH), 130.0 (CH), 129.4 (CH), 118.7 (CH₂), 71.7 (CH), 52.1 (CH₃), 19.9 (CH₃). IR (neat): v = 2985, 2952 (C-H), 1728 (C=O), 1638 cm⁻¹ (C=C). EIMS (70 eV) *m/z* (%): 210 ([M]⁺, 5), 179 ([M-Ch₃O]⁺, 15), 164 ([M-CH₂O₂]⁺, 60), 150 ([M-C₂H₄O₂]⁺, 35), 105 ([M-C₃H₃O₄]⁺, 100), 79 ([M-Ch₃O]⁺, 95). HRMS: calcd for C₁₁H₁₄O₄ [M]⁺: 210.0892; found: 210.0890.

(±)-Methyl (1S,2E)-1-Methylpenta-2,4-dien-1-yl Fumarate (18E)



A solution of DCC (2.862 g, 13.87 mmol, 1.13 equiv), DMAP (599.9 mg, 4.910 mmol, 0.4 equiv) and diethyl ether (30 mL) was added dropwise to a solution of hexa-3,5-dien-2-ol (**28**)¹ (1.205 g, 12.28 mmol, 1.0 equiv) and (*E*)-3-methoxycarbonylacrylic acid² (1.916 g, 14.73 mmol, 1.2 equiv) in diethyl ether (6mL) at 0 °C. The solution was allowed to warm to room temperature

and stirred for 16 h. The mixture was filtered, washed with a cooled solution of 2M HCl (16 mL), sat. aq. NaHCO₃ (16 mL), brine (16 mL), dried (Na₂SO₄) and concentrated *in vacuo*. The crude residue was subjected to column chromatography on silica (hexanes/ethyl acetate 9:1) to give fumarate **18***E* (1.620 g, 7.706 mmol, 63%) as a colourless oil. $R_f = 0.39$ (hexanes/ethyl acetate 90:10). ¹H NMR (400 MHz, CDCl₃): $\delta = 6.84$ (2H, m), 6.34-6.21 (2H, m), 5.68 (1H, dd, *J* = 14.0, 6.3 Hz), 5.48 (1H, m), 5.28-5.19 (1H, m), 5.13 (1H, s), 3.79 (3H, s), 1.37 (3H, d, *J* = 6.5 Hz). ¹³C

NMR (100 MHz, CDCl₃): $\delta = 165.5$ (C), 164.2 (C), 135.9 (CH), 134.2 (CH), 133.2 (CH), 132.8 (CH), 132.0 (CH), 118.9 (CH₂), 71.8 (CH), 52.3 (CH₃), 20.1 (CH₃). IR (neat): v = 3087, 2983, 2954 (C-H), 1732 (C=O), 1644 cm⁻¹ (C=C). EIMS (70 eV) *m*/*z* (%): 210 ([M]⁺, 20), 113 ([M-C₆H₉O]⁺, 100), 97 ([M-C₅H₅O₃]⁺, 20). HRMS: calcd for C₁₁H₁₅O₄ [M+H]⁺: 211.0970; found: 211.0974.

IMDA Reaction of Maleate 18Z in Toluene at 110 °C



A solution of maleate **18Z** (1.264 g, 6.012 mmol, 1.0 equiv) and BHT (132 mg, 0.601 mmol, 0.1 equiv) in toluene (600 mL) was stirred at 110 °C for 3 h. The reaction mixture was concentrated *in vacuo*, a portion of the residue dissolved in CDCl₃ and ¹H NMR analysis carried out. The residue contained *trans,lk*-IMDA adduct **23Z**, *trans,ul*-IMDA adduct **25Z**, *cis,lk*-IMDA adduct **24Z**,³ and *cis,ul*-IMDA adduct **26Z** (68:19:9:4, respectively). The residue was subjected to chromatography on silica (dichloromethane/diethyl ether 97:3) to give a mixture of the IMDA adduct **25Z**, *cis,lk*-IMDA adduct **25Z**, *trans,ul*-IMDA adduct **25Z** at t_R = 113.5 min, *cis,lk*-IMDA adduct **24Z**,³ at t_R = 116.0 min, and *cis,ul*-IMDA adduct **26Z** at t_R = 158.5 min. The mixture of *trans,lk*-IMDA adduct **25Z** and *trans,ul*-IMDA adduct **23Z** was separated by further HPLC [Alltech Altima C₁₈ column, eluting with water/methanol 60:40, 11.25 mL min⁻¹] to give *trans,ul*-IMDA adduct **25Z** at t_R = 29.6 min and *trans,lk*-IMDA adduct **23Z** at t_R = 34.1 min.

(±)-Methyl (3*S*,3*aR*,7*R*,7*aS*)-3-Methyl-1-oxo-3,3*a*,6,7,7*a*-hexahydro-7-isobenzofuran carboxylate (*trans*,*lk*-23*Z*): white crystalline solid after recrystallisation from hexanes/TBME 80:20. mp 87-89 °C. ¹H NMR (400 MHz, C_6D_6): $\delta = 5.33-5.26$ (2H, m), 3.55 (1H, dq, J = 10.3, 6.0 Hz), 3.22 (3H, s), 3.01 (1H, dd, J = 8.1, 3.5 Hz), 2.74 (1H, m), 2.36 (1H, m), 1.95-1.86 (1H, m), 1.81 (1H, dd, J = 13.5, 3.7 Hz), 1.46 (3H, d, J = 6.1 Hz). ¹³C NMR (100 MHz, C_6D_6): $\delta = 5.33-5.26$ (2H, m), 3.55 (1H, dq, J = 10.3, 6.0 Hz), 3.22 (3H, s), 3.01 (1H, dd, J = 8.1, 3.5 Hz), 2.74 (1H, m), 2.36 (1H, m), 1.95-1.86 (1H, m), 1.81 (1H, dd, J = 13.5, 3.7 Hz), 1.46 (3H, d, J = 6.1 Hz). ¹³C NMR (100 MHz, C_6D_6): $\delta = 5.33-5.26$ (2H, m), 3.55 (1H, m), 1.95-1.86 (1H, m), 1.81 (1H, dd, J = 13.5, 3.7 Hz), 1.46 (3H, d, J = 6.1 Hz). ¹³C NMR (100 MHz, C_6D_6): $\delta = 5.33-5.26$ (2H, m), 3.55 (1H, m), 5.5 (

172.9 (C), 172.2 (C), 128.3 (CH), 124.0 (CH), 78.9 (CH), 51.6 (CH₃), 45.4 (CH), 43.2 (CH), 35.8 (CH), 28.9 (CH₂), 18.2 (CH₃). IR (KBr): v = 2956 (C-H), 1789, 1732 cm⁻¹ (C=O). EIMS (70 eV): m/z (%) = 211 ([M+1]⁺, 2), 210 ([M]⁺, 2), 179 ([M-CH₃O]⁺, 20), 164 ([M-CH₂O₂]⁺, 85), 150 ([M-C₂H₄O₂]⁺, 50), 105 ([M-C₃H₅O₄]⁺, 100), 91 ([M-C₄H₇O₄]⁺, 50), 79 ([M-C₅H₇O₄]⁺, 75). Anal. calcd (%) for C₁₁H₁₄O₄ (210.1): C 62.85, H 6.71; found C 63.09, H 6.78.

(±)-Methyl (3*S*,3*a*,7*S*,7*a*)-3-Methyl-1-oxo-3,3*a*,6,7,7*a*-hexahydro-7-isobenzofuran carboxylate (*cis*,*lk*-24Z):³ white crystalline solid after recrystallisation from hexanes/ethyl acetate 60:40. mp 86-88 °C (lit. 153 °C after recrystallisation from water).^{3 1}H NMR (400 MHz, CDCl₃): δ = 5.85 (1H, m), 5.61 (1H, m), 4.36 (1H, dq, *J* = 6.5, 1.0 Hz), 3.75 (1H, s), 3.59 (1H, dd, *J* = 7.8, 4.2 Hz), 2.82 (1H, m), 2.75 (1H, ddd, *J* = 9.6, 6.9, 4.1 Hz), 2.38-2.25 (2H, m), 1.41 (3H, d, *J* = 6.5 Hz). ¹³C NMR (100 MHz, CDCl₃): δ = 175.7 (C), 172.8 (C), 128.4 (CH), 125.8 (CH), 80.6 (CH), 52.1 (CH₃), 42.2 (CH), 38.8 (CH), 36.7 (CH), 22.9 (CH₂), 20.2 (CH₃). IR (KBr): v = 3028, 2979, 2947, 2907 (C-H), 1766, 1738 cm⁻¹ (C=O). EIMS (70 eV): *m/z* (%) = 210 ([M]⁺, 5), 178 ([M-CH₄O]⁺, 10), 150 ([M-C₂H₄O₂]⁺, 10), 138 ([M-C₃H₄O₂]⁺, 20), 79 ([M-C₃H₇O₄]⁺, 100). Anal. calcd (%) for C₁₁H₁₄O₄(210.1): C 62.85, H 6.71; found C 62.78, H 6.85.

(±)-Methyl (3*S*,3*aS*,7*S*,7*aR*)-3-Methyl-1-oxo-3,3*a*,6,7,7*a*-hexahydro-7-isobenzofuran carboxylate (*trans*,*ul*-25*Z*): white crystalline solid after recrystallisation from hexanes/ethyl acetate 50:50. mp 122-124 °C. ¹H NMR (400 MHz, C₆D₆): $\delta = 5.32-5.27$ (1H, m), 5.23 (1H, m), 4.23 (1H, dq, *J* = 13.8, 6.9 Hz), 3.31-3.24 (1H, m), 3.24 (3H, s), 3.04 (1H, dd, *J* = 8.4, 3.9 Hz), 2.39 (1H, m), 2.02 (1H, dd, *J* = 14.1, 3.7 Hz), 1.91 (1H, m), 0.75 (3H, d, *J* = 6.7 Hz). ¹³C NMR (100 MHz, C₆D₆): $\delta = 173.2$ (C), 172.7 (C), 128.6 (CH), 124.7 (CH), 76.2 (CH), 51.6 (CH₃), 40.6 (CH), 38.1 (CH), 36.0 (CH), 29.0 (CH₂), 14.4 (CH₃). IR (KBr): v = 2955 (C-H), 1776, 1737 cm⁻¹ (C=O). EIMS (70 eV): *m*/*z* (%) = 210 ([M]⁺, 5), 178 ([M-CH₄O]⁺, 20), 150 ([M-C₂H₄O₂]⁺, 30), 105 ([M-C₃H₅O₄]⁺, 50), 79 ([M-C₃H₇O₄]⁺, 100). Anal. calcd (%) for C₁₁H₁₄O₄ (210.1): C 62.85, H 6.71; found C 62.93, H 6.93.

(±)-Methyl (3*S*,3a*S*,7*R*,7a*S*)-3-Methyl-1-oxo-3,3a,6,7,7a-hexahydro-7-isobenzofuran carboxylate (*cis*,*ul*-26*Z*): white crystalline solid after recrystallisation from hexanes/ethyl acetate 70:30. mp 110-111 °C. ¹H NMR (400 MHz, CDCl₃): $\delta = 5.98$ (1H, m), 5.60 (1H, m), 4.66 (1H, m), 3.76 (3H, s), 3.63 (1H, dd, J = 7.3, 7.9 Hz), 3.09 (1H, m), 2.73 (1H, ddd, J = 10.8, 6.7, 3.9 Hz), 2.43-2.32 (2H, m), 1.38 (3H, d, J = 6.5 Hz). ¹³C NMR (100 MHz, CDCl₃): $\delta = 175.7$ (C),

172.8 (C), 130.8 (CH), 121.9 (CH), 78.4 (CH), 52.2 (CH₃), 42.6 (CH), 40.8 (CH), 37.0 (CH), 22.9 (CH₂), 15.9 (CH₃). IR (KBr): v = 2950 (C-H), 1766, 1732 cm⁻¹ (C=O). EIMS (70 eV): *m/z* (%) = 210 ([M]⁺, 15), 178 ([M-CH₄O]⁺, 25), 150 ([M-C₂H₄O₂]⁺, 35), 138 ([M-C₃H₄O₂]⁺, 50), 79 ([M-C₅H₇O₄]⁺, 100). Anal. calcd (%) for C₁₁H₁₄O₄ (210.1): C 62.85, H 6.71; found C 62.69, H 6.71.

IMDA Reaction of Fumarate 18E in Toluene at 110 °C



A solution of fumarate **18***E* (1.335 g, 6.350 mmol, 1.0 equiv) and BHT (139.9 mg, 0.635 mmol, 0.1 equiv) in toluene (635 mL) was stirred at 110 °C for 57 h. The reaction mixture was concentrated *in vacuo*, a portion of the residue dissolved in CDCl₃ and ¹H NMR analysis carried out. The residue contained *trans*,*lk*-IMDA adduct **23***E*, *trans*,*ul*-IMDA adduct **25***E*, *cis*,*lk*-IMDA adduct **24***E*, and *cis*,*ul*-IMDA adduct **26***E* (56:16:12:16, respectively). The residue was subjected to chromatography on silica (dichloromethane) to give a mixture of the IMDA adduct **25***E*, *cis*,*lk*-IMDA adduct **24***E*, and *cis*,*ul*-IMDA adduct **26***E* (53:13:17:17)]. The mixture of IMDA adducts was separated by HPLC [Whatman Partisil column, eluting with hexanes/ethyl acetate 83:17, 13.5 mL min⁻¹] to give *cis*,*lk*-IMDA adduct **24***E* at t_R = 58.2 min, *trans*,*lk*-IMDA adduct **25***E* at t_R = 74.2 min.

(±)-Methyl (3S,3aR,7S,7aS)-3-Methyl-1-oxo-3,3a,6,7,7a-hexahydro-7-isobenzofuran carboxylate (*trans*,*lk*-**23***E*): white crystalline solid after recrystallisation from hexanes/dichloromethane 50:50. mp 135-137 °C. ¹H NMR (400 MHz, CDCl₃/CD₃OD 75:25): $\delta =$ 5.86 (1H, m), 5.78 (1H, m), 4.28 (1H, dq, J = 10.4, 6.2 Hz), 3.75 (3H, s), 2.84 (1H, ddd, J = 11.4, 10.0 Hz), 2.74 (1H, dd, J = 13.0, 11.5 Hz), 2.56 (1H, m), 2.45 (1H, m), 2.36-2.25 (1H, m), 1.46 (3H, d, J = 6.1 Hz). ¹³C NMR (50 MHz, CDCl₃/CD₃OD 75:25): $\delta = 175.7$ (C), 175.3 (C), 129.5 (CH), 123.8 (CH), 81.1 (CH), 52.5 (CH₃), 47.9 (CH), 46.4 (CH), 40.4 (CH), 31.1 (CH₂), 18.4 (CH₃). IR (KBr): v = 2975 (C-H), 1789, 1738 cm⁻¹ (C=O). EIMS (70 eV): m/z (%) = 210 ([M]⁺, 15), 178 ([M-CH₄O]⁺, 30), 165 ([M-CHO₂]⁺, 75), 151 ([M-C₂H₃O₂]⁺, 90), 105 ([M-C₃H₄O₂]⁺, 50), 79 ([M-C₅H₇O₄]⁺, 100). Anal. calcd (%) for C₁₁H₁₄O₄ (210.1): C 62.85, H 6.71; found C 63.04, H 6.89.

(±)-Methyl (3*R*,3*aS*,7*S*,7*aS*)-3-Methyl-1-oxo-3,3*a*,6,7,7*a*-hexahydro-7-isobenzofuran carboxylate (*cis*,*lk*-24*E*): colourless oil. ¹H NMR (400 MHz, CDCl₃): $\delta = 5.79$ (1H, m), 5.61 (1H, m), 4.33 (1H, dq, *J* = 6.7, 2.4 Hz), 3.69 (3H, s), 3.32 (dd, *J* = 8.0, 4.3 Hz, 1H), 3.10 (ddd, *J* = 6.9, 3.7, 3.7 Hz, 1H), 2.81 (m, 1H), 2.44 (m, 1H), 2.23 (m, 1H), 1.40 (d, *J* = 6.5 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): $\delta = 176.7$ (C), 173.7 (C), 127.2 (CH), 125.5 (CH), 81.0 (CH), 52.3 (CH₃), 39.9 (CH), 38.9 (CH), 36.7 (CH), 23.6 (CH₂), 20.4 (CH₃). IR (neat): v = 3028, 2953, 2849 (C-H), 1767, 1731 (C=O), 1651 cm⁻¹ (C=C). EIMS (70 eV): *m/z* (%) = 210 ([M]⁺, 35), 179 ([M-CH₃O]⁺, 25), 165 ([M-CHO₂]⁺, 30), 151 ([M-C₂H₃O₂]⁺, 30), 138 ([M-C₃H₄O₂]⁺, 100), 107 ([M-C₄H₇O₃]⁺, 45), 79 ([M-C₅H₇O₄]⁺, 95). Anal. calcd (%) for C₁₁H₁₄O₄ (210.1): C 62.85, H 6.71; found C 62.88, H 6.78.

(±)-Methyl (3*R*,3*aR*,7*S*,7*aS*)-3-Methyl-1-oxo-3,3*a*,6,7,7*a*-hexahydro-7-isobenzofuran carboxylate (*trans*,*ul*-25*E*): white crystalline solid after recrystallisation from hexanes/ethyl acetate 70:30. mp 112-113 °C. ¹H NMR (400 MHz, (CD₃)₂CO): $\delta = 5.90$ (1H, m), 5.79 (1H, m), 4.83 (1H, m), 3.69 (3H, s), 3.11 (1H, m), 2.85 (1H, ddd, *J* = 11.4, 10.2, 6.8 Hz), 2.74 (1H, dd, *J* = 13.5, 11.4 Hz), 2.55 (1H, m), 2.35-2.24 (1H, m), 1.28 (3H, d, *J* = 6.7 Hz). ¹³C NMR (50 MHz, (CD₃)₂CO): $\delta = 174.7$ (C), 174.5 (C), 129.7 (CH), 125.4 (CH), 78.1 (CH), 52.2 (CH₃), 42.9 (CH), 41.7 (CH), 40.8 (CH), 31.4 (CH₂), 14.8 (CH₃). IR (KBr): v = 3044, 2993, 2977, 2952, 2916 (KBr), 1769, 1726 (C=O), 1633 cm⁻¹ (C=C). EIMS (70 eV): *m/z* (%) = 210 ([M]⁺, 20), 178 ([M-CH₄O]⁺, 10), 165 ([M-CHO₂]⁺, 35), 151 ([M-C₂H₃O₂]⁺, 55), 79 ([M-C₅H₇O₄]⁺, 100). Anal. calcd (%) for C₁₁H₁₄O₄(210.1): C 62.85, H 6.71; found C 62.97, H 6.78.

(±)-Methyl (3*S*,3a*S*,7*R*,7a*S*)-3-Methyl-1-oxo-3,3a,6,7,7a-hexahydro-7-isobenzofuran carboxylate (*cis*,*ul*-26*E*): colourless oil. ¹H NMR (400 MHz, CDCl₃): $\delta = 5.86$ (1H, m), 5.54 (1H, m), 4.64 (1H, m), 3.65 (3H, s), 3.35 (1H, m), 3.16 (1H, m), 3.08 (1H, m), 2.46 (1H, m), 2.23 (1H, m), 1.32 (3H, d, J = 6.6 Hz). ¹³C NMR (100 MHz, CDCl₃): $\delta = 176.8$ (C), 173.6 (C), 129.2 (CH), 122.2 (CH), 78.5 (CH), 52.2 (CH₃), 41.9 (CH), 37.5 (CH), 36.5 (CH), 22.9 (CH₂), 15.9 (CH₃). IR (neat): v = 3032, 2983, 2953, 2852 (C-H), 1767, 1732 cm⁻¹ (C=O). EIMS (70 eV): *m/z* (%) = 211 ([M+1]⁺, 5), 210 ([M]⁺, 2), 179 ([M-CH₃O]⁺, 10), 165 ([M-CHO₂]⁺, 30), 151 ([M-CHO₂]⁺

 $C_2H_3O_2]^+$, 15), 79 ([M- $C_5H_7O_4$]⁺, 100). Anal. calcd (%) for $C_{11}H_{14}O_4$ (210.1): C 62.85, H 6.71; found C 62.63, H 6.57

Methyl (1*S*,2*E*)-3-Bromo-1-methylpenta-2,4-dien-1-yl Maleate (27*Z*)



Triethylamine (52 μ L, 0.37 mmol, 1.6 equiv), maleic anhydride (64 mg, 0.65 mmol, 2.8 equiv) and DMAP (3 mg, 0.03 mmol, 0.12 equiv) were added to a stirred solution of alcohol **29** (41 mg, 0.23 mmol, 1.0 equiv) in dichloromethane (2 mL) at 0 °C. The mixture was stirred at this temperature for 2.5 h. The solution was allowed to warm to room temperature before being diluted with diethyl ether (20

mL). The mixture was washed with 2M HCl (10 mL), sat. aq. NaHCO₃ (10 mL), brine (10 mL), dried (Na₂SO₄) and concentrated *in vacuo*. The crude material was diluted with tetrahydrofuran (5 mL) and cooled to -78 °C with stirring. An ethereal solution of diazomethane was added dropwise until tlc confirmed the reaction had gone to completion. Excess diazomethane was removed by bubbling N₂ gas through the solution. The solution was concentrated *in vacuo* and subjected to column chromatography on silica (hexanes/ethyl acetate 90:10) to give maleate **27Z** (27 mg, 0.09 mmol, 40%) as a colourless oil. [α] = +37.4 (c = 0.42, chloroform). ¹H NMR (300 MHz, C₆D₆): δ 6.03 (1H, dq, *J* = 7.7, 6.3 Hz), 5.90 (1H, ddd, *J* = 16.3, 10.3, 0.8 Hz), 5.79 (1H, dd, *J* = 7.7, 0.7 Hz), 5.68 (2H, d, *J* = 3.2 Hz), 5.58 (1H, dt, *J* = 16.3, 0.7 Hz), 4.94 (1H, d, *J* = 10.5 Hz), 3.31 (3H, s), 1.23 (3H, d, *J* = 6.5 Hz) ppm. ¹³C NMR (125 MHz, C₆D₆): δ 164.9, 163.7, 134.9, 133.4, 129.9, 129.0, 126.2, 119.5, 71.4, 51.1, 18.8 ppm. IR (thin film): ν 2918, 1788, 1731 cm⁻¹. EIMS (70 eV) *m/z* (%): 290 (2), 288 (2), 175 (15), 113 (100). HRMS: calcd for C₁₁H₁₃O₄⁷⁹Br [M]⁺: 287.9997; found: 288.0003.

Methyl (1S,2E)-3-Bromo-1-methylpenta-2,4-dien-1-yl Fumarate (27E)



To a stirred solution of alcohol **29** (54 mg, 0.31 mmol, 1.0 equiv) in diethyl ether (1.5 mL) at room temperature was added (*E*)-3-methoxycarbonylacrylic acid² (72 mg, 0.5 mmol, 1.8 equiv), DCC (127 mg, 0.61 mmol, 2.0 equiv) and DMAP (5.6 mg, 0.05 mmol, 0.15 equiv).

27E Stirring was continued for 3 h. The reaction mixture was filtered through celite and concentrated *in vacuo*. The crude residue was subjected to column chromatography on silica (hexanes/ethyl acetate 9:1) to give fumarate 27E (55.5 mg, 0.19 mmol, 63%) as a colourless oil. [α] = + 94.0 (c = 0.92, chloroform). ¹H NMR (300 MHz, CDCl₃): δ 6.85 (2H, s), 6.29 (1H, dd, *J* = 16.3, 10.4 Hz), 6.03 (1H, d, *J* = 7.9 Hz), 5.88 (1H, dq, *J* = 6.6, 6.3 Hz), 5.68

(1H, d, J = 16.3 Hz), 5.32 (1H, d, 10.5 Hz), 3.80 (3H, s), 1.42 (3H, d, J = 6.4 Hz) ppm. ¹³C NMR (75 MHz, CDCl₃): δ 165.5, 164.0, 134.9, 133.8, 133.6, 132.6, 126.8, 120.6, 72.0, 52.4, 19.5 ppm. IR (thin film): v 2953, 2849, 1723, 1645 cm⁻¹. EIMS (70 eV) m/z (%): 290 (18), 288 (20), 209 (25), 159 (50), 113 (95), 85 (80), 79 (90), 59 (75), 53 (100). HRMS: calcd for C₁₁H₁₃O₄⁷⁹Br [M]⁺: 287.9997; found: 288.0003.

IMDA Reaction of Maleate 27Z in Toluene at 110 °C



A solution of maleate **27Z** (12.2 mg, 42 μ mol, 1.0 equiv) and BHT (1 mg, 4.5 μ mol, 0.1 equiv) in toluene (4.2 mL) was stirred at 110 °C for 40 min. The reaction mixture was concentrated *in vacuo*. After column chromatography cycloadduct **30Z** (10.3 mg, 35 μ mol, 83%) was obtained as a single isomer.

Methyl (3S,3aR,7R,7aS)-4-Bromo-3-methyl-1-oxo-3,3a,6,7,7a-hexahydro-7-isobenzo furancarboxylate (**30**Z). White crystalline solid after recrystallistaion from hexane/dichloromethane. mp 86-88 °C $[\alpha] = -42.0$ (c = 0.82, chloroform). ¹H NMR (500 MHz, CDCl₃): δ 6.05 (1H, m), 4.36 (1H, dq, J = 9.7, 5.9 Hz), 3.74 (3H, s), 3.35 (1H, dd, J = 8.3, 3.8 Hz), 3.11 (1H, m), 2.77 (1H, m), 2.71 (1H, dd, J = 13.2, 3.5 Hz), 2.58 (1H, ddt, J = 19.1, 8.0, 3.7 Hz), 1.69 (1H, d, J = 6.1 Hz) ppm. ¹³C NMR (75 MHz, CDCl₃): δ 172.3, 172.0, 130.0, 116.4, 79.8, 52.6, 47.3, 47.3, 35.0, 31.2, 19.9 ppm. IR (thin film): v 2920, 1787, 1732 cm⁻¹. EIMS (70 eV) m/z (%): 290 (2), 244 (30), 228 (15), 105 (100), 77 (95). HRMS: calcd for $C_{11}H_{14}O_4^{81}Br$ [M+H]⁺: 289.0075; found: 289.0082.

IMDA Reaction of Fumarate 27E in Toluene at 110 °C



A solution of fumarate 27*E* (14.6 mg, 50 μ mol, 1.0 equiv) and BHT (1 mg, 4.5 μ mol, 0.1 equiv) in toluene (5 mL) was stirred at 110 °C for 9 h 50 min. The reaction mixture was concentrated *in vacuo*. After column chromatography cycloadduct **30***E* (10.4 mg, 36 μ mol, 71%) was obtained as a single isomer.

Methyl (3*S*,3*aR*,7*S*,7*aS*)-4-Bromo-3-methyl-1-oxo-3,3*a*,6,7,7*a*-hexahydro-7-isobenzofuran carboxylate (30*E*) White crystalline solid after recrystallisation from hepatane/dichloromethane. mp 181-182 °C. [α] = + 88.7 (c = 0.94, chloroform). ¹H NMR (500 MHz, CDCl₃): δ 6.09 (1H, q, J = 3.4 Hz), 4.41 (1H, dq, J = 10.0, 6.2 Hz), 3.78 (3H,s), 3.00 (1H, dd, J = 12.5, 11.7 Hz), 2.77 (1H, ddd, J = 11.7, 10.3, 7.0 Hz), 2.66 (1H, m), 2.53 (1H, dddd, J = 18.4, 6.8, 4.5, 2.7 Hz) 2.44 (1H, ddt, J = 18.4, 10.1, 3.7 Hz), 1.66 (3H, d, J = 6.2 Hz) ppm. ¹³C NMR (125 MHz, CDCl₃): δ 173.2, 172.0, 130.3, 115.6, 79.7, 52.5, 50.8, 47.6, 39.0, 32.7, 19.8 ppm. IR (thin film): v 2990, 2937, 1779, 1743 cm⁻¹. EIMS (70 eV) m/z (%): 288 (20), 230 (25), 213 (60), 105 (98), 77 (100). HRMS: calcd for C₁₁H₁₄O₄⁸¹Br [M+H]⁺: 289.0075; found: 289.0081.

Reductive Debromination of Methyl (3*S*,3a*R*,7*R*,7a*S*)-4-Bromo-3-methyl-1-oxo-3,3a,6,7,7ahexahydro-7-isobenzofurancarboxylate (30*Z*)



To a solution of cycloadduct **30Z** (10 mg, 30 μ mol, 1.0 equiv) in toluene (500 μ L) at room temperature was added tributyltin hydride (27 μ L, 0.10 mmol, 2.9 equiv) and AIBN (1.0 mg, 6 μ mol, 0.2 equiv) before warming to 80 °C for 3 h 50 min. The reaction mixture was then

concentrated *in vacuo*. The crude product was passed through a short pad of silica (dichloromethane) to give **23Z** (3.8 mg, 18 mmol, 59%), spectroscopically identical to the major product obtained upon IMDA reaction of **18Z**.

Reductive debromination of Methyl (3*S*,3*aR*,7*S*,7*aS*)-4-Bromo-3-methyl-1-oxo-3,3*a*,6,7,7*a*hexahydro-7-isobenzofurancarboxylate (30*E*)



To a solution of cycloadduct **30***E* (10 mg, 30 μ mol, 1.0 equiv) in toluene (500 μ L) at room temperature was added tributyltin hydride (27 μ L, 0.10 mmol, 2.9 equiv) and AIBN (1.0 mg, 6 μ mol, 0.2 equiv) before

warming to 80 °C for 2 h 40 min. The reaction

mixture was then concentrated *in vacuo*. The crude product was passed through a short pad of silica (dichloromethane) to give 23E (3.8 mg, 18 mmol, 59%), spectroscopically identical to the major product obtained upon IMDA reaction of 18E.

"Mix and Heat" Procedure for Hexa-3,5-dien-2-ol (28)



Maleic anhydride (156 mg, 1.59 mmol, 1.0 equiv) and BHT (35 mg, 0.16 mmol, 0.1 equiv) were added to a stirred solution of hexa-3,5-dien-2-ol 28 (156 mg, 1.59 mmol, 1.0 equiv) in toluene (3.2 mL) at RT. The reaction mixture was stirred at 110 °C for 2 h. After diazomethane treatment, ¹H NMR analysis of the crude product revealed four adducts 23Z, 25Z, 24Z and 26Z in 9:2:56:33 ratio. The residue was subjected chromatography silica а to on (dichloromethane/diethyl ether 97:3) to give a mixture of the four adducts (236 mg, 1.13 mmol, 71%; 23Z, 25Z, 24Z and 26Z = 10:1:57:32) eluting at $R_f = 0.24$. The product identities were determined by comparison of the GC and ¹H NMR spectra of the mixture to those of previously isolated and characterised compounds.

"Mix and Heat" Procedure for (S,Z)-4-bromohexa-3,5-dien-2-ol (29)



To a solution of **29**⁴ (22 mg, 0.13 mmol, 1.0 equiv) in toluene (1mL) was added maleic anhydride (18 mg, 0.18 mmol, 1.5 equiv). The mixture was heated at reflux for 5 h 30 min then concentrated *in vacuo*. The crude material was diluted with tetrahydrofuran (5 mL) and cooled to -78 °C with stirring. An ethereal solution of diazomethane was added dropwise until tlc confirmed the reaction had gone to completion. Excess diazomethane was removed by bubbling N₂ gas through the solution. The solution was concentrated *in vacuo* and subjected to column chromatography on silica (hexanes/ethyl acetate 88:12) to give a mixture of **30Z** and **31Z** 13:87 (21mg, 0.08 mmol, 58%).

"Mix and Heat" Procedure for ((*S*,*Z*)-4-bromohexa-3,5-dien-2-yloxy)(*tert*-butyl) dimethyl silane (35)



To a solution of 35^4 (30 mg, 0.10 mmol, 1.0 equiv) in toluene (1 mL) was added maleic anhydride (11 mg, 0.11 mmol, 1.1 equiv). The mixture was heated at reflux for 74h then concentrated *in vacuo*. The crude material was dissolved in

dichloromethane (2 mL) and trifluoroacetic acid (250 μ L) was added the reaction mixture was stirred at RT for 18h then concentrated *in vacuo*. The crude material was diluted with tetrahydrofuran (5 mL) and cooled to -78 °C with stirring. An ethereal solution of diazomethane was added dropwise until tlc confirmed the reaction had gone to completion. Excess diazomethane was removed by bubbling N₂ gas through the solution. The solution was concentrated *in vacuo* and subjected to column chromatography on silica (hexanes/ethyl acetate 88:12) to give **31Z** (17 mg, 0.06 mmol, 58%). [α] = +64.6 (c = 1.4, chloroform). ¹H NMR (500 MHz, CDCl₃): δ 6.25 (1H, m), 4.84 (1H, q, *J* = 6.8 Hz), 3.80 (3H,s), 3.74 (1H, ddd, *J* = 8.3, 4.4, 1.0 Hz), 3.07 (1H, dd, *J* = 8.3, 1.5 Hz), 2.83 (1H, m), 2.50-2.35 (3H, m), 1.48 (3H, d, *J* = 6.8 Hz) ppm. ¹³C NMR (125 MHz, CDCl₃): δ 174.7, 171.9, 131.2, 121.7, 79.6, 52.5, 49.6, 41.3, 36.3, 25.5, 20.6 ppm. IR (thin film): *v* 2929, 1771, 1735 cm⁻¹. ESIMS (positive ion) *m/z* (%): 313 (90), 311 (95), 289 (100). HRMS: calcd for C₁₁H₁₃O₄Br Na [M+Na]⁺: 310.9895; found: 310.9897.

Reductive debromination of Methyl (3*S*,3a*R*,7*S*,7a*R*)- 4-Bromo-3-methyl-1-oxo-3,3a,6,7,7ahexahydro-7-isobenzofurancarboxylate (31*Z*)



To a solution of cycloadduct **31Z** (5.5 mg, 19 μ mol, 1.0 equiv) in toluene (500 μ L) at room temperature was added tributyltin hydride (15 μ L, 0.06 mmol, 2.9 equiv) and AIBN (1.0 mg, 6 μ mol,

cis,lk-**31***Z cis,lk*-**24***Z* $(2.8 \text{ mg}, 14 \mu \text{mol}, 72\%)$.

3. ¹H and ¹³C NMR spectra of all new compounds











trans, lk 23*Z,* ¹H NMR C₆D₆ 400 MHz

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6

4 2 ⁰ 19









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3.617

2.471

1.529

50

3.889 68.851

2.304

4

100

7.392

150

0.906

Integral

. ppm 2.000 3.493 3.082



Ηį H () CO₂Me O trans, lk *E* ¹³C NMR CDCl₃/CD₃OD 3/1 100 MHz . resperanterior and representation of the second and the ____







trans, ul 25*E* ¹H NMR (CD₃)₂CO 400 MHz





cis, ul **26***E* ¹³C NMR CDCl₃ 100 MHz

4. Geometries of Fumarate Transition Structures

Figure S1. IMDA TSs from 18E with destabilising interactions identified. Distances between interacting atoms, and forming bond lengths are given in Angstroms (Å).

Figure S2. IMDA TSs from fumarate 27E with destabilising interactions identified. Distances between interacting atoms, and forming bond lengths are given in Angstroms (Å).

5. Computational Methods

Diels–Alder TSs were optimised using the B3LYP functional⁵ and the 6-31+G(d) basis set.⁶ Harmonic vibrational frequencies (at the same level of theory) were employed to characterize optimised geometries as either first order saddle structures (one negative Hessian eigenvalue) or minima (all frequencies real), and to provide Zero-Point Vibrational Energy (ZPVE; unscaled) corrections. ZPVE (0 K) corrected TS Boltzmann populations (383 K) were calculated from the electronic energies (ZPVE-corrected) using the electronic energies from optimized *cis,lk-, cis,ul-, trans,lk- and trans,ul-*IMDA TS isomers, and were used in place of enthalpies or free energies because they have been shown to give similar results.⁴ The Gaussian 98⁷ and 03⁸ program packages were used throughout. Optimised geometries (in Cartesian coordinate form) and their energies are provided in the following section.

The B3LYP functional, in conjunction with either the 6-31G(d) or 6-31+G(d) basis sets, is known to give acceptable relative energies and geometries for a broad variety of Diels-Alder reactions.^{9,10,11,12,13,14} Importantly, we have shown that the B3LYP/6-31+G(d) method correctly predicts *cis/trans* ratios for the IMDA reactions of several 9-substituted pentadienyl acrylates, often with an accuracy of 1 kJ/mol.⁹ This level of theory is, therefore, adequate for this study. In this work we focus exclusively on the influence of electronic, strain and steric factors on *cis/trans* selectivities of IMDA reactions, without considering solvent effects; consequently, we have used *gas phase* DFT calculations. The excellent agreement found between gas phase B3LYP/6-31+G(d) predicted IMDA *cis/trans* ratios and the experimental ratios, obtained using toluene as solvent, suggests that weakly polar solvents – which are often used in IMDA reactions – have no significant influence on *cis/trans* selectivities.⁹ A detailed computational and experimental study of solvent effects on IMDA stereoselectivity is currently underway in our laboratory.

6. Cartesian coordinates and energies of optimised TS geometries

(a) TSs for the IMDA reaction of 18Z:

C 0 0.461670 1.700012 0.226761	C 0 0.499130 1.489349 0.346863
C 0 -0.911896 1.926926 0.442108	C 0 -0.873611 1.760696 0.512604
C 0 -1.666016 1.157211 1.292633	C 0 -1.671692 1.056473 1.379974
C 0 -1.019653 -1.066956 0.208435	C 0 -1.045761 -1.237946 0.413284
C 0 0.354065 -1.109039 0.446991	C 0 0.329132 -1.279968 0.652039
C 0 1.377502 -1.380020 -0.645874	C 0 1.351990 -1.555618 -0.442871
O 0 1.263702 -2.244125 -1.476715	O 0 1.235443 -2.403015 -1.289154
O 0 2.522507 -0.658676 -0.552048	O 0 2.499359 -0.832932 -0.336533
C 0 2.580811 0.355881 0.484528	C 0 2.565155 0.064865 0.798813
C 0 -1.519028 -0.647430 -1.101212	C 0 -1.549088 -0.859344 -0.907730
O 0 -0.855835 -0.042480 -1.928604	O 0 -0.890549 -0.283371 -1.758774
O 0 -2.823624 -0.974533 -1.282364	0 0 -2.855164 -1.192230 -1.071533
C 0 -3.374161 -0.590073 -2.548920	C 0 -3.412155 -0.849594 -2.347000
C 0 3.473969 -0.134460 1.618896	C 0 3.574800 1.152359 0.454636
H 0 0.937302 0.570557 1.967514	H 0 0.864151 0.453888 2.164368
H 0 0.915359 2.149353 -0.654037	H 0 0.975998 1.863983 -0.554749
H 0 -1.422592 2.597595 -0.244904	H 0 -1.348969 2.402466 -0.225296
H 0 -1.226913 0.598206 2.109482	H 0 -1.273346 0.525848 2.235550
H 0 -2.747284 1.255798 1.320023	H 0 -2.750183 1.184814 1.369446
H 0 -1.719406 -1.511902 0.904785	H 0 -1.745560 -1.657500 1.125275
H 0 0.638412 -1.613571 1.372070	H 0 0.614410 -1.774628 1.583176
H 0 3.052322 1.212021 -0.009705	H 0 2.944794 -0.516754 1.650100
H 0 -4.401200 -0.957535 -2.546646	H 0 -4.436905 -1.223175 -2.330185
H 0 -3.357925 0.497879 -2.664825	H 0 -3.403931 0.234451 -2.496292
H 0 -2.807251 -1.039108 -3.368927	H 0 -2.845245 -1.319366 -3.155319
H 0 4.444809 -0.450867 1.227264	H 0 4.544556 0.701340 0.223511
H 0 3.636307 0.667450 2.348038	H 0 3.250732 1.729340 -0.415802
H 0 3.021896 -0.986526 2.139938	H 0 3.697021 1.834579 1.302338

(b) TSs for the IMDA reaction of 18E:

trans, lk-23E

trans, ul-25E

cis, ul-26E

• trans,lk- 23E-TS	• trans,ul-25E-TS
B3LYP/6-31G(d) (a.u.): -728.4148331	B3LYP/6-31G(d) (a.u.): -728.4129474
C1 -0.8395200212 -0.710657828 -0.5016493918	C1 -0.7117298233 -0.9496180635 -0.1015331944
C2 -1.5521042058 1.7338846802 -0.4653332126	C2 -2.1604317958 1.1343968972 -0.2466943096
C3 -0.3046640326 2.2981152621 -0.606189805	C3 -1.1916425104 2.0138346968 -0.6733767409
C4 0.7797865186 1.9839130588 0.2390772945	C4 0.035119965 2.1960576681 -0.0004399981
C5 0.6267786742 1.0435702945 1.2522009163	C5 0.3288452463 1.4368734919 1.1273969552
C6 0.3202748008 -0.7139815652 0.2682829869	C6 0.4806456881 -0.4764580573 0.43845711
C7 1.7245036912 0.4685860104 2.1104246551	C7 1.6367575645 1.3828383364 1.8832469543
C8 0.4258710948 -1.4493248128 1.579216467	C8 0.9927518623 -0.9114972993 1.7878047981
O9 1.3033142851 -0.8794709366 2.4563529972	O9 1.7298582329 0.0379607185 2.4335442989
C10 -0.7078876728 -0.6156099748 -1.9614764422	C10 -0.8093414558 -1.0787563082 -1.5615621389
011 0.3259895923 -0.364290773 -2.5590267739	011 0.0039399095 -0.6444895422 -2.3611697248
012 -0.1673287153 -2.457285299 1.8711609983	012 0.8182226169 -1.9950227834 2.2867399888

	O13 -1.8894000829 -0.8545922831 -2.5877347619 C14 -1.8385223619 -0.8100654557 -4.0195139997 C15 1.9659909433 1.2094211904 3.4199995833 H16 -1.7878362236 -1.0375361611 -0.0907691252 H17 -1.9154371501 1.3556796212 0.4820159549 H18 -2.3095430252 1.8703274363 -1.2308693623 H19 -0.0849851589 2.8498557797 -1.5172510045 H20 1.7801808382 2.2726236176 -0.0787250605 H21 0.415002600 1.01201645 1.7517251029	O13 -1.9235024044 -1.7617460435 -1.9315800779 C14 -2.0754688676 -1.9580267901 -3.3433575377 C15 2.8960313563 1.7275848125 1.0979319531 H16 -1.4420650415 -1.4662775644 0.5105730947 H17 -2.2599325682 0.8375207166 0.7898908843 H18 -3.0125287367 0.9027289672 -0.8781361532 H19 -1.2830968171 2.4418861527 -1.6690043176 H20 0.8289710716 2.7311720591 -0.5159750884
	H21 -0.3415025688 1.013619645 1.7512792824 H22 1.2496018576 -0.6816279072 -0.2995391984 H23 2.6598590427 0.4002022262 1.5385352922 H24 -2.8490764972 -1.0449663852 -4.3563987551 H25 -1.1261183296 -1.5444977384 -4.4053062086 H26 -1.5407482827 0.1836126466 -4.3674075418 H27 2.7024543505 0.6738553231 4.0268661381 H28 1.0372423748 1.2893497237 3.9941027559 H29 2.3422633664 2.2175113464 3.2172128442	H21-0.5128060965 1.190339172 1.7726578485 H22 1.2607969477 -0.2767049137 -0.2934393908 H23 1.5803358943 2.0249113057 2.7709652707 H24 -2.9919675659 -2.5375246844 -3.4619735206 H25 -1.2214647327 -2.5043094029 -3.7532509435 H26 -2.1598062035 -0.9985595033 -3.8624319309 H27 3.7764597043 1.5382643053 1.7185733786 H28 2.8945627719 2.7873866608 0.8203626895 H29 2.9851711554 1.1321716615 0.1836691929
	• cis,lk- 24E-TS	• cis,ul-26E-TS
ľ	B3LYP/6-31G(d) (a.u.): -728.4131212 C1 -0.5576915629 1.2732652236 1.2767235224	B3LYP/6-31G(d) (a.u.): -728.4133542 C1 -1.0540564724 1.431044978 0.1714866709
	C3 -0.8831172494 2.2889987716 -0.9373742926 C4 0.3442086444 1.8873819904 -1.4153526942 C5 0.1240002063 -0.5337815708 -0.9789702821 C6 -0.200061103 -0.5924689843 0.3710637956 C7 -1.5369198077 -1.0756829727 0.8539182704 O8 -2.2327221711 -1.8799088479 0.2826583616 O9 -1.9274214356 -0.552625788 2.0505496484 C10 -1.2152073571 0.6429937393 2.4901863285 C11 1.53141061 -0.7131385932 -1.3723924481 O12 2.4891938747 -0.6137396608 -0.6218935171 O13 1.6483359809 -0.9922455856 -2.6928234177 C14 2.9898529012 -1.1993033695 -3.1582657409 C15 -0.2633177838 0.3026837969 3.6302589502 H16 0.5138720453 1.4495118 1.3218372864	C3 1.0521157777 2.0576599629 -0.9159962181 C4 1.8367962247 1.4201128254 0.0197370549 C5 0.8323324205 -0.8334164444 -0.1449065811 C6 -0.526369123 -0.5892197117 0.019773505 C7 -1.5065772294 -0.7483248184 -1.1072744952 O8 -1.3788043094 -1.4943109346 -2.0471905487 O9 -2.614788391 0.0420552782 -0.9947075978 C10 -2.5226122289 1.0731796498 0.0293908981 C11 1.6134053821 -1.2652114338 1.0254830926 O12 1.2573898465 -1.1504941199 2.1878251397 O13 2.8042855967 -1.7996996323 0.6632668901 C14 3.6239743509 -2.2581718707 1.7482304176 C15 -3.4592986108 2.2008072097 -0.3844326854 H16 -0.6582710834 1.4870047037 1.1823594326
	H17 -2.3906944972 2.1044395817 0.5693514287 H18 -1.6178975995 2.6730286752 -1.6422897339 H19 1.1870845351 1.713083991 -0.7576685917 H20 0.5883447503 2.0013511177 -2.4676704336 H21 -0.6370710272 -0.6700288787 -1.7373197474 H22 0.6328219052 -0.7956464825 1.0418965057 H23 -2.0136543179 1.2922975512 2.8667038134 H24 2.8999840931 -1.4090610214 -4.2246660583 H25 3.4521598337 -2.0436327203 -2.6396554952 H26 3.5997542592 -0.3068743136 -2.9918484655 H27 0.563124503 -0.3320297194 3.292914403 H28 -0.7996321303 -0.2267640055 4.4229155531 H29 0.16110998 1.2207999055 4.0520653369	H17 -0.8885789653 2.3196903928 -1.7679999004 H18 1.5149683128 2.3936536715 -1.8418398599 H19 1.5020890065 1.2606752083 1.0373696246 H20 2.9048429845 1.308278355 -0.1435968878 H21 1.2479540917 -1.0073931461 -1.129556779 H22 -0.9228975336 -0.7865588777 1.015257143 H23 -2.8767786589 0.6396301074 0.9735285504 H24 4.5282975244 -2.6536417556 1.2844695214 H25 3.1112751254 -3.0396982163 2.3156055039 H26 3.8676830231 -1.4341450873 2.4248084236 H27 -4.4786701412 1.818997737 -0.4959530707 H28 -3.4604019064 2.9862909587 0.3785410689 H29 -3.1516800268 2.6397659478 -1.3377548106
- 1		

(c) TSs for the IMDA reaction of 27Z:

C 0 -1.585190 1.085007 1.501221	C 0 -1.780853 1.013809 1.793686
C 0 -0.935394 -1.171204 0.419952	C 0 -1.152084 -1.260132 0.873672
C 0 0.441010 -1.171204 0.662643	C 0 0.226532 -1.260117 1.116745
C 0 1.490036 -1.451859 -0.403809	C 0 1.286621 -1.544662 0.060303
O 0 1.388809 -2.305511 -1.249298	O 0 1.187561 -2.362076 -0.819046
O 0 2.641220 -0.749786 -0.258774	O 0 2.449936 -0.862473 0.255569
C 0 2.669754 0.248047 0.799011	C 0 2.448151 -0.008514 1.428345
C 0 3.454300 -0.285080 1.993027	C 0 3.622116 0.957870 1.335800
Br 0 1.331604 2.539597 -1.040024	Br 0 1.193054 2.246658 -0.773117
C 0 -1.472229 -0.801071 -0.891541	C 0 -1.700806 -0.976273 -0.457596
O 0 -0.865509 -0.151688 -1.728760	O 0 -1.121567 -0.359756 -1.335846
O 0 -2.746414 -1.237305 -1.061859	O 0 -2.962921 -1.460678 -0.591507
C 0 -3.345367 -0.925873 -2.331192	C 0 -3.579483 -1.240875 -1.871536
H 0 0.958496 0.547073 2.174469	H 0 0.680084 0.538208 2.610275
H 0 -1.345078 2.529648 -0.033661	H 0 -1.466675 2.362091 0.186188
H 0 -1.153610 0.513214 2.312805	H 0 -1.394714 0.503906 2.666855
H 0 -2.664597 1.203949 1.531509	H 0 -2.859344 1.142380 1.766907
H 0 -1.614792 -1.622314 1.133423	H 0 -1.825500 -1.693436 1.603973
H 0 0.722183 -1.657455 1.598862	H 0 0.504822 -1.726166 2.065475
H 0 3.207993 1.088608 0.353989	H 0 2.623688 -0.660767 2.295593
H 0 2.945480 -1.129669 2.472656	H 0 4.553146 0.386154 1.262253
H 0 4.443481 -0.622894 1.670059	H 0 3.543808 1.615250 0.470490
H 0 3.585632 0.507600 2.739258	H 0 3.664000 1.570480 2.243774
H 0 -2.742752 -1.334290 -3.146835	H 0 -2.973511 -1.682846 -2.666855
H 0 -3.434219 0.157257 -2.457993	H 0 -3.695984 -0.169815 -2.062317
H 0 -4.331024 -1.391953 -2.307922	H 0 -4.553131 -1.728485 -1.811111

(d) TSs for the IMDA reaction of 27E:

 trans,lk-30E-TS 	 trans,ul-32E-TS
B3LYP/6-31+G(d) (a.u.): -3299.349663	0 B3LYP/6-31+G(d) (a.u.): -3299.34161
C 0 -0.909729 -0.786896 0.009720	C 0 -0.978088 -0.780563 0.534515
C 0 -1.378342 1.605957 0.903320	C 0 -1.499756 1.493469 1.544083
C 0 -0.288712 2.214127 0.325790	C 0 -0.455841 2.183655 0.972656
C 0 1.030441 1.742630 0.500229	C 0 0.896942 1.786255 1.085541
C 0 1.279419 0.602005 1.257309	C 0 1.215118 0.632813 1.797089
C 0 0.464462 -0.908051 0.219543	C 0 0.395142 -0.901627 0.744202
C 0 2.586838 -0.121841 1.454239	C 0 2.513245 -0.103027 2.071793
C 0 1.039825 -1.902649 1.201157	C 0 0.950729 -1.887024 1.741867
O 0 2.220398 -1.500916 1.750992	O 0 2.103424 -1.481064 2.340866
C 0 3.429596 0.398666 2.609970	C 0 3.635666 -0.102615 1.040390
O 0 0.550369 -2.966660 1.493546	O 0 0.459412 -2.955856 2.016724
Br 0 2.378311 2.446945 -0.640640	Br 0 2.128189 2.690460 -0.046555
C 0 -1.378098 -0.369705 -1.316940	C 0 -1.441971 -0.335175 -0.785812
O 0 -0.664185 0.081451 -2.201843	O 0 -0.726807 0.155853 -1.647766
0 0 -2.714233 -0.557755 -1.465057	O 0 -2.772430 -0.541077 -0.953033
C 0 -3.254944 -0.211502 -2.751007	C 0 -3.306961 -0.165176 -2.233734
H 0 -1.625427 -1.227585 0.694946	H 0 -1.691086 -1.257889 1.197540

H 0 -1 314224 0 992294 1 792847	H 0 -1 389633 0 861496 2 416290
$H_0 = 2380539 \pm 912247 \pm 0.619156$	$H_0 = 2.521606 + 762207 + 292725$
H = 0.0453842.2.966644.0.440063	$H_{0} = 0.683685 2.955856 0.243454$
110 - 0.433042 2.900044 - 0.440003	H 0 0 527070 0 492202 2 626956
H = 0.022400 0.493340 2.119904	H = 0.037779 0.463292 2.030630
H U 1.081314 -0.758072 -0.008259	H 0 1.015215 -0.744781 -0.157544
H 0 3.174332 -0.120209 0.529037	H 0 2.914429 0.233994 3.035202
H 0 4.312546 -0.233551 2.747772	H 0 4.360992 -0.870422 1.328781
H 0 2.853424 0.401093 3.541443	H 0 4.145233 0.863556 1.021545
H 0 3.758728 1.420471 2.393570	H 0 3.279877 -0.322784 0.029861
H 0 -2.755005 -0.777649 -3.541443	H 0 -2.791794 -0.701294 -3.035202
H 0 -3.130798 0.858292 -2.943848	H 0 -3.196121 0.911377 -2.394135
H 0 -4.312561 -0.472366 -2.699341	H 0 -4.360992 -0.442429 -2.199265
• cis,lk- 31E-TS	• <i>cis,ul-33E-TS</i>
P2I VD $(6,21+C(d),(n,u))$; 2200 245640	P2I VD / $(6.21 + C(4))$ (c.u.); 2200 242207
$D_{3L}(17)^{-31+O(0)}(a.u.)$; -5299.545049	$D_{2} = 170 - 31 + O(0) (a.u.): -5299.542207$
C 0 1.028813 1.113320 0.410041	C 0 1.383423 1.109373 0.339932
C 0 1.02/191 2.0/2006 -0.403900	C 0 0.801254 2.082245 -0.325211
C 0 -0.356033 2.334808 -0.364900	C 0 -0.583298 2.339615 -0.303085
C 0 -1.215393 1.649307 0.462708	C 0 -1.450867 1.672989 0.535600
C 0 -0.630753 -0.657974 -0.300583	C 0 -0.875565 -0.606033 -0.157562
C 0 0.740768 -0.699997 -0.062439	C 0 0.498184 -0.648148 0.080978
C 0 1.746964 -0.910767 -1.163010	C 0 1.501984 -0.829132 -1.028534
O 0 1.543091 -1.526291 -2.182480	O 0 1.292618 -1.379486 -2.082900
O 0 2.972580 -0.381592 -0.902557	O 0 2.731979 -0.313675 -0.740204
C 0 3.031418 0.586670 0.188797	C 0 2.752640 0.519653 0.452698
C 0 3 677887 -0 033386 1 421814	C 0 3 983856 1 415604 0 405075
Br 0 1 973511 2 807297 -1 890396	Br 0 1 694397 2 669800 -1 910934
C = 1.5755112.00725771.050550	C 0 1 780536 1 153510 0 858566
$0.0 \pm 1.53000 \pm 1.170013 = 0.110703$	$0.0 \ 1.502287 \ 1.252707 \ 2.021082$
0.0 - 2.775919 - 1.420500 - 0.05229	0.0 - 1.505367 - 1.552707 2.051062
0 0 -2.775818 -1.459590 0.205558	0 0 - 3.014433 - 1.409897 0.341322
C 0 - 3.737305 - 2.003342 1.115128	C 0 - 3.976715 - 1.972961 1.251007
H 0 1.246872 1.066696 1.433853	H 0 0.966278 1.191238 1.564606
H 0 -0.771271 2.963684 -1.147461	H 0 -0.995880 2.927216 -1.118515
H 0 -0.893234 1.181641 1.384628	H 0 -1.143585 1.251816 1.484818
H 0 -2.287277 1.791473 0.356339	H 0 -2.521484 1.807892 0.408356
H 0 -1.016434 -0.526840 -1.304977	H 0 -1.256256 -0.499374 -1.166824
H 0 1.026230 -1.150116 0.888000	H 0 0.789871 -1.093475 1.032928
H 0 3.680481 1.375351 -0.201645	H 0 2.857193 -0.150360 1.316269
H 0 3.058792 -0.822113 1.863068	H 0 4.880920 0.792191 0.329727
H 0 4.645767 -0.467728 1.154160	H 0 3.959900 2.099700 -0.443481
H 0 3 845154 0 738403 2 182480	H 0 4 046356 1 999603 1 330521
H 0 3 915161 1 324600 1 954041	H = 1.01000 H = 1.0000 H = 1.00000 H = 1.00000 H = 1.0000 H = 1.00000 H = 1.00000 H = 1.00000 H =
$U_0 = 2.21020 - 2.062694 + 4.09194$	110 - 7.10 + 10 + 10 + 1200 + 52.002000 110 - 2.616440 - 2.0027021 - 1.644219
110 - J.J01707 - 2.70J004 1.470104 110 - 4.645702 - 2.126108 0.526002	110-3.010440-2.7272311.044310
n u -4.043/82 -2.130108 U.320993	п v -4.000920 -2.11/338 V.039042

(e) TSs for the IMDA reaction of 34:

• trans,lk- 36-TS	• trans,ul- 38-TS

B35/W6-31-C(0) (0.01-153:1394 B35/W6-31-C(0) (0.01-153:1394 00.05 50279 - 2.000551 (19.04) B35/W6-31-C(0) (0.01-153:13945 C0.0021120 (10.0020 0.070057 C0.002202 0.033541 (1.37997) C0.0125440 (0.0028) (3.07035 C1.114486 (1.78258) (3.07335 C0.0224540 (0.0028) (3.07035 C1.114486 (1.78258) (3.07335 C0.0224540 (0.0028) (3.07035 C1.114486 (1.78258) (3.07335) C0.0224540 (0.0028) (3.06425) (3.0641) C1.23449 (0.123449) (3.1314 C0.024490 (0.35489) (3.13146 C1.021632 (3.07224) (3.05284) C0.034897 (0.12713) (3.0657) C0.34898 (1.3146) C0.034897 (0.12713) (3.0657) C0.34898 (1.3146) C0.127297 (0.1273) (1.56377) C0.213918 (4.37864) (1.85693 C0.13897 (0.7285 (0.6561) C1.13897 (1.63989) (1.8628) C0.13997 (0.7285 (0.6561) C1.414118 (0.53846 (0.78778) C0.13997 (0.7285 (0.6561) C1.414118 (0.53846 (0.78778) C0.13997 (0.7285 (0.671) (3.7584) C0.43985 (1.11470) C0.13997 (0.7285 (0.671) (3.7584) C0.43985 (1.01470) C0.13997 (0.7285 (0.671) (3.7584) C0.43985 (1.01470) C0.13997 (0.72978) C0.43985 (1.01470) C0.13997 (0.729778) C0.43985 (0.7788) <	BN.YP6-31-6G(d) (au.): -1251-3244 BN.YP6-31-6G(d) (au.): -1251-3248 C00.9729 2.40005.01-2051-32244 C00.97001 2.01700.02095 C01.23401 0.05280.037265 C00.97001 2.01700.02095 C01.23401 0.05280.037265 C01.23401 0.05280.037265 C01.23401 0.05280.037265 C02.410671 0.35900 0.043197 C01.23401 0.05280.037265 C02.410671 0.35900 0.043197 C01.23401 0.05462 0.145876 C02.23401672.165881 1.95889 C01.36820 1.075881 0.98835 C01.447008 1.318861 (93887) C01.36820 1.075881 0.98835 C01.447008 1.318861 (93887) C01.36820 1.075881 0.98835 C01.129864 7.287788 1.988835 C01.129864 7.287788 1.98835 C01.129864 7.287788 1.988835 C01.129871 0.07887 0.618988 C01.129874 7.287788 1.99976 C01.129871 0.079882 0.618988 C01.457186 1.98860 7.87788 C01.129871 0.079870 0.72855 0.60805 C01.47118 0.538460 7.87788 C01.29971 0.37888 0.61888 C01.47118 0.538460 7.87788 C01.29971 0.79882 0.61898 C01.47118 0.53846 7.87788 C01.29971 0.79882 0.61898 C01.47118 0.53846 7.287788 C01.29971 0.79882 0.61898 C01.47118 0.53846 7.287788 C01.29971 0.79882 0.618981 C01.29981 0.49885 0.17878		
BM_YP6-31+G60 (a.u.s 1251.32948 BM_YP6-31+G60 (a.u.s 1251.32948 C00.050202 - 2,40005 0.19655 C00.057870 - 2,30105 0.19655 C00.057870 - 2,30105 0.32968 C00.050202 - 2,40005 0.19655 C00.057870 - 2,30105 0.32968 C00.057870 - 2,30105 0.32968 C00.050202 - 2,12720 0.30131 C0 2,56864 - 1,000028 1.358857 C0 2,56864 - 1,000028 1.358857 C00.05202 - 2,073782 1.958325 C0 4,47035 1.358651 C0 4,47035 1.358651 C00.05202 - 4,07384 - 1,27128 C0 0,57870 - 2,301270 0.35286 C00.052838 - 3,15500 1.845427 C0 0,12809 - 2,740792 1.182263 C00.052838 - 3,15500 1.84547 C0 0,12809 - 2,740792 1.182263 C00.128280 - 2,71788 - 1,278128 C0 0,12820 - 4,07281 - 1,28633 C00.128280 - 2,71788 - 1,278128 C0 0,12820 - 4,07281 - 1,28633 C00.128280 - 2,71788 - 1,278128 C0 - 1,47118 - 0,24660 - 2,14884 C0.128280 - 2,07281 - 2,073810 C0 - 1,28718 - 2,0710 - 3,0884 C0.128280 - 1,0784 - 1,2711 - 2,47112 - 2,0714 C0 - 2,19911 - 5,08685 C0.297910 - 3,69912 - 2,07740 C0 - 2,19911 - 3,08921 - 8,0733 C0.128280 - 2,07140 - 3,07484 C0 - 1,07116 - 2,071407 - 3,07145 C0.297910 - 3,08951 - 0,07013 H0 - 0,07215 - 3,07466 C0.297910 - 3,08951	Image: Construction of the construction of		
BLXPR-31-060 BLXPR-31-0600 0.000290-2.00050 0.300.05 C0.000290-2.00050 0.300.05 0.00071412.010092 0.47037 C0.000220 0.730381 1.37039 C0.01071412.010092 0.47037 C0.000220 0.730831 1.37039 C0.01071412.010092 0.47037 C0.000220 0.73081 1.37039 C0.012710.017781 1.57881 5788 588 50 0.234833 1.51104 7.232822 58835 50 0.234833 1.51104 7.232822 58835 50 0.234833 1.51104 7.232822 58835 50 0.234833 1.51104 7.23282 58835 50 0.234833 1.51104 7.23282 58835 50 0.234833 1.51104 7.23282 5883 51 51104 7.23282 5883 51 51104 7.23282 5883 51 51104 7.23282 5883 51 51104 7.23282 5883 51 51104 7.23282 51 5100 7104 50 0.23458 51 51 0.05737 0.83808 51 0.02345 51 0.05737 0.83808 51 0.05738	Bit YP6-31+G(d) Gaup-1251-3244 Bit YP6-31+G(d) Gaup-1251-3244 C 00.50209 - 2.00055 0.150655 C 0.057907 - 2.001270 0.382065 C 00.07442 0.04082 0.947007 C 0.00228 0.20381 1.37793 C 01.225490 0.6528 0.57655 C 0.017482 0.04022 0.947007 C 0.007442 0.04082 0.947007 C 0.00228 0.20381 1.37793 C 0.1245490 0.0528 0.54842 C 0.114480 0.79538 0.93887 C 0.125728 1.57828 1.57828 C 0.00787 0.104567 C 0.125752 1.57828 1.578525 C 0.017085 1.326457 1.095669 C 0.017087 1.326457 0.95769 C 0.017082 1.20487 0.95769 C 0.0121602 1.20477 1.21782 0.977213 D 0.125974 - 207701 1.09976 C 0.13807 0.21782 1.578517 C 0.215714 - 207701 1.49977 0.977213 D 0.132839 - 21728 1.578517 C 0.215714 - 207701 1.49976 C 0.138070 0.74632 0.65215 C 0.141118 0.535846 C 0.138070 0.74851 2.005712 C 0.215714 - 207701 1.49976 C 0.138070 0.74851 2.005712 C 0.215915 - 37782 0.052639 C 0.138070 0.74851 2.005712 C 0.215915 - 3778381 C 0.138970 0.75852 0.616086 C 0.239815 2.10156 0.716333 C 0.239701 1.548673 C 0.239801 1.236879 0.022664 C 0.1499711 1.44824 1.28007 H 0.022757 0.25780 0.920606<		
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C D 2 43167 0.058800 0 55903 C D 2 43167 0.05802 0 84397 C D 2 66580 C 000028 1.36422 C D 2 43167 0.05802 0 84397 C D 2 66580 C 000028 1.3642 C D 2 005907 0 - 76452 1.55541 C 0 1 84523 C 0 2 44602 - 3.517280 1 959535 C 0 4 40705 - 3.138867 1 95849 C 0 2 43167 0 0.55802 0 84397 C 0 2 00505 - 3.38867 1 95849 C 0 2 43167 0 0.55802 0 84397 C 0 2 00505 - 3.38867 1 95849 C 0 2 43167 0 0.55802 0 84397 C 0 2 00505 - 0.55841 C 0 1 36233 - 2.00721 - 3.22580 1 80356 C 0 4.47190 - 3.28224 C 0 0.30007 - 2.04452 - 1.182587 C 0 0.21592 - 2.07703 - 1.989525 C 0 - 1.20373 1 .58617 C 0 2.315918 - 4.378021 1.85629 C 0 - 1.20373 1 .58617 C 0 3.45954 - 2.20703 - 1.99976 C 0 - 1.20373 1 .58617 C 0 3.45954 - 2.20703 - 1.99976 C 0 - 1.20373 1 .69131 - 0.429959 C 0 - 1.41118 0.53466 0.781708 S 0 - 2.50584 2 .63102 C 0 .141118 0.53466 0.781708 C 0 - 2.97130 0 .79852 0.61808 C 0 - 2.97313 0 .10536 - 1.299759 C 0 - 2.97130 0 .79852 0.61808 C 0 - 3.29832 3 .15107 - 0.728637 C 0 - 2.97130 0 .79852 0.61808 C 0 - 3.29321 .25808 - 1.261459 C 0 - 2.97130 0 .79852 0.61808 C 0 - 3.29320 .128687 - 2.07703 H 0 - 0.216721 .26667 0 .077313	C 0 2-399490 0088660 0.559065 C 0 2-341671 0.359620 0.843397 C 0 2-65590 - 0758521 6.506841 C 0 2.386524 - 2.30124 0.62266 C 0 3.86552 - 1.57828 1.598649 C 0 2.386524 - 2.30124 0.62266 C 0 3.46553 - 1.38567 1.985649 C 0 2.486578 - 1.38567 1.985649 C 0 2.46672 - 1.38567 1.985649 C 0 2.46672 - 1.38567 1.985649 C 0 2.46672 - 1.38567 1.985649 C 0 2.470273 - 1.38567 1.985649 C 0 0.470382 - 1.73488 - 2.12128 C 0 0.213623 - 2.06722 - 0.967224 O 0 0.74382 - 1.73488 - 2.12128 C 0 0.02076 - 1.68339 - 1.886235 O 0 1.32833 - 2.06722 - 0.967224 O 0 0.21761 - 1.68339 - 1.886235 O 0 1.32833 - 2.06722 - 0.967245 O 0 0.21761 - 1.68339 - 1.886235 O 0 1.32833 - 2.06722 - 0.967245 O 0 0.21761 - 1.885236 O 0 - 1.2383 - 2.07731 - 1.99976 C 0 1.41731 - 1.38623 - 1.886235 O 0 - 1.2383 - 2.07731 - 1.99976 C 0 - 1.41731 - 0.238245 O 0 - 1.2383 - 2.07731 - 1.99976 C 0 - 1.41731 - 0.238546 O 0 - 23751 - 0.56823 - 1.61868 C 0 - 3.418718 - 0.237470 O - 1.29371 - 2.09713 - 3.09746 C 0 - 3.45835 - 1.571708 O - 0.26721 - 2.09713 - 0.275458 H 0 - 0.02751 - 2.75830 - 0.275830 O - 0.26712 - 2.76617 0.875458 H 0 - 0.02772 - 2.77830 - 0.275800 H 0 - 0.1	C = 0.0371112 = 0.0000000000000000000000000000000000	C 0 1 114868 0 708538 0 503887
C 0 - 24-9999 00.86000 (1.45387) C 0 - 24-0101 (1.05000 (1.45387) C 0 2 - 66000 (1.45	$ \begin{array}{llllllllllllllllllllllllllllllllllll$	C = 0.2400406 = 0.092660 = 0.572055	C 0 2 421(71 0 2(2(02 0 942507
C 0.2.060300 1.060028 1.948522 C 0.2.080079 0.76832 6.7632 C 0.3.066222 1.737828 1.958623 C 0.2.081679 0.67832 1.633661 C 0.3.066222 1.737828 1.958623 C 0.2.06207 0.0216728 1.322258 1.603561 C 0.0.1.06307 1.445624 1.202583 C 0.0140792 1.82216 1.603561 C 0.0.1.06307 2.16781 2.318724 C 0.0120677 1.022159 1.009765 C 0.0.1.06307 2.16781 2.318724 C 0.0120677 1.022159 1.009765 C 0.1.120171 1.84067 2.581824 C 0.1.114118 0.022559 C 0.1.114118 0.022559 C 0.1.120171 1.84087 1.208725 1.009765 1.009765 1.009765 C 0.1.120171 1.870871 C 0.1.114118 0.023561 1.0177 0.014149 1.00976 C 0.1.120171 1.870871 1.104455 0.022559 C 0.1.11118 0.022559 C 0.1.11118 0.023561 1.0177 0.0171785 1.00976 0.014340 0.002775 0.022559 C 0.1.411118 0.0237607 0.0063251	C 0.2.060380 1.000028 1.245422 C 0.2.08070/90.70832 1.25664 C 0.3.08122 1.2737828 1.598625 C 0.2.08170/90.76851 3.286671 9.58666 C 0.0.3.08122 1.2377828 1.598625 C 0.2.08170/90.76851 3.58667 9.58625 C 0.0.3.0807 2.144623 1.18577 C 0.0.214623 2.007224 0.09724 C 0.0.3.0807 2.146423 1.185671 C 0.0.214532 1.586251 0.09724 2.007224 C 0.0.3.08073 2.121628 1.280257 0.0924572 1.988255 0.00241592 1.586253 0.00241592 1.586253 0.0024552 1.09976 C 0.51706 1.996460 2.418844 C 0.141118 0.835466 0.731708 0.025559 C 0.141118 0.835466 0.731708 0.025593 C 0.141118 0.746553 1.09976 C 0.2306783 1.00455 0.2305747 0.688303 1.024554 1.09976 C 0.51706 1.09455 0.025598 C 0.141118 0.835466 0.731708 0.0272572 2.72580 1.092455 C 0.141118 0.835466 0.731708 0.746553 2.005777 0.0147497 0.265747	C 0 2.499496 0.088669 0.579605	C 0 2.4310/1 0.303002 0.84339/
C 01.381790 - 2521729 0.36133 C 0.0396622 - 7.2773828 1.595649 C 0.0464020 - 354498 1.318416 C 0.0336552 - 0.272684 - 2.302526 C 0.0464020 - 354498 1.31841 C 0.0336901 - 2764579 - 2.82236 C 0.021623 - 2.005722 - 0.67224 C 0.021623 - 2.00572 - 0.67234 C 0.0128203 - 2.11628 - 1.82587 C 0.012823 - 2.11628 - 1.82587 C 0.0121623 - 2.00572 - 0.67234 C 0.0121623 - 2.00576 - 1.63359 C 0.1411180.053546 0.781708 C 0.1407310 - 0.72455 0.636213 C 0.1411180.053466 0.781708 C 0.120073 1.09511 - 0.20559 S 0.01256584 - 2.61302 - 0.035846 C 0.2307310 3.76982 0.61808 C 0.230883 3.15107 - 0.282822 S 0.0256842 2.613102 - 0.035846 C 0.2307310 3.76982 0.61808 C 0.2307310 5.44406 - 2.19455 C 0.2307310 5.44406 - 2.19455 C 0.2307310 5.44406 - 2.19455 H 0.012721 - 2.76501 0.02569 C 0.420231 1.5468 - 1.51459 H 0.012721 - 2.76501 0.02569 C 0.420231 1.5468 - 1.51459 H 0.012721 - 2.76501 0.02569 C 0.420231 1.5468 - 1.51459 H 0.012721 - 2.76501 0.02765 H 0.012721 - 2.77501 H 0.156902 - 2.77503 H 0.156902 - 2.77503 H 0.156902 - 2.77503 H 0.156971 - 2.95120 - 3.75671 H 0.156971 - 2.77503 H 0.156971 - 2.95120 - 3.75671 H 0.15775 - 0.25684 H 0.02777 - 2.95120 - 3.75671 H 0.	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C 0 2.665680 -1.060028 1.364822	C 0 2.680679 -0.764542 1.636841
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$ \begin{array}{llllllllllllllllllllllllllllllllllll$	C 0.2.444020 3.54498 1.31346 C 0.2.702011 3.262891 6.03361 $C 0.0.305582$ 0.0.213621 2.005722 0.06724 0.007224 $C 0.0.30807$ 2.044632 1.182587 C 0.0.213623 2.005722 0.06724 $C 0.0.30807$ 2.216281 2.18024 C 0.0.213623 2.009724 0.099976 $C 0.1.468531$ 0.1.422830 2.036653 C 0.1.409719 1.996460 2.41884 $C 0.1.473190$ 2.92782 2.95517 C 0.1.401700 1.124455 0.0926559 $C 0.1.400710$ 6.03911 0.029996 C 0.1.4017180 0.024554 1.099564 $C 0.1.400710$ 6.03910 0.014353 1.01176 0.024554 1.01556 $C 0.2.70101$ 2.050445 1.015751 0.024574 1.01564 0.014353 1.015767 0.014356 1.015751 0.0143564 1.015751 0.024574 1.015751 0.024574 1.015751 0.024574 1.015751 0.024574 1.015751 1.0027670 1.0047708570 1.00477076 1.0245776 1.0017707 1.015751 1.00177077 1.017811 1.00577	C 0 3.986252 -1.757828 1.595825	C 0 4.047058 -1.338867 1.958649
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0.00.23942 - 1.73048 - 2.128128 0.0.020776 - 1.639359 - 1.890353 0.01.98020 - 4.07331 1.580517 0.0.213918 - 4.78021 1.85293 0.01.323339 - 2.12163 - 1.281021 0.0.1129547 - 2.207703 - 1.09976 0.01.330370 - 0.25755 0.65815 0.0.1129547 - 2.207703 - 1.09976 0.01.30070 0.072455 0.658215 0.0.14118 0.583460 - 728178 0.01.25727 2.20753 1.60931 0.40259 0.0.145285 0.5151 (0.0.14118 0.583460 - 728178 0.01.25073 1.60931 0.40259 0.0.145285 0.5151 (0.0.145285) 0.01.25073 7.56852 0.610808 0.0.145285 0.5151 (0.0.7405839) 0.01.13397 0.76852 0.610808 0.0.2075 7.278580 1.09266 0.01.13397 0.46829 0.150808 0.0.2075 7.278580 1.09266 10.01.13573 1.16480 0.319933 10.02705 7.27850 10.09266 10.01.1339 1.16480 0.319933 10.02795 7.278580 1.07266 10.02.0121 1.1273 1.224852 10.02705 7.273500 10.02.0121 1.1273 1.224852 10.02754 2.27850 1.09266 10.113753 1.167931 0.6892/4 10.258478 2.16057 0.273500 10.247112 2.42077 1.0 5.8447 10.0258478 2.16057 0.273500 10.24872 2.44877 1.44340 2.19456 10.15733 2.66666 10.147701 2.240273 0.58447 10.42753 2.261696 3.136061 10.247112 2.42077 1.058848 10.15733 2.66663	C = 0.030807 - 2.044632 - 1.182587	C 0 0 213623 2 005722 0 967224
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$ \begin{array}{llllllllllllllllllllllllllllllllllll$	00 1.9282/2 - 401/2.31 1.3860/1 00 2.13918 - 3.7802/1 1.8502/3 00 1.12857 - 2.2773 2.72782 7.97517 00 -1.129547 - 2.2773 1.099976 00 1.120547 - 2.2773 2.72782 7.97517 00 -1.129547 - 2.2773 0.20559 00 1.120547 - 2.2773 2.77517 00 -1.129547 - 2.2773 0.20559 00 1.120547 - 2.27782 7.97517 00 -1.129547 - 2.2778 0.20559 00 1.120547 - 2.07730 0.672455 0.636215 00 -1.41118 0.583466 0.781708 00 1.120547 - 2.07790 0.75435 00 -1.29547 - 2.077940 00 1.120547 - 2.077910 0.875436 00 -1.290537 4.14078 0.21955 00 0.1432 0.42724 1.280007 10 0.007345 0.42727 0.205200 10 0.114340 - 0.42742 1.80007 10 0.007345 0.42727 0.202920 10 0.114340 - 0.42742 1.80007 10 0.007345 0.427273 0.129406 10 0.114340 - 0.42742 1.80007 10 0.007345 0.427273 0.129406 10 0.12497 - 1.42731 2.234955 10 0.190734 0.00600 0.224453 10 0.247160 - 1.47731 2.234955 10 0.190734 0.00600 0.224453 10 0.247160 - 1.47102 - 2.40074 0.54847 11 0.05474 - 2.00602 - 2.47636 10 - 2.4074 0.54847 10 0.24760 - 1.2713 - 2.2178 - 2	0 0 0.743942 -1.750464 -2.126126	0 0 0.920770 -1.059539 -1.898283
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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C 0 - 1.303070 0.672455 0.686215 C 0 - 1.411118 0.583466 0.781708 O 0 - 1.200715 1.60911 - 0.420959 O - 1.452315 1.511047 - 0.282822 Si 0 - 2.565842 2.63102 - 0.838846 Si 0 - 2.89085 2.410156 - 0.746333 C 0 - 2.973190 3.769852 0.618088 C 0 - 2.3068805 3.502747 0.688309 C 0 - 4.20320 1.255801 1.022066 H 0 - 0.216721 - 2.766617 0.875458 H 0 0 - 0.216721 - 2.766617 0.875458 H 0 - 0.02705 - 2.725801 1.092066 H 0 1.115753 1.16489 0.391953 H 0 0.02708 - 2.725801 1.092067 H 0 2.012497 - 1.42731 2.214983 H 0 1.95594 1.54588 - 0.178131 H 0 3.20334 0.772400 0.223465 H 0 0.210592 - 3.73500 H 0 2.012497 - 1.142731 2.244983 H 0 1.95514 - 0.09600 2.472763 H 0 2.47711 2 - 4.20273 0.548447 H 0 2.658478 - 3.16057 0.072300 H 0 - 1.71191 - 2.481522 H 0 - 2.722173 - 2.21786 - 2.3144696 H 0 - 1.602684 - 0.819763 - 2.885727 H 0 - 1.500473 - 0.900093 - 2.73210 H 0 5.66002 - 2.37663 - 3.132609 H 0 - 1.500473 - 0.900093 - 2.73240 H 0 5.66002 - 1.971191 - 2.481527 H 0 - 1.500473 - 0.900093 - 2.73240 H 0 5.66002 - 1.971091 - 2.481527 H 0 - 5.425018 - 0.065720 0.882462 H 0 - 1.47173 - 2.260481 - 3.312609 H 0 - 1.500473 - 0.900693 - 2.73240 H 0 - 5.425018 - 0.86703 H 0 - 4.272	C 0 4.779190 -1.257278 2.795517	C 0 5.147003 -1.124435 0.926559
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C 0 -1.303070 0.672455 0.636215	C 0 -1 411118 0 583466 0 781708
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N0 - 2.300842 2.00082 2.000740 C0 - 2.199615 3.40106 0.008309 C0 - 1.20015 3.000512 - 2.300740 C0 - 2.199615 3.40106 0.008309 C0 - 2.07109 3.708852 0.618098 C0 - 3.268005 3.20740 0.068309 C0 - 2.07211 - 2.766617 0.875458 H0 - 0.022705 - 2.72580 1.261459 H0 0 - 0.114349 0.391953 H0 0 - 0.022370 2.020200 H0 1.115753 1.416489 0.391953 H0 0 0.975400 0.223405 H0 0 2.07121 2.276661 7.0875458 H0 0.95594 1.545883 - 0.1773400 0.223405 H0 0 2.014349 0.480274 1.2832007 H0 0.95514 - 0.906800 - 2.072300 H0 1.0331070 0.048615 0.0773103 H0 3.2263340 - 7.220108 - 0.273500 H0 2.47112 - 2.40273 - 0.58447 H0 2.2658478 - 2.161057 - 0.273500 H0 - 1.467102 - 2.540451 - 3.321609 H0 - 1.175523 - 2.065693 - 3.136261 H0 - 1.620546 - 0.819763 - 2.885727 H0 0 - 1.30073 0.906693 - 2.732910 H0 - 1.620547 - 0.29170 - 2.448152 H0 0 - 1.37207 - 1.29120 - 0.005720 H0 - 1.500473 - 0.986693 - 2.732910 H0 0 - 1.500473 - 0.986693 - 2.732910 H0 - 1.620547 - 0.22107 - 2.448152 H0 0 - 1.37217 - 1.44320 - 0.075790 H0 - 1.500473 - 0.986693 - 2.732910 H0 0 - 1.500473 - 0.986693 - 2.732910 H0 - 1.50247 - 1.29120 - 3.705612 H0 0 - 3.8707 - 1.469630 - 1.216465 H0 - 1.50247 - 1.29120 - 3.705612 H	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	S: 0, 2,565942,2,622102, 0,925946	S: 0 2 902095 2 410156 0 746252
$ \begin{array}{c} 0.1 - 1.920173 3.009312 \cdot 2.305740 \\ \hline C 0.2.97319 0.3769852 0.0518088 \\ \hline C 0.4.092041 1.619995 1.297913 \\ \hline C 0.4.209301 .258408 \\ \hline C 0.4.209301 .258408 + .261459 \\ \hline H 0.0.114349 - 0.482742 1.820007 \\ \hline H 0.0.070435 - 0.423742 1.820007 \\ \hline H 0.0.070435 - 0.42383 - 0.178131 \\ \hline H 0.3.30700 - 0.408615 - 0.073013 \\ \hline H 0.2.20730 - 0.484477 \\ \hline H 0.2.20730 - 0.484477 \\ \hline H 0.2.20730 - 0.484477 \\ \hline H 0.2.2658478 - 2.16169 \\ \hline H 0.1.17352 - 2.40805 - 2.47383 \\ \hline H 0.2.27700 - 1.49731 - 2.24985 \\ \hline H 0.1.467102 - 2.540451 - 3.321609 \\ \hline H 0.1.467103 - 2.95102 - 3.705612 \\ \hline H 0.540271 - 1.29512 - 3.705612 \\ \hline H 0.540271 - 1.29512 - 3.705612 \\ \hline H 0.540271 - 1.29512 - 3.705612 \\ \hline H 0.5420518 - 0.025270 - 8.000292 - 1.687363 \\ \hline H 0.1.92158 - 2.003277 \\ \hline H 0.1.82178 - 2.244406 \\ \hline H 0.1.971152 - 0.37270 - 0.520279 \\ \hline H 0.1.82178 + 2.203157 \\ \hline H 0.1.82178 + 2.203157 \\ \hline H 0.1.82178 + 2.2033157 \\ \hline H 0.1.82178 + 2.2033157 \\ \hline H 0.1.82178 + 2.2033157 \\ \hline H 0.2.081797 - 4.34080 - 0.95715 \\ \hline H 0.2.081797 - 4.34080 - 0.95715 \\ \hline H 0.3.84549 - 1.00303 - 0.462006 \\ \hline H 0.2.081797 - 4.34080 - 0.95715 \\ \hline H 0.3.345459 - 3.203157 \\ \hline H 0.3.345459 - 3.203157 \\ \hline H 0.3.345459 - 3.203157 \\ \hline H 0.3.345459 - 3.20327 \\ \hline H 0.3.345459 - 3.203157 \\ \hline H 0.3.345459 - 3.203157 \\ \hline H 0.4.32764 + 1.09240 - 0.57758 \\ \hline H 0.4.32764 + 1.093403 - 0.462006 \\ \hline H 0.4.201797 - 4.34925 - 1.05783 \\ \hline H 0.3.345459 - 2.00327 \\ \hline H 0.3.345459 - 3.203157 \\ \hline H 0.3.345459 - 2.00327 \\ \hline H 0.3.34549 - 1.00403 - 0.462006 \\ \hline H 0.4.20159 - 2.00327 \\ \hline H 0.3.345459 - 2.00127 \\ \hline H 0.3.345459 - 2.00127 \\ \hline H 0.3.34549 - 0.5085037 + 8.3524 - 1.587067 \\ \hline \bullet cis, lk-37-TS \\ \hline cis, lk-37-TS \\ \hline cis, lk-37-TS \\ \hline cis, lk-37-TS \\ \hline C 0.3.12149 0.0.644464 - 0.517609 \\ \hline \end{array}$	$ \begin{array}{c} 0.1.920175.3007912-2.50740 \\ \hline C 0.2.973190.370882 0.018088 \\ \hline C 0.3.306880 3.502747 0.068809 \\ \hline C 0.4.092041 1.61995 - 1.297913 \\ \hline C 0.4.092041 1.61995 - 1.297913 \\ \hline H 0 0.114349 - 0.482742 1.820007 \\ \hline H 0 0.216721 - 1.467312 2.34985 \\ \hline H 0 0.207043 - 0.423279 2.009600 \\ - 2.47000 - 4.096800 2.472763 \\ \hline H 0 0.20454 - 1.096800 2.472763 \\ \hline H 0 0.20454 - 1.20732 0.689224 \\ \hline H 0 - 2.47600 - 1.97191 - 2.481522 \\ \hline H 0 - 2.47600 - 1.97191 - 2.481522 \\ \hline H 0 - 2.47600 - 1.97191 - 2.44152 \\ \hline H 0 - 1.626846 - 0.819763 - 2.885727 \\ \hline H 0 - 1.669022 - 1.876800 2.947830 \\ \hline H 0 - 1.66904 - 0.819763 - 2.885727 \\ \hline H 0 - 1.609045 - 0.05750 \\ \hline H 0 - 1.71594 + 1.20841 - 3.321609 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 2.081797 + 3.302512 \\ \hline H 0 - 2.081797 + 3.31268154 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.952957 - 0.18009 0.386703 \\ \hline H 0 - 1.281494 + 1.00331 - 2.681854 \\ \hline H 0 - 2.081797 + 3.302512 \\ \hline H 0 - 3.34549 3.216171 - 1.499502 \\ \hline H 0 - 1.381494 + 1.03333 - 1.681854 \\ \hline H 0 - 3.910614 - 0.08524 - 2.003157 \\ \hline H 0 - 2.051794 + 1.23621 - 1.038774 \\ \hline H 0 - 4.201094 + 1.033397 - 1.590485 \\ \hline H 0 - 3.21785 \\ \hline \hline H 0 - 2.081797 - 0.590485 \\ \hline H 0 - 3.218494 - 0.0377304 \\ \hline H 0 - 4.201094 + 1.048791 - 1.551.32724 \\ \hline C 0 2.2608797 0.077058 \\ \hline C 0 1.81249 0.085144 - 0.051542 \\ \hline C 0 - 2.060785 + 1.054305 \\ \hline C 0 - 0.40785 + 1.054382 \\ \hline C 0 - 0.40785 + 1.354305 \\ \hline C 0 - 0.40785 + 1.354305 \\ \hline C 0 - 0.40785 + 1.354708 \\ \hline \end{array}$	510 - 2.303642 2.055102 - 0.653640	510-2.805085 2.410150-0.740555
$ \begin{array}{c} C0 - 2973190 3.769852 \ 0.618088 \\ \hline C0 - 3.368803 - 3.502474 \ 0.688309 \\ \hline C0 - 4.002011 1.61995 - 1.259713 \\ \hline C0 - 4.00201 1.561617 0.875458 \\ \hline H 0 - 0.0114349 \ -0.482742 1.830007 \\ \hline H 0 - 0.0114349 \ -0.482742 1.830007 \\ \hline H 0 - 0.073013 \\ \hline H 0 - 0.95594 - 1.54884 \ -1.26173 0 \ 0.223465 \\ \hline H 0 - 2.02739 \ -0.073013 \\ \hline H 0 - 2.02739 \ -0.73013 \\ \hline H 0 - 2.02739 \ -0.7300 \ -0.73013 \\ \hline H 0 - 2.02739 \ -0.7300 \ -0.273500 \\ \hline H 0 - 1.0268478 \ -2.161057 \ -0.273500 \\ \hline H 0 - 2.02739 \ -0.273500 \\ \hline H 0 - 1.47312 \ -2.47007 \ -2.37400 \\ \hline H 0 - 1.47312 \ -2.47007 \ -2.37400 \\ \hline H 0 - 1.47312 \ -2.47007 \ -2.37400 \\ \hline H 0 - 1.46512 \ -2.472137 \ -2.21763 \\ \hline H 0 - 1.47372 \ -2.21763 \ -2.34496 \\ \hline H 0 - 1.17352 \ -2.54645 \ -3.132601 \\ \hline H 0 - 1.17352 \ -2.54645 \ -3.132601 \\ \hline H 0 - 1.17352 \ -2.54760 \ -2.34495 \\ \hline H 0 - 1.17352 \ -2.54760 \ -2.34496 \\ \hline H 0 - 1.17352 \ -2.56649 \ -3.136261 \\ \hline H 0 - 1.17352 \ -2.56649 \ -3.136261 \\ \hline H 0 - 1.17352 \ -2.56649 \ -3.136261 \\ \hline H 0 - 1.17352 \ -2.56649 \ -3.136261 \\ \hline H 0 - 1.17352 \ -2.56649 \ -3.136261 \\ \hline H 0 - 1.17352 \ -2.5760 \ -1.6445 \\ \hline H 0 - 1.17152 \ -2.57190 \ -1.64939 \ -2.732910 \\ \hline H 0 - 1.171594 \ -2.085462 \ -1.0005730 \\ \hline H 0 - 1.271594 \ -1.28080 \ -2.732910 \\ \hline H 0 - 1.71594 \ -1.28080 \ -2.73291 \ -1.6445 \ -1.00097790 \\ \hline H 0 - 1.37526 \ -2.085462 \ -1.064875 \ -1.0007790 \\ \hline H 0 - 2.67847 \ -2.68184 \ -1.0007790 $	$\begin{array}{c} \text{C} 0-2.973190 3.769852 0.618088 \\ \text{C} 0-3.368805 3.502747 0.088309 \\ \text{C} 0-4.209201 1.528408 - 1.261459 \\ \text{H} 0-0.216721 - 2.766617 0.875458 \\ \text{H} 0-0.216721 - 2.766617 0.875458 \\ \text{H} 0-0.216721 - 2.766617 0.875458 \\ \text{H} 0-0.070435 - 0.482742 1.258408 - 1.261459 \\ \text{H} 0-0.070435 - 0.482742 1.258408 - 1.261459 \\ \text{H} 0-0.322705 - 2.725830 - 1.261457 \\ \text{H} 0-0.322705 - 2.725830 - 1.261457 \\ \text{H} 0-0.222705 - 2.725830 - 1.261457 \\ \text{H} 0-0.222705 - 2.725830 - 1.27140 - 0.223465 \\ \text{H} 0-1.267172400 - 0.223465 \\ \text{H} 0-2.658478 - 2.161057 - 0.273500 \\ \text{H} 0-1.467102 - 2.440251 - 3.548447 \\ \text{H} 0-2.658478 - 2.161057 - 0.273500 \\ \text{H} 0-1.476172 - 2.240251 - 3.548447 \\ \text{H} 0-2.658478 - 2.20176 - 2.27360 \\ \text{H} 0-1.476172 - 2.264541 - 3.312609 \\ \text{H} 0-1.17532 - 2.265649 - 3.136261 \\ \text{H} 0-1.476172 - 2.2540451 - 3.31609 \\ \text{H} 0-1.17532 - 2.265649 - 3.136261 \\ \text{H} 0-1.476172 - 2.264541 - 3.31609 \\ \text{H} 0-1.17532 - 2.265649 - 3.136261 \\ \text{H} 0-1.266844 - 0.819763 - 2.885727 \\ \text{H} 0-5.69902 - 2.372910 \\ \text{H} 0-5.69902 - 2.372910 \\ \text{H} 0-5.69902 - 2.37621 - 0.69630 - 2.72910 \\ \text{H} 0-5.69902 - 2.37621 - 0.69630 - 2.72910 \\ \text{H} 0-5.265710 - 0.22107 - 2.666549 - 3.136261 \\ \text{H} 0-4.37297 - 0.500279 \\ \text{H} 0-1.87207 - 0.180690 - 0.32707 - 0.500279 \\ \text{H} 0-1.87207 - 0.180690 - 0.32707 - 0.500279 \\ \text{H} 0-1.87218 - 2.007578 \\ \text{H} 0-1.87218 - 2.007578 \\ \text{H} 0-3.372456 - 2.94237 - 3.129730 \\ \text{H} 0-1.87218 - 2.007578 \\ \text{H} 0-3.2797 - 0.500279 \\ \text{H} 0-3.345459 - 3.216171 + 1.489502 \\ \text{H} 0-3.372456 - 2.94237 - 3.129730 \\ \text{H} 0-1.87218 - 2.007578 \\ \text{H} 0-3.27979 - 0.50077 \\ \text{H} 0-1.88454 \\ \text{H} 0-3.310952 - 10.63073 \\ \text{H} 0-4.255710 0 + 0.18333 - 1.891129 \\ \text{H} 0-2.55710 0 + 0.18333 - 1.891129 \\ \text{H} 0-3.257190 + 0.181249 - 0.033730 \\ \text{H} 0-4.255710 0 + 0.181249 - 0.037370 \\ \text{H} 0-4.255710 0 + 0.181249 - 0.203377 \\ \text{H} 0-3.285719 - 0.11020 - 0.4144587 \\ \text{H} 0-3.285719 - 0.11020 - 0.41785 \\ \text{H} 0-3.285719 - 0.11020 - 0.41785 \\ \text{H} 0-3.285719 - 0.11020 - 0.418429 \\ \text{H} 0-3.285719 - 0.20337$	C 0 -1.920/15 3.609512 -2.305/40	C 0 -2.199615 3.444046 -2.194565
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	$ \begin{array}{c} C0 + 0.021671 \\ 1.61995 + 1.297913 \\ H 0 - 0.21672 \\ 1.276617 0 875458 \\ H 0 - 0.021762 \\ 1.07531 \\ 14494 \\ 0.482742 \\ 1.820007 \\ H 0 - 0.070435 \\ 0.020485 \\ 10 - 0.021702 \\ 1.092544 \\ 0.095594 \\ 0.0965804 \\ 0.72763 \\ H 0 \\ 0.224760 \\ 1.14731 \\ 1.242073 \\ 0.588447 \\ H 0 \\ 1.99514 \\ - 0.996800 \\ 0.224760 \\ 1.17152 \\ 4.0906800 \\ 0.224760 \\ 1.17152 \\ 4.0906800 \\ 0.224760 \\ 1.17152 \\ 4.0906800 \\ 0.224760 \\ 1.17152 \\ 4.0906800 \\ 0.224760 \\ 1.17152 \\ 4.090680 \\ 0.224760 \\ 1.17152 \\ 4.090680 \\ 0.224760 \\ 1.17152 \\ 4.0905840 \\ 0.223469 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.05194 \\ 1.17152 \\ 4.01275 \\ 1.$	C 0 -2.973190 3.769852 0.618088	C 0 -3.368805 3.502747 0.688309
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	C 0 -4.092041 1.619995 -1.297913	C 0 -4.209320 1.258408 -1.261459
$\begin{array}{r c c c c c c c c c c c c c c c c c c c$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H 0 -0.216721 -2.766617 0.875458	H 0 -0.022705 -2.725830 1.092606
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$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$ \begin{array}{llllllllllllllllllllllllllllllllllll$	H = 0.2012407 + 1.142721 + 2.224085	H = 0.1 = 0.05514 = 0.006800 = 0.472762
$ \begin{array}{r llllllllllllllllllllllllllllllllllll$	$ \begin{array}{llllllllllllllllllllllllllllllllllll$	H 0 2.012497 -1.142731 2.234963	H = 0.25314 + 0.900800 + 2.472703
H 0 4.605194 -1.716524 0.689224 H 0 4.387543 -0.97005 2935243 H 0 -1.267100 -197119 - 2.481522 H 0 -2.722137 -2.2178 -2.344696 H 0 -1.467102 -2.540451 - 3.321609 H 0 -1.173523 - 2.665649 - 3.136261 H 0 -1.626846 - 0.819763 - 2.885727 H 0 -1.003279 - 2.072910 H 0 5.669022 - 1.876800 - 2.947830 H 0 6.033997 - 1.696930 1.214645 H 0 4.170776 - 1.295120 3.705612 H 0 5.425018 -0.065262 0.882462 H 0 -1.711594 1.124084 1.558670 H 0 -1.887711 1.000992 1.687363 H 0 -1.952957 - 0.180969 0.386703 H 0 -1.887711 1.000992 1.687363 H 0 -1.032761 4.192551 - 2.033157 H 0 -1.381409 4.108383 - 1.891129 H 0 - 2.067497 4.30805 0.935715 H 0 -2.557190 4.153625 1.036789 H 0 - 3.345459 3.216171 1.489502 H 0 -3.71955 2.916200 1.546875 H 0 - 3.345459 3.216171 1.489502 H 0 -3.71955 2.91620 1.546875 H 0 - 3.356510 0.950623 - 2.142426 H 0 -3.90614 0.61151 - 2.095337 H 0 - 4.40594 1.003403 - 0.462006 H 0 -4.355690 0.611100 - 0.437256 H 0 - 4.921539 2.277420 - 1.590485 H 0 -5.085037 1.835236 - 1.587067 • cis, lk-37-TS • cis, lk-37-TS • cis, lk-37-TS • cis, lk-39-TS • cis, lk-377-TS • cis, lk-39-TS • cis, lk-3754 - 0.082672 c.0713058 <td< th=""><th>$\begin{array}{r l} H 0 4.387 (34.009105) 2.935243 \\ H 0 -3.976 (00 - 197119) - 2.481522 \\ H 0 -1.467102 -2.540451 -3.321609 \\ H 0 -1.467102 -2.540451 -3.321609 \\ H 0 -1.77323 -2.65549 -3.136261 \\ H 0 -1.77323 -2.65549 -3.136261 \\ H 0 -1.77323 -2.65549 -3.136261 \\ H 0 -1.60639 - 2.732910 \\ H 0 -1.60639 - 2.732910 \\ H 0 -1.60639 - 2.732910 \\ H 0 -1.82708 - 0.22107 - 2.67075 \\ H 0 -1.82711 - 1.463420 - 0.075790 \\ H 0 -1.7711594 - 1.24084 - 1.558670 \\ H 0 -1.82771 - 1.43420 - 0.075790 \\ H 0 -1.82771 - 1.43420 - 0.075790 \\ H 0 -1.82771 - 1.43420 - 0.075790 \\ H 0 -1.82771 - 1.434237 - 1.443420 - 0.075790 \\ H 0 -1.82771 - 1.434237 - 1.443420 - 0.075790 \\ H 0 -1.82771 - 1.43420 - 0.07579 \\ H 0 -1.82771 - 1.60899 - 0.386703 \\ H 0 -1.92575 - 0.180969 0.386703 \\ H 0 -1.925157 - 0.180969 0.386703 \\ H 0 -1.827438 - 2.806584 - 3.005753 \\ H 0 -1.321409 + 1.08383 - 1.891129 \\ H 0 -3.05661 + 0.08838 - 3.005753 \\ H 0 -1.321409 + 1.08383 - 1.891129 \\ H 0 -3.05661 + 0.08883 - 1.891129 \\ H 0 -3.05661 + 0.08838 - 3.005761 \\ H 0 -3.345459 + 3.016111 + 4.9502 \\ H 0 -3.3719955 - 2.916260 + 1.546875 \\ H 0 -3.910614 + 0.611511 - 2.095337 \\ H 0 -4.32569 + 1.003430 - 0.462006 \\ H 0 -3.3910614 + 0.611100 - 0.437256 \\ H 0 -3.3910614 + 0.61110 - 0.437256 \\ H 0 -3.3910614 + 0.61110 - 0.437256 \\ H 0 -3.910614 + 0.611511 - 2.95337 \\ H 0 -5.085037 + 1.835236 - 1.587067 \\ \bullet \ cis, lk - 37 - TS \ cis, ll - 39 - TS \\ cis, ll - 39 - TS \\ cis, ll - 390 - TS \\ cis, ll - 306872 + 0.713058 \\ co 2.060879 + 0.068744 + 0.068746 + 0.01681 - 0.01691 \\ co 2.080897 + 0.087962 - 0.165842 \\ co 2.080897 + 0.579823 - 0.165842 \\ co 0.0460785 + 0.57183 + 0.420654 \\ co 0.0460785 + 0$</th><th>H 0 2.4//112 -2.4202/3 -0.54844/</th><th>H 0 2.658478 -2.161057 -0.273500</th></td<>	$\begin{array}{r l} H 0 4.387 (34.009105) 2.935243 \\ H 0 -3.976 (00 - 197119) - 2.481522 \\ H 0 -1.467102 -2.540451 -3.321609 \\ H 0 -1.467102 -2.540451 -3.321609 \\ H 0 -1.77323 -2.65549 -3.136261 \\ H 0 -1.77323 -2.65549 -3.136261 \\ H 0 -1.77323 -2.65549 -3.136261 \\ H 0 -1.60639 - 2.732910 \\ H 0 -1.60639 - 2.732910 \\ H 0 -1.60639 - 2.732910 \\ H 0 -1.82708 - 0.22107 - 2.67075 \\ H 0 -1.82711 - 1.463420 - 0.075790 \\ H 0 -1.7711594 - 1.24084 - 1.558670 \\ H 0 -1.82771 - 1.43420 - 0.075790 \\ H 0 -1.82771 - 1.43420 - 0.075790 \\ H 0 -1.82771 - 1.43420 - 0.075790 \\ H 0 -1.82771 - 1.434237 - 1.443420 - 0.075790 \\ H 0 -1.82771 - 1.434237 - 1.443420 - 0.075790 \\ H 0 -1.82771 - 1.43420 - 0.07579 \\ H 0 -1.82771 - 1.60899 - 0.386703 \\ H 0 -1.92575 - 0.180969 0.386703 \\ H 0 -1.925157 - 0.180969 0.386703 \\ H 0 -1.827438 - 2.806584 - 3.005753 \\ H 0 -1.321409 + 1.08383 - 1.891129 \\ H 0 -3.05661 + 0.08838 - 3.005753 \\ H 0 -1.321409 + 1.08383 - 1.891129 \\ H 0 -3.05661 + 0.08883 - 1.891129 \\ H 0 -3.05661 + 0.08838 - 3.005761 \\ H 0 -3.345459 + 3.016111 + 4.9502 \\ H 0 -3.3719955 - 2.916260 + 1.546875 \\ H 0 -3.910614 + 0.611511 - 2.095337 \\ H 0 -4.32569 + 1.003430 - 0.462006 \\ H 0 -3.3910614 + 0.611100 - 0.437256 \\ H 0 -3.3910614 + 0.61110 - 0.437256 \\ H 0 -3.3910614 + 0.61110 - 0.437256 \\ H 0 -3.910614 + 0.611511 - 2.95337 \\ H 0 -5.085037 + 1.835236 - 1.587067 \\ \bullet \ cis, lk - 37 - TS \ cis, ll - 39 - TS \\ cis, ll - 39 - TS \\ cis, ll - 390 - TS \\ cis, ll - 306872 + 0.713058 \\ co 2.060879 + 0.068744 + 0.068746 + 0.01681 - 0.01691 \\ co 2.080897 + 0.087962 - 0.165842 \\ co 2.080897 + 0.579823 - 0.165842 \\ co 0.0460785 + 0.57183 + 0.420654 \\ co 0.0460785 + 0$	H 0 2.4//112 -2.4202/3 -0.54844/	H 0 2.658478 -2.161057 -0.273500
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H0 4.170776 - 1.295120 3.705612 H 0 5.425018 - 0.065262 0.882462 H0 5.095840 - 0.222107 2.627075 H 0 5.425018 - 0.065262 0.882462 H0 - 1.71594 1.124084 1.558670 H 0 - 1.83771 1.40362 0 - 0.075790 H0 - 1.952957 - 0.180969 0.386703 H 0 - 1.83711 1.00092 1.687363 H0 - 1.952957 - 0.180969 0.386703 H 0 - 1.83711 1.00092 1.687363 H0 - 1.952957 - 0.180969 0.386703 H 0 - 1.83711 1.00092 1.687363 H0 - 1.361701 - 1.00556 2.942337 - 3.129730 H 0 - 1.83711 1.00092 1.687363 H0 - 1.361409 4.10383 - 3.1817 H 0 - 1.381409 4.103838 - 1.891129 H0 - 2.01797 4.340805 0.935715 H 0 - 3.305661 4.068695 - 2.600327 H0 - 3.3752365 4.491104 0.338074 H 0 - 3.719955 2.10260 1.546875 H0 - 3.3752365 4.491104 0.338074 H 0 - 4.201004 4.148087 0.377304 H0 - 4.201004 4.148087 0.377304 H 0 - 4.201004 4.148087 0.377304 H0 - 4.921539 2.277420 - 1.590485 H 0 -5.085037 1.835236 - 1.587067 • cis,lk-37-TS • cis,lk-37-TS • cis,ul-39-TS	H0 4,170776 - 1.295120 3,705612 H0 5,425018 -0.065262 0,882462 H0 5,095840 -0.22107 2,627075 H0 4,442377 - 1,44320 -0.075700 H0 -1,952957 -0.180969 0,386703 H0 -1,87771 - 1,409092 1,687363 H0 -1,952957 -0.180969 0,386703 H0 -1,87771 - 1,43420 - 0.075700 H0 -1,952957 -0.180969 0,386703 H0 -1,87771 - 1,43420 - 0.07570 H0 -1,052957 -0.180969 0,386703 H0 -1,87771 - 1,43420 - 0.075730 H0 -1,052957 -0.180969 0,386703 H0 -1,87711 - 1,00902 1,687363 H0 -1,052957 -0.180969 0,386703 H0 -1,87711 - 1,00902 1,687363 H0 -1,052161 4,19251 - 2,033157 H0 -1,381409 4,108383 - 1,891129 H0 -2,07197 4,340805 0,935715 H0 -3,305661 4,068695 - 2,600327 H0 -3,375265 4,491104 0,338074 H0 -2,557190 4,153625 1,036789 H0 -3,3752365 4,491104 0,338074 H0 -4,201509 0,511100 - 0,437256 H0 -3,31061 0,95062 - 2,142426 H0 -3,910614 0,01151 - 2.095337 H0 -4,921539 2,277420 - 1,590485 H0 -5,085037 1,835236 - 1,587067 • cis,lk-37-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-3064 0,015100 0,020140 0,01590	H 0 5.669022 -1.876800 2.947830	H 0 6.033997 -1.696930 1.214645
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$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$ \begin{array}{c} 10 \ 0.303 \ 100 \ 1.021 \ 0.001 \ 1.001 \ 0.0$	H = 0.5005840 + 0.222107 + 2.627075	H = 0.125010 = 0.005202 = 0.002102 H = 0.4842377 = 1.443420 = 0.075700
In 0 - 1./11394 1.124084 1.338070 In 0 - 1.887/111100992 1.85365 In 0 - 1.95957 - 0.180990 0.386703 In 0 - 1.887/111100992 1.85365 In 0 - 1.640656 2.942337 - 3.129730 In 0 - 1.827438 2.806854 - 3.005753 In 0 - 1.032761 4.192551 - 2.033157 In 0 - 1.827438 2.806854 - 3.005753 In 0 - 2.071774 3.40805 0.935715 In 0 - 3.0561 4.068805 - 2.600327 In 0 - 3.345493 3.216171 1.489502 In 0 - 3.07304 In 0 - 3.3555 4.491104 0.0338074 In 0 - 4.216875 In 0 - 3.32565 4.491104 0.338074 In 0 - 4.216875 In 0 - 3.32565 4.91104 0.338074 In 0 - 4.216875 In 0 - 4.921539 2.277420 - 1.590485 In 0 - 3.910614 0.611511 - 2.095337 In 0 - 4.921539 2.277420 - 1.590485 In 0 - 5.085037 1.835236 - 1.587067 In 0 - 4.921539 2.277420 - 1.590485 In 0 - 5.085037 1.835236 - 1.587067 In 0 - 3.1287540082672 0.713058 In 0 - 2.286392 - 0.246490 (a.u.): -1251.32724 In 0 - 3.1287540082672 0.713058 In 0 - 2.286392 - 0.246490 0.45056 In 2.269879 0.8799623 - 0.155482 In 1.812149 0.684464 0.517609	H 0 - 1,711294 1.124064 1.536070 H 0 - 1,827181 1.03092 1.687363 H 0 - 1,92557 - 0.180969 0.386703 H 0 - 1,971252 - 0.327927 0.520279 H 0 - 1,032761 4.192551 - 2.033157 H 0 - 1,827438 2.806854 - 3.005753 H 0 - 1,032761 4.192551 - 2.033157 H 0 - 1,827438 2.806854 - 3.005753 H 0 - 2.091797 4.340805 0.935715 H 0 - 3.30561 (- 0.66869 - 2.600327) H 0 - 3,34549 3.216171 1.489502 H 0 - 3.71955 2.916260 1.546875 H 0 - 3.32554 .491104 0.338074 H 0 - 4.201004 4.148087 0.37304 H 0 - 4.446594 1.003403 - 0.462006 H 0 - 4.3016014 0.611511 - 2.095337 H 0 - 4.921539 2.277420 - 1.590485 H 0 - 5.085037 1.835236 - 1.587067 • cis,lk-37-TS • cis,ul-39-TS • cis,lk-37-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-087902 - 0.713058 C 0 2.286392 - 0.246490 1.454056 C 0 2.286392 - 0.246490 1.454056 C 0 1.812149 0.684464 0.517609 C 0 0.28870 0.068714 0.600159 C 0 - 0.528138 0.520654	II 0 5.093040 -0.222107 2.027075	110 + .0+2.577 - 1.++5+20 - 0.075750
H 0 - 1.922957 - 0.180969 0.388703 H 0 - 1.927252 - 0.327927 0.22792 H 0 - 1.922957 - 0.180959 0.388703 H 0 - 1.927282 - 0.327927 0.22792 H 0 - 1.032761 4.192551 - 2.033157 H 0 - 1.381409 4.108383 - 1.891129 H 0 - 2.678497 4.308731 - 2.681854 H 0 - 3.005661 4.068605 - 2.600327 H 0 - 3.345459 3.216171 1.489502 H 0 - 3.300561 4.068605 - 2.600327 H 0 - 3.3752365 4.491104 0.338074 H 0 - 4.201004 4.148087 0.377304 H 0 - 4.201004 4.148087 0.377304 H 0 - 4.355690 0.611100 - 0.37256 H 0 - 4.921539 2.277420 - 1.590485 H 0 - 5.085037 1.835236 - 1.587067 • cis,lk-37-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • 0.8312YP/6-31+G(d) (a.u.): -1251.327191 B312YP/6-31+G(d) (a.u.): -1251.32724 C 0 3.128754 - 0.082672 0.713058 C 0 2.286392 - 0.246490 1.454056 C 0 2.286392 - 0.246490 1.454056 C 0 1.812149 0.684464 0.517609	H 0 - 1, 952957 - 0.180969 0.3867/03 H 0 - 1, 972257 - 0.320279 H 0 - 1, 952957 - 0.180969 0.3867/03 H 0 - 1, 97225 - 0.320279 H 0 - 1, 022761 4.192551 - 2.033157 H 0 - 1, 381409 4.108383 - 1.891129 H 0 - 2.678497 4.308731 - 2.681854 H 0 - 1, 381409 4.108383 - 1.891129 H 0 - 2.678497 4.308731 - 2.681854 H 0 - 1.381409 4.108383 - 1.891129 H 0 - 3.345459 3.216171 1.489502 H 0 - 3.3752365 4.491104 0.338074 H 0 - 3.3752365 4.491104 0.338074 H 0 - 4.201004 4.148087 0.377304 H 0 - 4.321539 2.277420 - 1.590485 H 0 - 4.201004 4.148087 0.377304 H 0 - 4.921539 2.277420 - 1.590485 H 0 - 5.085037 1.835236 - 1.587067 • cis, lk-37-TS • cis, ul-39-TS 0 B3LYP/6-31+G(d) (a.u.): -1251.327191 C 0 3.128754 - 0.082672 0.713058 C 0 2.286392 - 0.246490 1.454056 C 0 2.286392 - 0.246490 1.454056 C 0 2.286392 - 0.246490 1.45605 C 0 1.812149 0.684464 0.517609 C 0 1.251511 1.231628 - 0.221100 C 0 - 0.528180 0.5446	H 0 -1./11594 1.124084 1.558670	H 0 -1.88//11 1.000992 1.08/303
H 0 - 1.640656 2.942337 - 3.129730 H 0 - 1.827438 2.806854 - 3.005753 H 0 - 1.032761 4.192551 - 2.033157 H 0 - 1.381409 4.108383 - 1.891129 H 0 - 2.091797 4.340805 0.935715 H 0 - 3.005661 4.068695 - 2.600327 H 0 - 3.345459 3.216171 1.489502 H 0 - 3.719955 2.916260 1.546875 H 0 - 3.3752365 4.491104 0.338074 H 0 - 4.201004 4.148087 0.377304 H 0 - 4.921539 2.277420 - 1.590485 H 0 - 4.355690 0.611100 - 0.437256 H 0 - 4.921539 2.277420 - 1.590485 H 0 - 5.085037 1.835236 - 1.587067 • cis,lk-37-TS • cis,ul-39-TS • 0 B3LYP/6-31+G(d) (a.u.): -1251.327191 C 0 3.128754 - 0.082672 0.713058 C 0 3.128754 - 0.082672 0.713058 C 0 2.286392 - 0.246490 1.454056 C 0 2.868979 0.8790 0.879053 C 0 2.886427 0.713058	H 0 - 1.640656 2.942337 - 3.129730 H 0 - 1.827438 2.806854 - 3.005753 H 0 - 1.032761 4.192551 - 2.033157 H 0 - 1.381409 4.108383 - 1.891129 H 0 - 2.091797 4.340805 0.935715 H 0 - 3.05661 4.068695 - 2.600327 H 0 - 3.345459 3.216171 1.489502 H 0 - 3.05661 4.068695 - 2.600327 H 0 - 3.352365 4.491104 0.338074 H 0 - 4.2557190 4.153625 1.036789 H 0 - 4.446594 1.003403 - 0.462006 H 0 - 4.235690 0.611100 - 0.437256 H 0 - 4.921539 2.277420 - 1.590485 H 0 - 5.085037 1.83236 - 1.587067 • cis, lk-37-TS • cis, ul-39-TS • cis, lk-37-TS • cis, ul-39-TS • cis, lk-27-L120104 B3LYP/6-31+G(d) (a.u.): -1251.327191 C 0 3.128754 - 0.082672 0.713058 C 0 2.286392 - 0.246490 1.454056 C 0 2.286392 0.879623 - 0.15482 C 0 1.812149 0.684464 0.517609 C 0 0.25810 0.065214 0.600159 C 0 - 0.5781430 0.420054	H 0 -1.952957 -0.180969 0.386703	H 0 -1.971252 -0.327927 0.520279
H 0 -1.032761 4.192551 - 2.033157 H 0 -1.381409 4.108383 - 1.891129 H 0 -2.678497 4.308731 - 2.681854 H 0 -3.005661 4.068695 - 2.600327 H 0 -3.345459 3.216171 1.489502 H 0 -3.05561 4.068695 - 2.00327 H 0 -3.752365 4.491104 0.338074 H 0 -2.557190 4.153625 1.036789 H 0 -3.752365 4.491104 0.338074 H 0 -4.201004 4.148087 0.377304 H 0 -4.446594 1.003403 - 0.462006 H 0 -4.355690 0.611100 - 0.437256 H 0 -4.921539 2.277420 - 1.590485 H 0 -5.085037 1.835236 - 1.587067 • cis,lk-37-TS • cis,ul-39-TS • 0 B3LYP/6-31+G(d) (a.u.): -1251.327191 C 0 3.128754 - 0.082672 0.713058 C 0 3.128754 - 0.082672 0.713058 C 0 2.286392 - 0.246490 1.454056 C 0 1.812149 0.684464 0.517609 C 0 1.812149 0.684464 0.517609	H 0 -1.032761 4.192551 -2.033157 H 0 -1.381409 4.108383 -1.891129 H 0 -2.0678497 4.308731 -2.681854 H 0 -3.005661 4.068695 -2.600327 H 0 -3.345459 3.216171 1.489502 H 0 -3.752365 4.491104 0.338074 H 0 -3.45594 1.003403 -0.462006 H 0 -4.201004 4.148087 0.377304 H 0 -4.921539 2.277420 -1.590485 H 0 -4.201004 4.148087 0.377304 • cis,lk-37-TS • cis,ul-39-TS • cis,lk-37-TS • cis,ul-39-TS • cis,lk-37-TS • cis,ul-39-TS • cis,lk-37-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • colored and an and an and an and an	H 0 -1.640656 2.942337 -3.129730	H 0 -1.827438 2.806854 -3.005753
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H 0 -1.032761 4.192551 -2.033157	H 0 -1.381409 4.108383 -1.891129
H 0 -2.091797 4.340805 0.935715 H 0 -3.345459 3.216171 1.489502 H 0 -3.345459 3.216171 1.489502 H 0 -3.719955 2.916260 1.546875 H 0 -3.752365 4.491104 0.338074 H 0 -4.201004 4.148087 0.377304 H 0 -4.45954 1.003403 -0.462006 H 0 -4.253569 0.611100 -0.437256 H 0 -3.886810 0.950623 -2.142426 H 0 -3.910614 0.611511 -2.095337 H 0 -4.921539 2.277420 -1.590485 H 0 -5.085037 1.835236 -1.587067 • cis,lk-37-TS • cis,ul-39-TS 0 B3LYP/6-31+G(d) (a.u.): -1251.327191 B3LYP/6-31+G(d) (a.u.): -1251.32724 C 0 3.128754 -0.082672 0.713058 C 0 2.286392 -0.246490 1.454056 C 0 2.809879 0.879623 -0.165482 C 0 1.812149 0.684464 0.517609	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H 0 -2.678497 4.308731 -2.681854	H 0 -3.005661 4.068695 -2.600327
H 0 -3.345459 3.216171 1.489502 H 0 -3.752365 4.491104 0.338074 H 0 -3.752365 4.491104 0.338074 H 0 -4.446594 1.003403 -0.462006 H 0 -4.446594 1.003403 -0.462006 H 0 -4.535690 0.611100 -0.437256 H 0 -4.921539 2.277420 -1.590485 H 0 -3.910614 0.611511 -2.095337 • cis,lk-37-TS • cis,ul-39-TS • 0.812VP/6-31+G(d) (a.u.): -1251.327191 B3LYP/6-31+G(d) (a.u.): -1251.32714 C 0 3.128754 -0.082672 0.713058 C 0 2.286392 -0.246490 1.454056 C 0 1.812149 0.684464 0.517609 C 0 1.812149 0.684464 0.517609	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H 0 -2.091797 4.340805 0.935715	H 0 -2.557190 4.153625 1.036789
H 0 3.752365 4.91104 0.338074 H 0 4.446594 1.003403 -0.462006 H 0 -3.886810 0.950623 2.142426 H 0 -4.921539 2.277420 -1.590485 • cis, lk - 37-TS • cis, ul - 39-TS • cis, lk - 37-TS • cis, ul - 39-TS • cis, lk - 37-TS • cis, ul - 39-TS • $cis, ul-39-TS$ •	H 0 3.572365 4.491104 0.388074 H 0 -4.446594 1.003403 -0.462006 H 0 -3.886810 0.950623 -2.142426 H 0 -4.921539 2.277420 -1.590485 • cis,lk-37-TS • cis,ul-39-TS • cis,lk-37-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-TS • cis,ul-39-Cis,ul-30-C	H 0 -3 345459 3 216171 1 489502	H 0 - 3.719955 2.916260 1.546875
In 0 - 3.15230 + 4.25130	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$H_0 = 3.752365 A A9110A 0 33807A$	H = 4.201004.4.148087 = 377304
In 0 -4.40394 1,003403 -0.402000 In 0 -4.40339 1,003403 -0.402000 In 0 -4.40394 1,003403 -0.402000 In 0 -4.40339 1,0014 0,611101 -2.095337 In 0 -4.921539 2.277420 -1.590485 In 0 -3.910614 0,611511 -2.095337 In 0 -4.921539 2.277420 -1.590485 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.835236 -1.587067 In 0 -5.085037 1.587067 In 0 -5.08507 0.31+G(d) (a.u.): -1251.327191 In 0 -5.286392 -0.246490 1.454056 In 0 -5.08507 0.87908790 0.879623 -0.165482 In 0 -5.84864 0.517609	In 0 = 4.440594 (1.005405 = 0.4402006) In 0 = 4.353090 (0.011100 = 0.37250) In 0 = 4.921539 2.277420 = 1.590485 In 0 = 4.353090 (0.011101 = 0.057250) In 0 = 4.921539 2.277420 = 1.590485 In 0 = 3.910614 0.611511 = 2.095337 In 0 = 5.085037 1.835236 = 1.587067 In 0 = 6.5, lk = 37 - TS In 0 = 6.5, lk = 37 - TS In 0 = 6.5, lk = 37 - TS In 0 = 6.5, lk = 37 - TS In 0 = 8.1, lk = 37 - TS In 0 = 6.5, lk = 37 - TS In 0 = 8.1, lk = 37 - TS In 0 = 6.5, lk = 37 - TS In 0 = 8.1, lk = 37 - TS In 0 = 6.5, lk = 39 - TS In 0 = 8.1, lk = 37 - TS In 0 = 6.5, lk = 3.1, lk = 3.1	110 - 3.752505 + .+5110 + 0.55007 +	110 - 4.201004 + .140007 0.377304
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H 0 -4.921539 2.277420 -1.590485 H 0 -5.085037 1.835236 -1.587067 • cis,lk-37-TS • cis,ul-39-TS • 0 B3LYP/6-31+G(d) (a.u.): -1251.327191 B3LYP/6-31+G(d) (a.u.): -1251.32724 C 0 3.128754 -0.082672 0.713058 C 0 2.286392 -0.246490 1.454056 C 0 2.609879 0.879623 -0.165482 C 0 1.812149 0.684464 0.517609	H 0 -4.921539 2.277420 -1.590485 H 0 -5.085037 1.835236 -1.587067 • cis,lk-37-TS • cis,ul-39-TS • 0 B3LYP/6-31+G(d) (a.u.): -1251.327191 B3LYP/6-31+G(d) (a.u.): -1251.32724 C 0 3.128754 -0.082672 0.713058 C 0 2.286392 -0.246490 1.454056 C 0 1.2515111 1.231628 -0.221100 C 0 0.460785 1.054138 0.420654 C 0 0.460785 1.054138 0.547668 1.239532	H 0 -3.886810 0.950623 -2.142426	H 0 -3.910614 0.611511 -2.095337
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C 0 0.877563 -1.791016 0.008804	C 0 0.032028 -1.946259 0.750702
C 0 2.254013 -1.833084 0.247818	C 0 1.409439 -1.988327 0.989900
C 0 3.250610 -2.102066 -0.849060	C 0 2.402634 -2.244690 -0.114410
O 0 3.040634 -2.746338 -1.849900	O 0 2.189133 -2.854553 -1.135315
0 0 4.481552 -1.576080 -0.605453	0 0 3.635239 -1.720000 0.141846
C 0 4.540939 -0.598541 0.482407	C 0 3.676041 -0.848785 1.313232
C 0 -0.026077 -2.248856 1.061249	C 0 -0.873962 -2.368210 1.815628
O 0 0.275345 -2.421356 2.237244	O 0 -0.572052 -2.512848 2.995255
O 0 -1.287048 -2.461197 0.592743	O 0 -2.138733 -2.577682 1.355469
C 0 -2.226624 -2.989212 1.544174	C 0 -3.083572 -3.063522 2.323929
C 0 5.214478 -1.207855 1.705750	C 0 4.832993 0.121567 1.119598
C 0 -1.177444 0.973114 0.453079	C 0 -1.987030 0.848800 1.044617
O 0 -1.456253 1.655243 -0.751526	O 0 -2.228149 1.482742 -0.193954
Si 0 -2.996078 2.070068 -1.304886	Si 0 -3.748947 1.878876 -0.809830
C 0 -2.686142 2.900665 -2.961380	C 0 -3.385742 2.640000 -2.488937
C 0 -3.814957 3.257614 -0.083862	C 0 -4.599426 3.117752 0.336166
C 0 -4.054031 0.517563 -1.498032	C 0 -4.806549 0.322600 -0.971725
H 0 2.755539 -0.106461 1.735077	H 0 1.876144 -0.215897 2.461411
H 0 3.238464 1.197174 -0.997910	H 0 2.452454 0.943619 -0.324081
H 0 0.911041 1.848770 -1.048004	H 0 0.145950 1.637558 -0.440155
H 0 0.562546 0.222183 1.544815	H 0 -0.283859 0.124466 2.209167
H 0 0.483856 -1.681366 -0.994629	H 0 -0.360229 -1.861755 -0.255569
H 0 2.526855 -2.296890 1.196121	H 0 1.688965 -2.444458 1.941345
H 0 5.175354 0.195847 0.075256	H 0 3.880493 -1.483307 2.185303
H 0 -3.159241 -3.110565 0.991852	H 0 -4.018784 -3.189163 1.776993
H 0 -1.879898 -3.952728 1.927856	H 0 -2.749237 -4.019302 2.736816
H 0 -2.359802 -2.299164 2.382370	H 0 -3.205978 -2.346069 3.140610
H 0 4.608810 -2.003998 2.152618	H 0 5.769989 -0.431519 0.997650
H 0 6.185669 -1.630112 1.429886	H 0 4.922363 0.772461 1.996567
H 0 5.376785 -0.433792 2.465271	H 0 4.685318 0.746857 0.234222
H 0 -1.492371 1.579010 1.322296	H 0 -2.315170 1.494995 1.879318
H 0 -1.737030 0.026550 0.508911	H 0 -2.559311 -0.088165 1.126923
H 0 -2.186371 2.216263 -3.657486	H 0 -2.867783 1.926071 -3.140625
H 0 -2.048035 3.785233 -2.846069	H 0 -2.747894 3.526810 -2.390747
H 0 -3.626526 3.224060 -3.425873	H 0 -4.310333 2.946579 -2.994720
H 0 -3.203003 4.155533 0.068726	H 0 -3.988586 4.019302 0.470642
H 0 -3.979248 2.794373 0.897537	H 0 -4.795197 2.695389 1.330231
H 0 -4.795410 3.583817 -0.455276	H 0 -5.566818 3.431396 -0.077942
H 0 -4.244568 0.023514 -0.536819	H 0 -5.025665 -0.133179 0.002228
H 0 -3.571808 -0.213455 -2.158554	H 0 -4.308426 -0.434784 -1.589355
H 0 -5.031006 0.766602 -1.933105	H 0 -5.769989 0.556641 -1.443756

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