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Supporting Information

Scandium and Lanthanum Hydride Complexes Stabilized by Super-bulky Penta-arylcyclopentadienyl Ligands

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Experimental Procedures

General remarks

All reactions were carried out under a dry and oxygen-free nitrogen atmosphere using Schlenk techniques and a Vigor glovebox. The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves (4 Å) catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by O_2 (GE) / H_2O (Xentaur) to ensure both were always below 0.1 ppm. Toluene, hexane and Et_2O were purified by use of a Vigor VSPS-5 solvent purification system, and dried over fresh Na chips in the glovebox. THF and C_6D_6 were distilled from Na/K alloy/benzophenone, degassed by the freeze-pump-thaw method (three times), and dried over fresh Na chips in the glovebox. $(Cp^{Ar5})H$ ($Cp^{Ar5} = C_5Ar_5$; Ar = 3,5-^{i}Pr$_2$-C$_6$H$_3$),[1] K(*p*-CH$_2$-C$_6$H$_4$-Me)[2] and $[(Cp^{Ar5})Sc(p\text{-}CH_2\text{-}C_6H_4\text{-}Me)_2(THF)]$[3] (**1**) were synthesized according to the published procedures. $K(Cp^{Ar5})$ was generated *in situ* from the reaction of $(Cp^{Ar5})H$ with excess KH in THF, and used directly after filtration. Other reagents were purchased and used without purification.

Samples for NMR spectroscopic measurements were prepared in the glovebox by use of J. Young valve NMR tubes. ^1H and ^{13}C NMR spectra were recorded on the Bruker AV400 or AV500 spectrometer and referenced to the resonances of the solvent used. IR spectra were recorded as KBr pellets on a Nicolet iS5 FT-IR spectrometer. The UV-Vis spectra were recorded on CARY500. The elemental analyses were performed on Elementar Vario EL cube (WO_3 was used as pro-oxidant) at National Analytical Research Centre of Changchun Institute of Applied Chemistry (CIAC).

Synthesis of [(Cp^{Ar5})Sc(H)(μ-OC_4H_9)]$_2$ (2).

In the glovebox, [(Cp^{Ar5})Sc(*p*-CH_2-C_6H_4-Me)$_2$(THF)] (**1**) (600 mg, 0.5 mmol) in hexane (5 mL) were charged into a glass tube in a medium-pressure autoclave with a magnetic stirring bar. The autoclave was transferred outside of the glovebox and pressurized with H_2 to 20 atm. The mixture was stirred at room temperature for 12 h. Pressure was released and the autoclave was quickly returned to the glovebox. After filtration, all the volatiles were removed under vacuum. The residue was washed with cold hexane (1 mL) and dried under vacuum to give **2** (335 mg, 0.17 mmol, 68% yield) as a pale-yellow solid. Single crystals of **2** suitable for X-ray analysis, were grown from hexane at -30 °C. ^{1}H NMR (500 MHz, C_6D_6, 25 °C): δ = 7.22 (s, 20H, C_5Ar_5), 6.87 (s, 10H, C_5Ar_5), 4.04 (br, 2H, Sc–*H*), 2.76 (sept, 20H, C*H*Me$_2$), 2.40 (m, 4H, O(C*H*$_2$)$_3$CH$_3$), 2.30 (m, 4H, O(C*H*$_2$)$_3$CH$_3$), 1.33 (m, 4H, O(C*H*$_2$)$_3$CH$_3$), 1.12 (d, 120H, CH*Me*$_2$), 0.48 (m, 6H, O(CH$_2$)$_3$C*H*$_3$). ^{13}C {^{1}H} NMR (126 MHz, C_6D_6, 25 °C): δ = 147.79 (*C*$_5$*Ar*$_5$), 136.22 (C_5Ar_5), 130.18 (C_5Ar_5), 128.17 (C_5Ar_5), 122.24 (C_5Ar_5), 69.55 (O(*C*H$_2$)$_3$CH$_3$), 37.13 (O(*C*H$_2$)$_3$CH$_3$), 34.11 (*C*HMe$_2$), 24.01 (CH*Me*$_2$), 17.86 (O(*C*H$_2$)$_3$CH$_3$), 13.37 (O(CH$_2$)$_3$*C*H$_3$). Anal. calcd. for (**2**) $C_{138}H_{190}O_2Sc_2$ (1970.80): C, 84.10; H, 9.72; found: C, 84.62; H, 9.95. FT-IR (KBr, cm^{-1}): 3612, 2958, 2868, 1767, 1595, 1467, 1380, 1361, 1336, 1313, 1188, 1131, 1100, 1067, 939, 920, 872, 763, 713.

Synthesis of [(Cp^{Ar5})Sc(D)(μ-OC_4H_8D)]$_2$ (2-D).

In the glovebox, [(Cp^{Ar5})Sc(*p*-CH_2-C_6H_4-Me)$_2$(THF)] (**1**) (100 mg, 0.08 mmol) in hexane (5 mL) were charged into a glass tube in a medium-pressure autoclave with a magnetic stirring bar. The autoclave was transferred outside of the glovebox and pressurized with D_2 to 10 atm. The mixture was stirred at room temperature for 3 days. Pressure was released and the autoclave was quickly returned to the glovebox. After filtration, all the volatiles were removed under vacuum to give **2-D** (43 mg, 0.03 mmol, 74% yield) as a pale-yellow solid. ^{2}H NMR (500 MHz, C_6H_6, 25 °C): δ = 4.04 (s, 2D, Sc–*D*), 0.46 (s, 2D, O(CH$_2$)$_3$C*D*H$_2$). FT-IR (KBr, cm^{-1}): 3623, 2958, 2868, 1767, 1595, 1467, 1380, 1361, 1338, 1314, 1188, 1131, 1100, 1067, 939, 920, 872, 763, 713.

Synthesis of [(Cp^{Ar5})La(*p*-CH_2-C_6H_4-Me)$_2$(THF)] (3).

$LaBr_3$ (379 mg, 1 mmol) in THF (20 mL) was stirred at 75 °C for 5 h in a 100mL Schlenk-flask. The Schlenk-flask was quickly returned to the glovebox. K(Cp^{Ar5}) (1.00 mmol) in 10 mL THF solution was added dropwise to the stirred solution of $LaBr_3$. The resulting slurry was stirred at room temperature for 12 h. Solid of K(*p*-CH_2-C_6H_4-Me) (288 mg, 2.00 mmol) was

added to the resulting pale-yellow slurry in several portions, which afforded a yellow brown colored solution that was stirred at room temperature for 3 h. The mixture was then filtered through a Celite-padded coarse frit to remove the insoluble salts. The yellow brown filtrate was collected and the volatiles were removed under reduced pressure to give a yellow solid. This solid was extracted with hexane (2 x 5 mL). The obtained extract was concentrated to 3 mL, and kept at -30 °C to give **3** (965 mg, 0.75 mmol, 75% yield) as pale-yellow crystals. Single crystals of **3** • (C_6H_{14}) suitable for X-ray analysis, were grown from hexane at -30 °C. ^{1}H NMR (500 MHz, C_6D_6, 25 °C): δ = 7.09 (s, 10H, C_5Ar_5), 6.99 (d, J = 10 Hz, 4H, C_6H_4), 6.84 (s, 5H, C_5Ar_5), 6.59 (d, J = 10 Hz, 4H, C_6H_4), 2.99 (br, 4H, α-THF), 2.68 (m,10H, CHMe$_2$), 2.29 (s, 4H, CH_2-C_6H_4), 2.16 (s, 6H, C_6H_4-Me), 1.22 (br, 4H, β-THF),1.09 (d, J = 5 Hz, 60H, CHMe_2). ^{13}C {^{1}H} NMR (126 MHz, C_6D_6, 25 °C): δ = 148.18 (C_5Ar_5), 147.04 (C_6H_4), 137.82 (C_5Ar_5), 132.68 (C_6H_4), 128.48 (C_5Ar_5), 126.91 (C_6H_4), 123.29 (C_6H_4), 122.54 (C_5Ar_5), 69.70 (CH$_2$-C_6H_4), 69.21 (α-THF), 34.71 (CHMe$_2$), 25.63 (β-THF), 24.44 (CHMe_2), 20.89 (C_6H_4-Me). Anal. calcd. for (**3**) $C_{85}H_{111}O_1La_1$ (1287.64): C, 79.28; H, 8.69; found: C, 79.42; H, 8.81. FT-IR (KBr, cm^{-1}): 3616, 2959, 2933, 2860, 1593, 1520, 1467, 1382, 1363, 1336, 1305, 1252, 1187, 1106, 1067, 1029, 944, 925, 872, 826, 768, 714.

Synthesis of [(Cp^{Ar5})La(μ-H)]$_2$ (4).

In the glovebox, [(Cp^{Ar5})La(p-CH$_2$-C$_6$H$_4$-Me)$_2$(THF)] (**3**) (965 mg, 0.75 mmol) in hexane (5 mL) were charged into a glass tube in a medium-pressure autoclave. The autoclave was transferred outside of the glovebox and pressurized with H_2 to 20 atm. The mixture was kept at room temperature for 12 h. Pressure was released and the autoclave was quickly returned to the glovebox. After filtration, the solid was washed with cold hexane (1 mL) and dried under vacuum to give **4** (566 mg, 0.28 mmol, 75% yield) as a brown-purple solid. Single crystals of **4** suitable for X-ray analysis, were grown from benzene at room temperature. ^{1}H NMR (500 MHz, C_6D_6, 25 °C): δ = 8.03 (s, 4H, C_5Ar_5), 7.00 (s, 2H, C_5Ar_5), 6.73 (s, 12H, C_5Ar_5), 6.59 (s, 4H, C_5Ar_5), 6.28 (s, 4H, C_5Ar_5), 5.55 (s, 4H, C_5Ar_5), 2.93 (m, 4H, CHMe$_2$), 2.54 (m, 8H, CHMe$_2$), 2.17 (m, 4H, CHMe$_2$), 1.91 (m, 4H, CHMe$_2$), 1.33 (d, J = 5 Hz, 12H, CHMe_2), 1.31 (d, J = 5 Hz, 12H, CHMe_2), 1.26 (d, J = 5 Hz, 12H, CHMe_2), 1.01 (d, J = 5 Hz, 24H, CHMe_2), 0.97 (d, J = 5 Hz, 24H, CHMe_2), 0.90 (d, J = 5 Hz, 12H, CHMe_2), 0.63 (d, J = 5 Hz, 12H, CHMe_2), 0.18 (d, J = 5 Hz, 12H, CHMe_2), -2.10 (br, 2H, La-H). ^{13}C {^{1}H} NMR (126 MHz, C_6D_6, 25 °C): δ = 147.89 (C_5Ar_5), 147.85 (C_5Ar_5), 147.48 (C_5Ar_5), 146.44 (C_5Ar_5), 140.78 (C_5Ar_5), 137.95 (C_5Ar_5), 132.73 (C_5Ar_5), 130.48 (C_5Ar_5), 130.31 (C_5Ar_5), 129.65 (C_5Ar_5), 126.18 (C_5Ar_5), 124.52 (C_5Ar$_5$), 121.62 (C_5Ar_5), 119.92 (C_5Ar_5), 117.88 (C_5Ar_5), 114.73 (C_5Ar$_5$), 104.25 (C_5Ar$_5$), 35.07 (CHMe$_2$),

34.66 (*C*HMe$_2$), 33.61 (*C*HMe$_2$), 33.21 (*C*HMe$_2$), 25.81 (CH*Me*$_2$), 25.03 (CH*Me*$_2$), 24.89 (CH*Me*$_2$), 24.81 (CH*Me*$_2$), 24.76 (CH*Me*$_2$), 24.01 (CH*Me*$_2$), 22.26 (CH*Me*$_2$), 20.37(CH*Me*$_2$). Anal. calcd. for (**4**) $C_{130}H_{172}La_2$ (2012.49): C, 77.58; H, 8.61; found: C, 78.04; H, 9.04. FT-IR (KBr, cm^{-1}): 3404, 2959, 2933, 2888, 2869, 1767, 1595, 1466, 1382, 1362, 1335, 1314, 1255, 1187, 1105, 1069, 940, 921, 894, 874, 824, 766, 713. UV-Vis (Cyclohexane, 25 °C): (1) 0.001 mg/mL: λ_{max} (E, mM^{-1}cm^{-1}) = 210 nm (1.12); λ = 260 nm (0.34); λ = 330 nm (0.10). (2) 0.1 mg/mL: λ_{max} (E, mM^{-1}cm^{-1}) = 470 nm (0.12); λ = 740 nm (0.08).

At room temperature, powdered samples of complex **4** gave an EPR spectrum with a very weak rhombic signal at *g* = 2.02, indicating the potential additional electron in complex **4**. When we took magnetic measurement of powdered samples of complex **4** by SQUID magnetometry, a series of attempts for RSO centering were failed. Thus, complex **4** can be regard as diamagnetic complex.

Synthesis of [(Cp^{Ar5})La(μ-D)]$_2$ (4-D).

In the glovebox, [(Cp^{Ar5})La(*p*-CH$_2$-C$_6$H$_4$-Me)$_2$(THF)] (**3**) (300 mg, 0.23 mmol) in hexane (5 mL) were charged into a glass tube in a medium-pressure autoclave with a magnetic stirring bar. The autoclave was transferred outside of the glovebox and pressurized with D_2 to 10 atm. The mixture was stirred at room temperature for 3 days. Pressure was released and the autoclave was quickly returned to the glovebox. After filtration, all the volatiles were removed under vacuum to give **4-D** (182 mg, 0.09 mmol, 78% yield) as a brown-purple solid. ^{2}H NMR (500 MHz, C_6H_6, 25 ^{o}C): δ = -2.10 (s, 2D, La–*D*). FT-IR (KBr, cm^{-1}): 3456, 2959, 2933, 2888, 2869, 1766, 1595, 1466, 1382, 1362, 1336, 1315, 1255, 1187, 1105, 1069, 957, 940, 921, 895, 873, 824, 766, 713.

2. Selected NMR Spectra

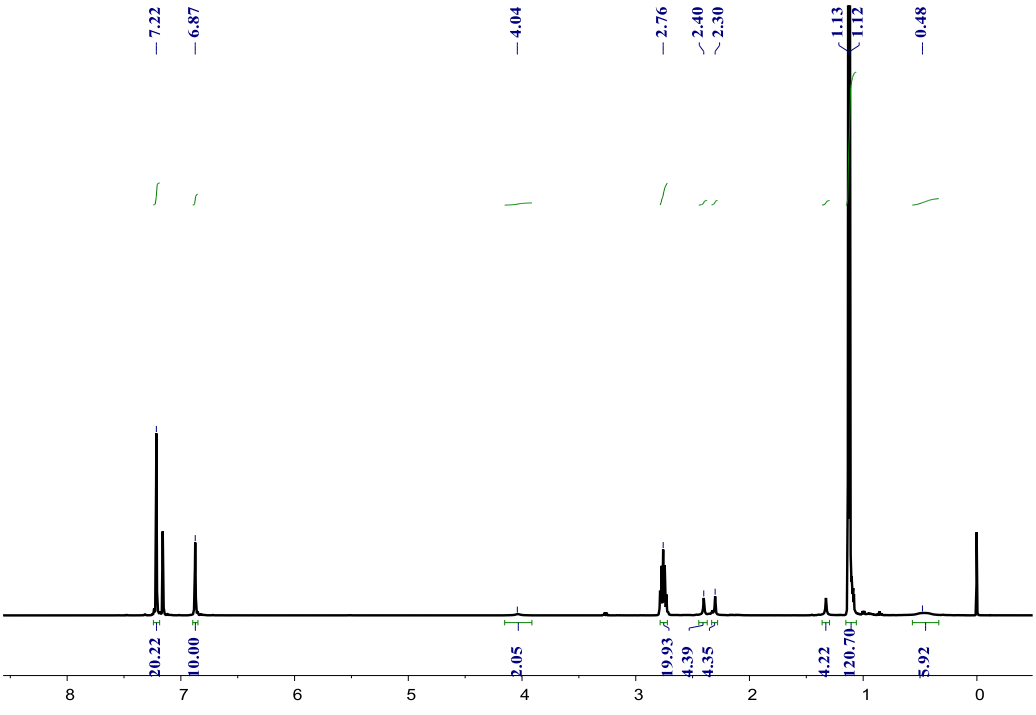


Figure S1. ^{1}H NMR spectrum (500 MHz) of complex **2** in C_6D_6 at 25 °C.

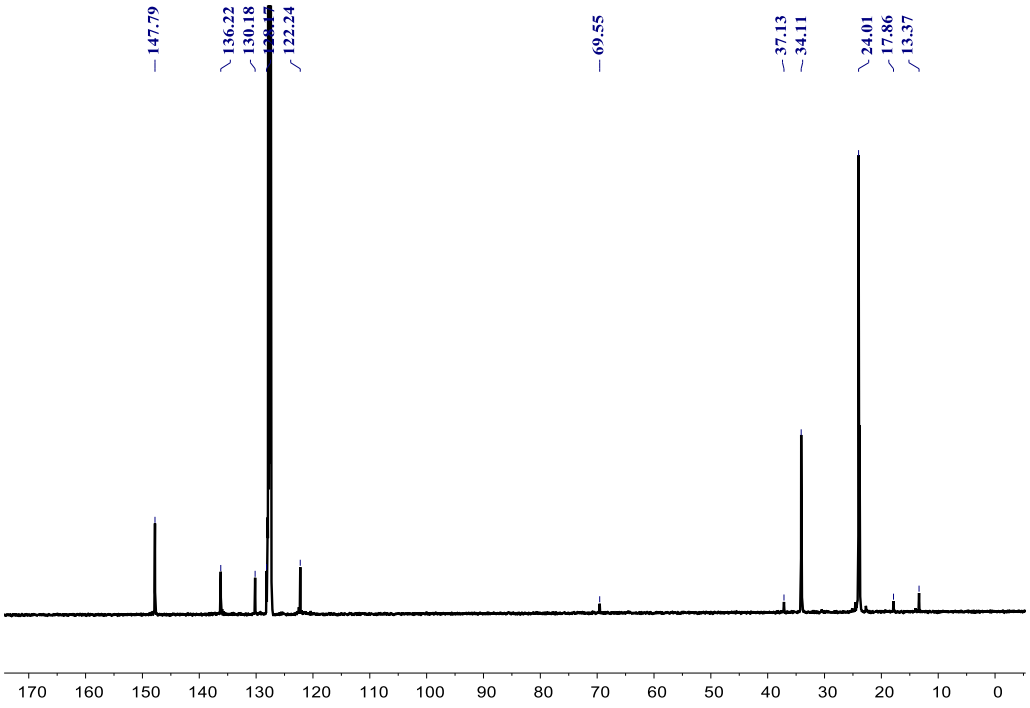


Figure S2. ^{13}C {^{1}H} NMR spectrum (101 MHz) of complex **2** in C_6D_6 at 25 °C.

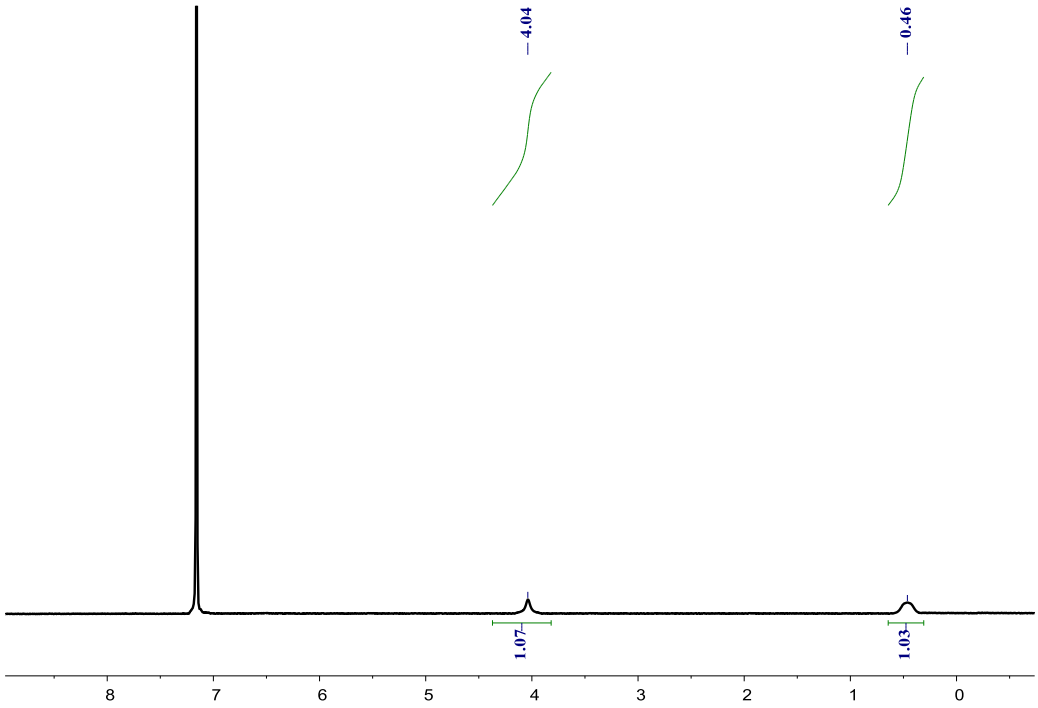


Figure S3. ^{2}H NMR spectrum (500 MHz) of complex **2-D** in C_6H_6 at 25 ^{o}C. (Drops of C_6D_6 were added as internal standard)

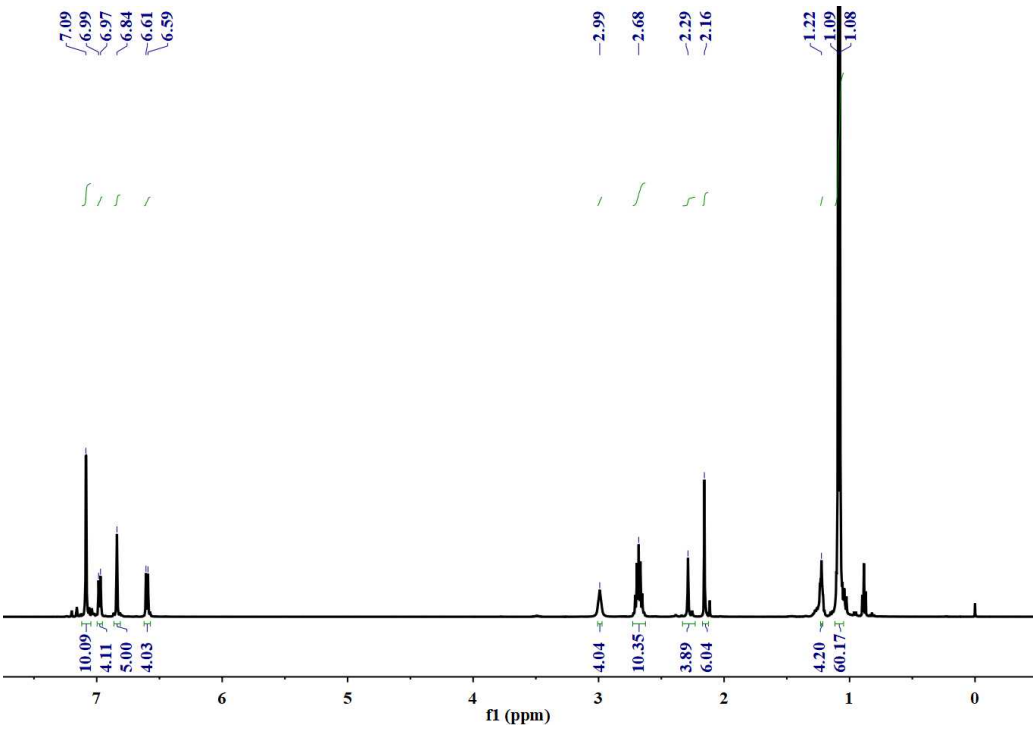


Figure S4. ^{1}H NMR spectrum (500 MHz) of complex **3** in C_6D_6 at 25 °C.

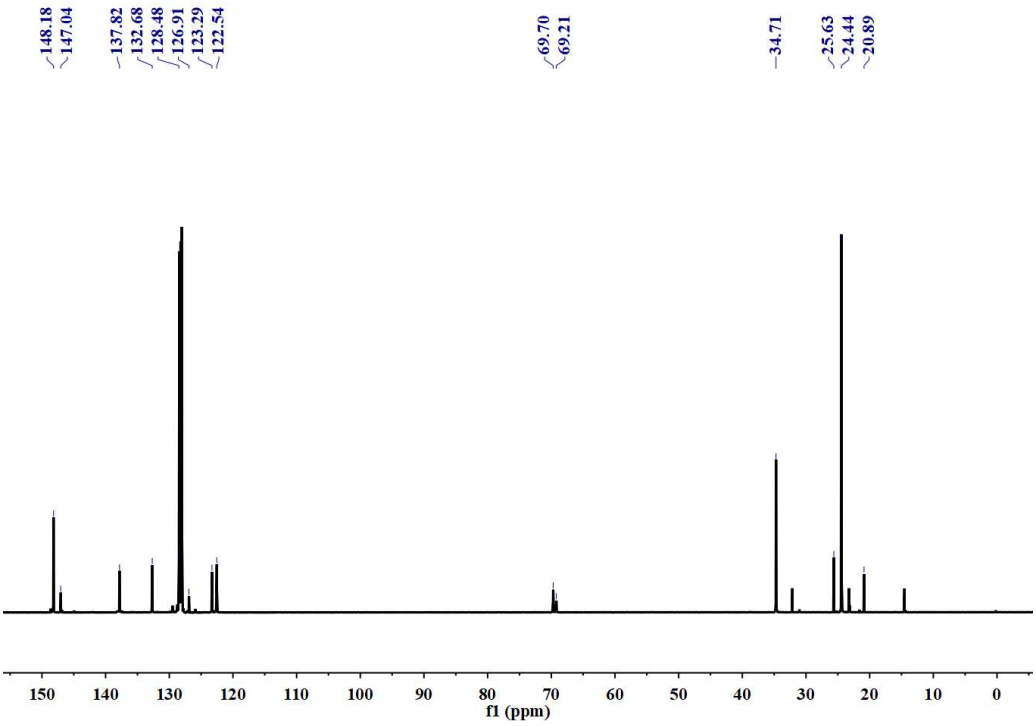


Figure S5. ^{13}C {^{1}H} NMR spectrum (126 MHz) of complex **3** in C_6D_6 at 25 °C.

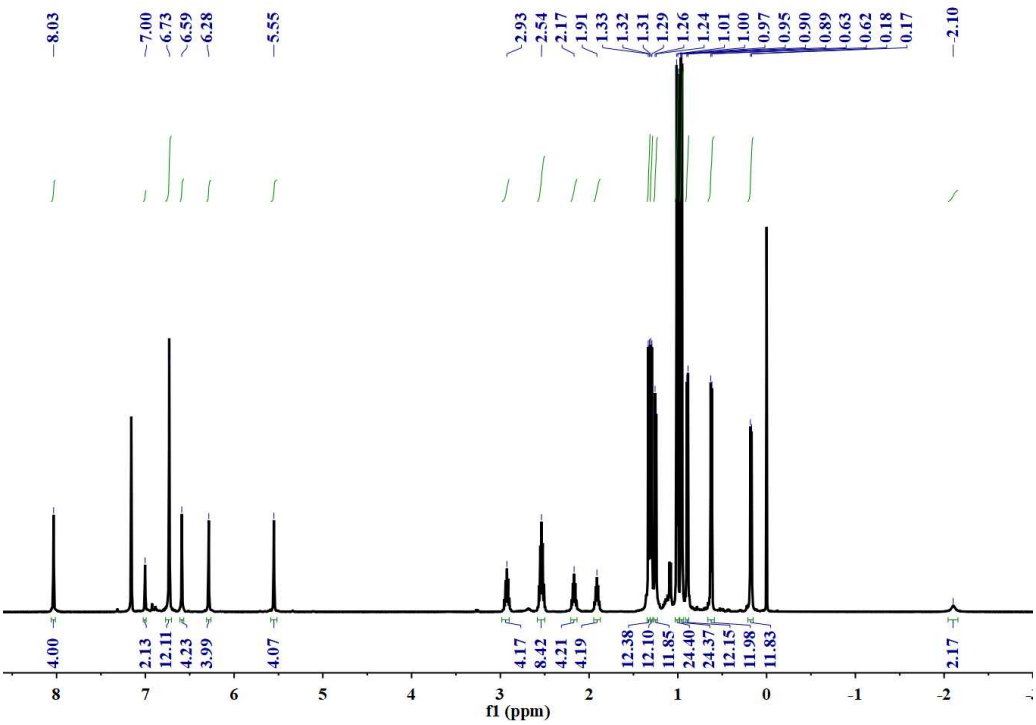


Figure S6. ^{1}H NMR spectrum (500 MHz) of complex **4** in C_6D_6 at 25 °C.

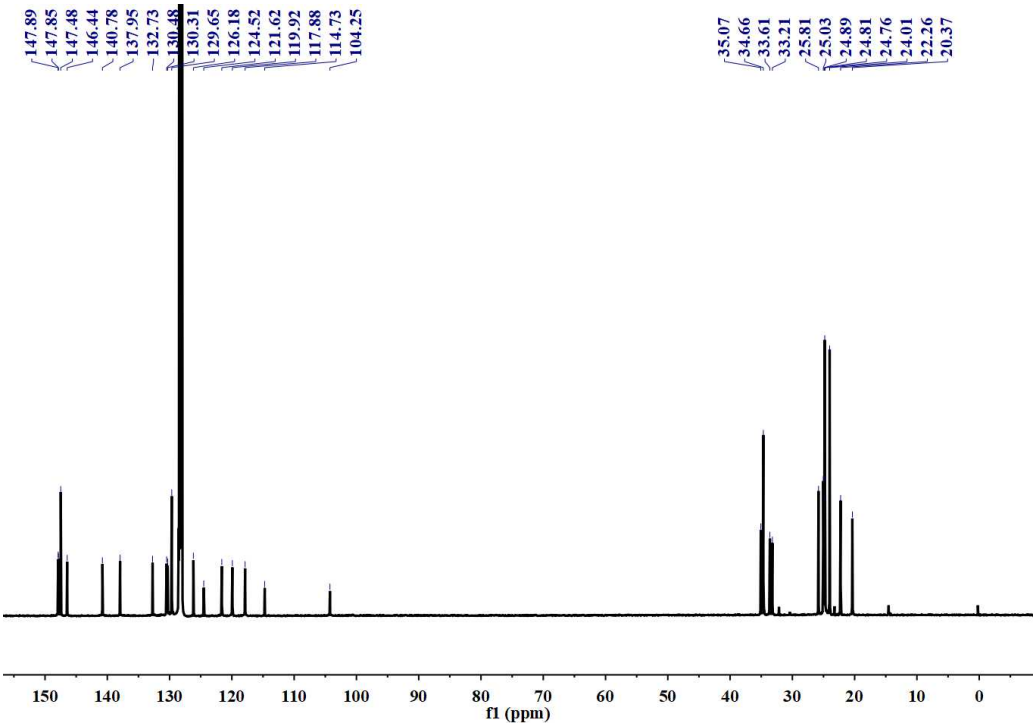


Figure S7. ^{13}C {^{1}H} NMR spectrum (126 MHz) of complex **4** in C_6D_6 at 25 °C.

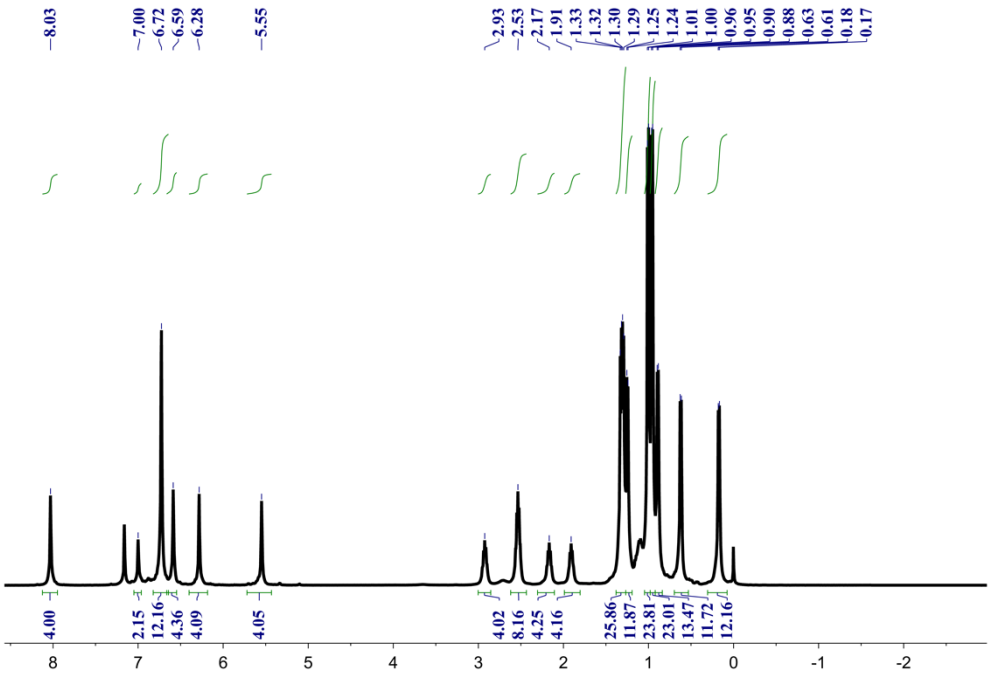


Figure S8. ^{1}H NMR spectrum (500 MHz) of complex **4-D** in C_6D_6 at 25 °C.

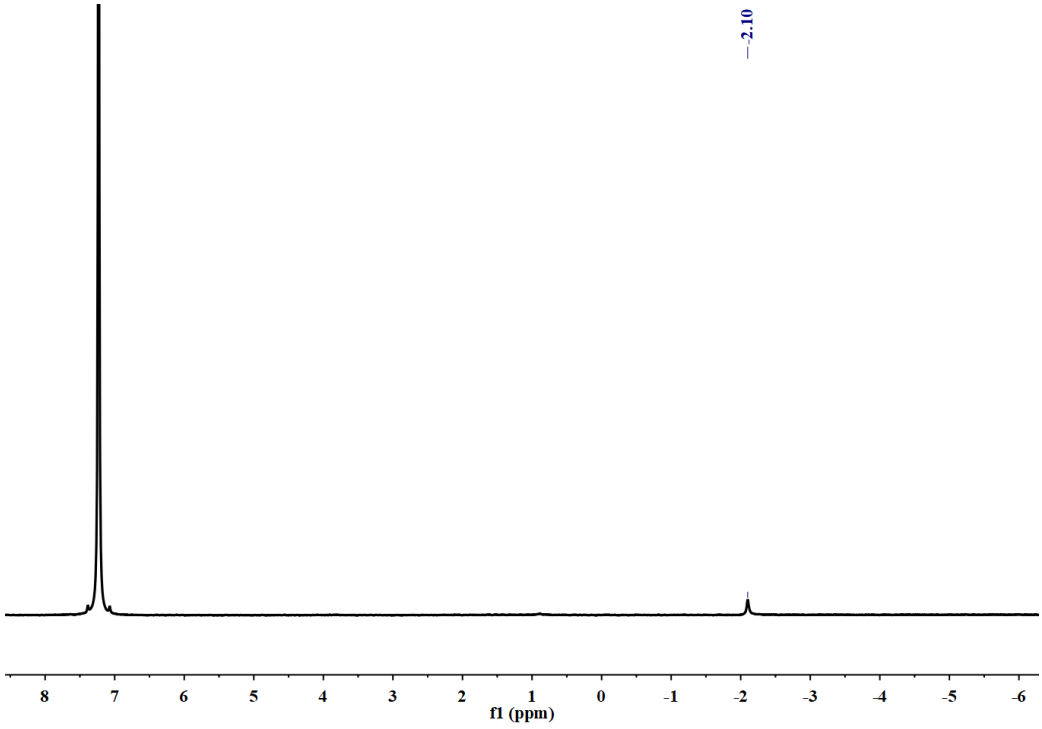


Figure S9. ^{2}H NMR spectrum (500 MHz) of complex **4-D** in C_6H_6 at 25 °C. (Drops of C_6D_6 were added as internal standard)

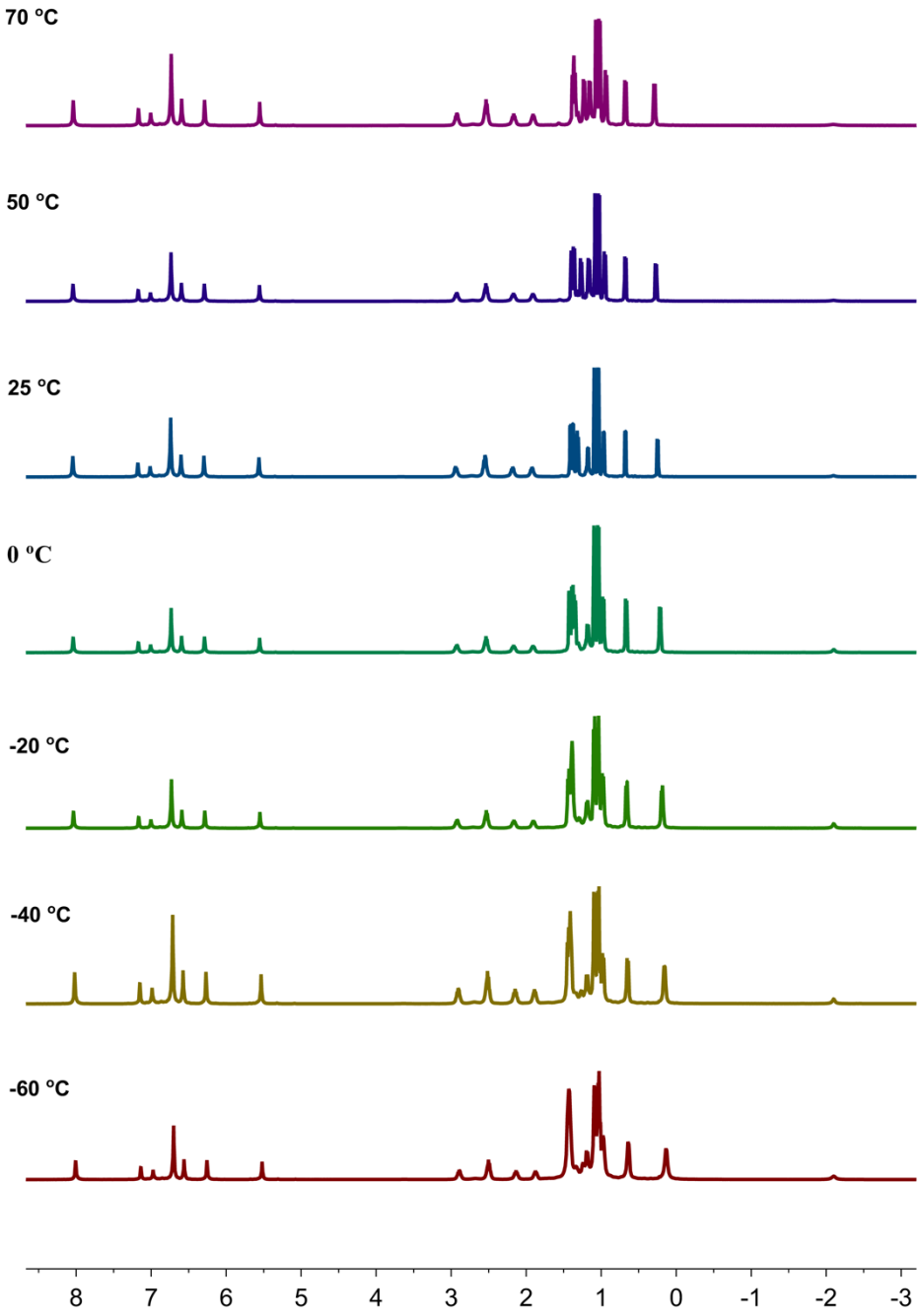


Figure S10. Stacked ^{1}H NMR spectrum (500 MHz) of complex **4** in d_8-toluene at varied temperatures.

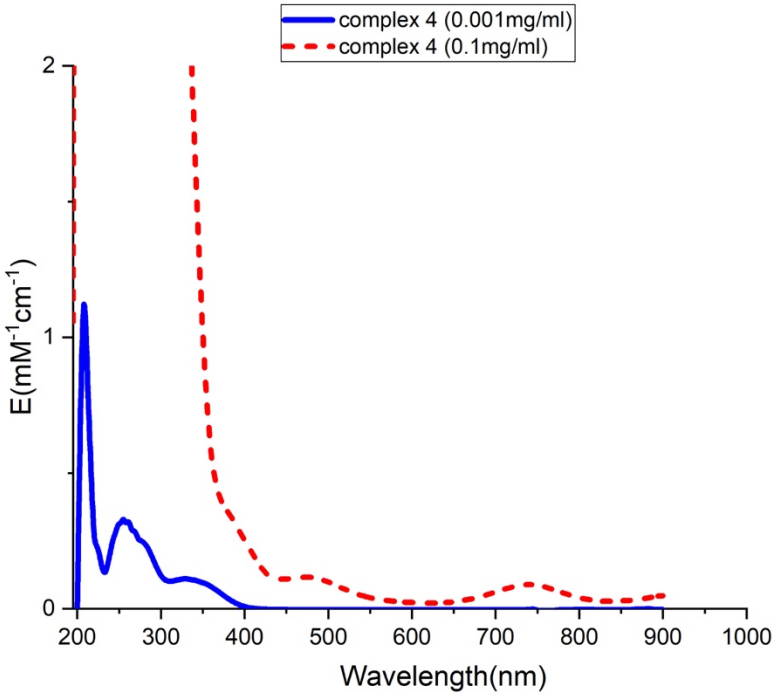


Figure S11. Experimental UV-visible spectra of complex **4** in cyclohexane at 25 °C.

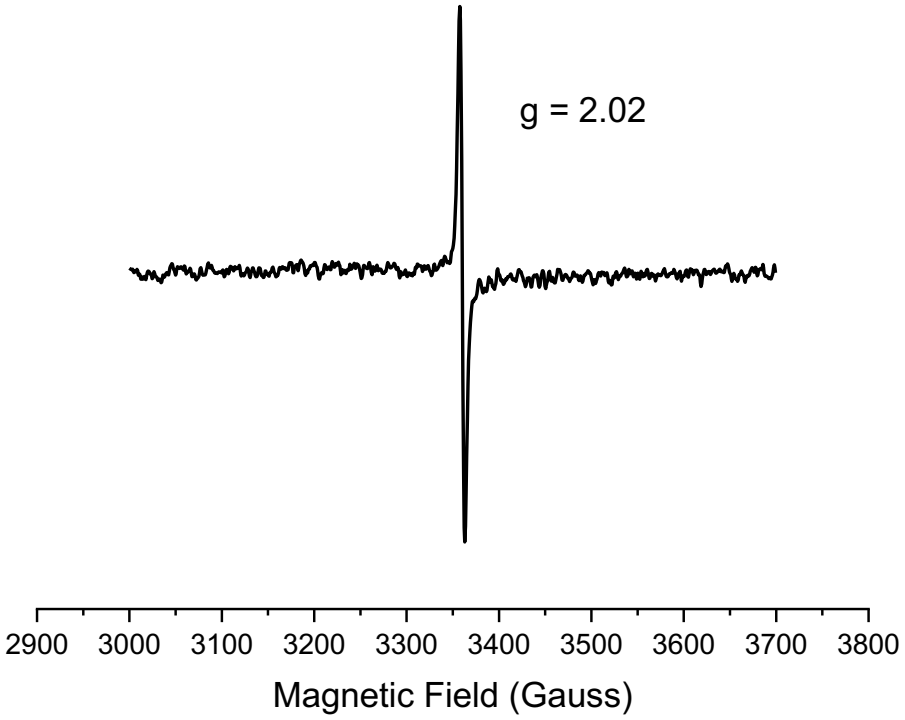


Figure S12. X-band EPR spectrum of complex **4** at 25 ^{o}C, recorded on a powdered sample.

At room temperature, powdered samples of complex **4** gave X-band EPR spectra with a weak rhombic signal at g = 2.02. This could arise from a minor impurity in the sample, and cannot be confidently assigned; DFT calculations predict that complex **4** has an EPR-silent singlet ground state. Magnetic measurements of powdered samples of complex **4** were attempted by SQUID magnetometry, but unfortunately a series of attempts for RSO centering failed. This is consistent with, but not conclusive proof of, a diamagnetic ground state for complex **4**.

3. X-Ray Crystallographic Studies

Single crystals suitable for X-Ray analysis were obtained as described in the preparation. The crystals were manipulated in the glovebox under a microscope in the glovebox, data collection was performed at -80 °C on a Bruker SMART APEX diffractometer with a CCD area detector, using graphite monochromated Mo K_α radiation (λ = 0.71073 Å). The determination of the crystal class and unit cell parameters was carried out by the SMART program packages.[4] The raw frame data were processed using SAINT[5] and absorption corrections using SADABS[6] to yield the reflection data file. The structures were solved by using SUPERFLIP[7] in the WinGX program package.[8] Refinements were performed on F^2 anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method using SHELXL-2018 program.[9]

Refinement of **2**: Three ^{i}Pr groups in the Cp^{Ar5} ligand were disordered. C42~C44 and C42'~C44' disordered over two sites with occupancies 0.638:0.362. C59~C61 and C59'~C61' disordered over two sites with occupancies 0.657:0.343. C66~C68 and C66'~C68' disordered over two sites with occupancies 0.399:0.601. The terminal hydride (H1) was located by difference Fourier syntheses, and refined.

Refinement of **3**: The SQUEEZE[10] routine of the program PLATON[11] was implemented to remove the contributions of one disordered hexane to the observed structure factors. Four ^{i}Pr groups in the Cp^{Ar5} ligand and the THF ligand were disordered. C17~C20 and C17'~C20' disordered over two sites with occupancies 0.543:0.457. C41~C43 and C41'~C43' disordered over two sites with occupancies 0.503:0.497. C53~C55 and C53'~C55' disordered over two sites with occupancies 0.362:0.638. C58~C60 and C58'~C60' disordered over two sites with occupancies 0.378:0.622. C77~C79 and C77'~C79' disordered over two sites with occupancies 0.677:0.323.

Refinement of **4**: The SQUEEZE[10] routine of the program PLATON[11] was implemented to remove the contributions of two disordered benzenes to the observed structure factors. The bridging hydrides (H1 and H2) were located by difference Fourier syntheses, and refined. Nine ^{i}Pr groups in the Cp^{Ar5} ligand were disordered. C19~C21 and C19'~C21' disordered over two sites with occupancies 0.725:0.275. C54~C56 and C54'~C56' disordered over two sites with occupancies 0.396:0.604. C59~C61 and C59'~C61' disordered over two sites with occupancies 0.360:0.640. C71~C73 and C71'~C73' disordered over two sites with occupancies 0.563:0.437. C120~C122 and C220~C222 disordered over two sites with occupancies 0.430:0.570. C132~C134 and C232~C234 disordered over two sites with occupancies 0.516:0.484. C137~C139 and C237~C239 disordered over two sites with

occupancies 0.752:0.248. C144~C146 and C244~C246 disordered over two sites with occupancies 0.576:0.424. C149~C151 and C249~C251 disordered over two sites with occupancies 0.373:0.627.

Other hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. The residual electron densities were of no chemical significance. Crystal data and analysis results are listed in **Table S1-3**.

CCDC number 2049193 (**2**), 1912747 (**3**) and 1912748 (**4**) contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement for complex **2.**

Identification code	D160
CCDC number	2049193
Empirical formula	$C_{138}H_{190}O_2Sc_2$
Formula weight	1970.80
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
a	16.5086(13) Å
b	26.3426(19) Å
c	15.7814(12) Å
α	90 °
β	114.8710(10) °
γ	90 °
Volume	6226.5(8) $Å^3$
Z, Calculated density	4, 1.051 Mg/m^3
Absorption coefficient	0.157 mm^{-1}
F(000)	2152
Crystal size	0.220 x 0.180 x 0.130 mm
Theta range for data collection	1.546 to 24.999 °
Limiting indices	-19<=h<=16, -31<=k<=21, -17<=l<=18
Reflections collected / unique	31757 / 10920 [R(int) = 0.0645]
Completeness to theta	(24.999 °) 99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.980 and 0.967
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10920 / 16 / 626
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0827, wR2 = 0.2029
R indices (all data)	R1 = 0.1375, wR2 = 0.2406
Largest diff. peak and hole	0.679 and -0.389 e. $Å^{-3}$

Table S2. Crystal data and structure refinement for complex **3.**

Identification code	D157
CCDC number	1912747
Empirical formula	$C_{85}H_{111}O_1La_1$
Formula weight	1287.64
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
a	10.7515(7) Å
b	29.6409(19) Å
c	25.5920(17)
α	90 °
β	99.774(10) °
γ	90 °
Volume	8037.4(9) $Å^3$
Z, Calculated density	4, 1.064 Mg/m^3
Absorption coefficient	0.571 mm^{-1}
F(000)	2744
Crystal size	0.240 x 0.190 x 0.160 mm
Theta range for data collection	1.594 to 24.999 °
Limiting indices	-6<=h<=12, -35<=k<=33, -30<=l<=28
Reflections collected / unique	40657 / 14036 [*R*(int) = 0.0309]
Completeness to theta	(25.00 °) 99.1 %
Absorption correction	Empirical
Max. and min. transmission	0.913 and 0.878
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14036 / 30 / 779
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R_1 = 0.0432, wR_2 = 0.1079
R indices (all data)	R_1 = 0.0557, wR_2 = 0.1156
Largest diff. peak and hole	0.956 and -0.412 e. $Å^{-3}$

Table S3. Crystal data and structure refinement for Complex **4.**

Identification code	D235
CCDC number	1912748
Empirical formula	$C_{130}H_{172}La_2$
Formula weight	2012.49
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
a	20.0516(5)Å
b	19.8615(5) Å
c	31.0309(8) Å
α	90 °
β	93.7520(10) °
γ	90 °
Volume	12331.7(5) $Å^3$
Z, Calculated density	4, 1.084 Mg/m^3
Absorption coefficient	0.727 mm^{-1}
F(000)	4264
Crystal size	0.230 x 0.210 x 0.180 mm
Theta range for data collection	1.445 to 24.499 °
Limiting indices	-23<=h<=23, -23<=k<=23, -35<=l<=36
Reflections collected / unique	74455 / 19696 [*R*(int) = 0.0425]
Completeness to theta	(24.499 °) 96.1 %
Absorption correction	Empirical
Max. and min. transmission	0.877 and 0.846
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19696 / 61 / 1179
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R_1 = 0.0501, wR_2 = 0.1312
R indices (all data)	R_1 = 0.0716, wR_2 = 0.1463
Largest diff. peak and hole	1.032 and -0.931 e. $Å^{-3}$

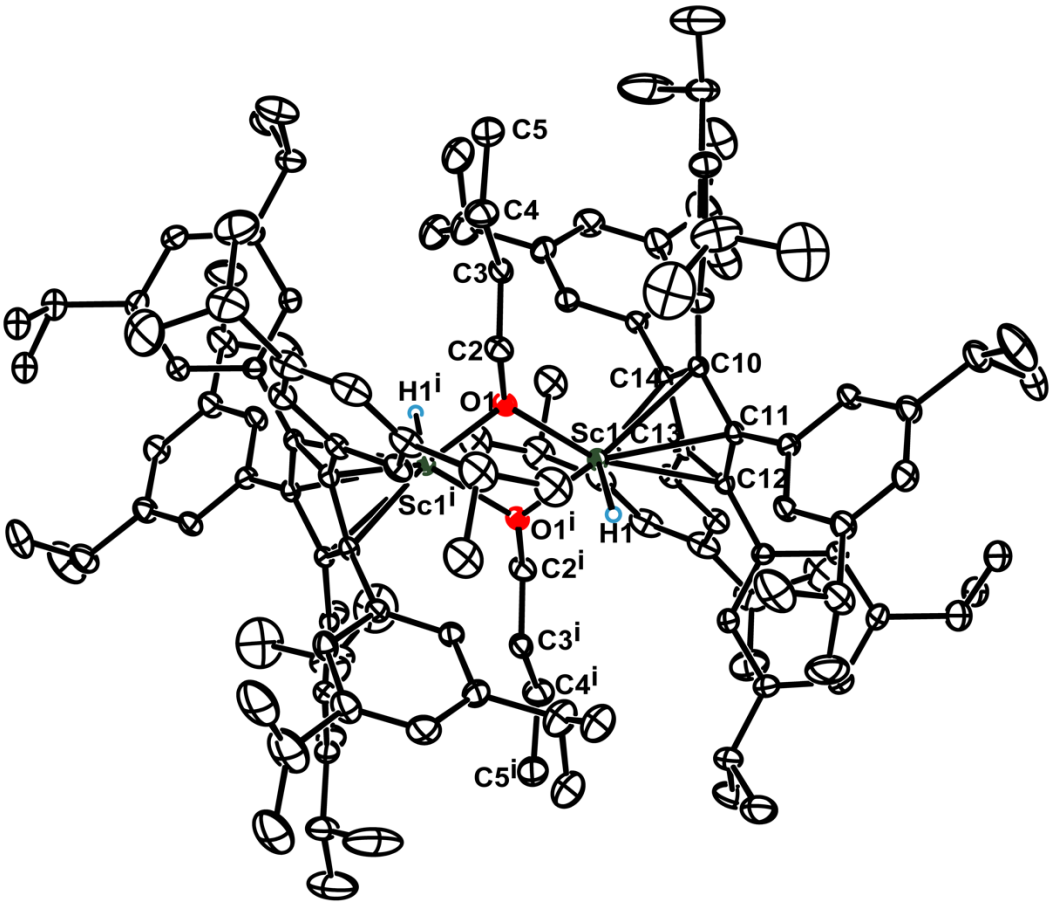


Figure S13. ORTEP plot (20% probability) of $[(Cp^{Ar5})Sc(H)(\mu\text{-}OC_4H_9)]_2$ (**2**). All the hydrogen atoms, except the terminal hydrides (H1 and $H1^i$) are omitted for clarity. Selected interatomic distances [Å]: Sc1–H1 2.28(4), Sc1–O1 2.057(3), Sc1–$O1^i$ 2.060(2), Sc1–C10 2.520(3), Sc1–C11 2.559(3), Sc1–C12 2.545(3), Sc1–C13 2.527(3), Sc1–C14 2.488(3), Sc1–$Sc1^i$ 3.1952(14), Sc1–Cent1 2.218.

- Cent1: Centre of the Cp^{Ar5} ring (C10~C14).

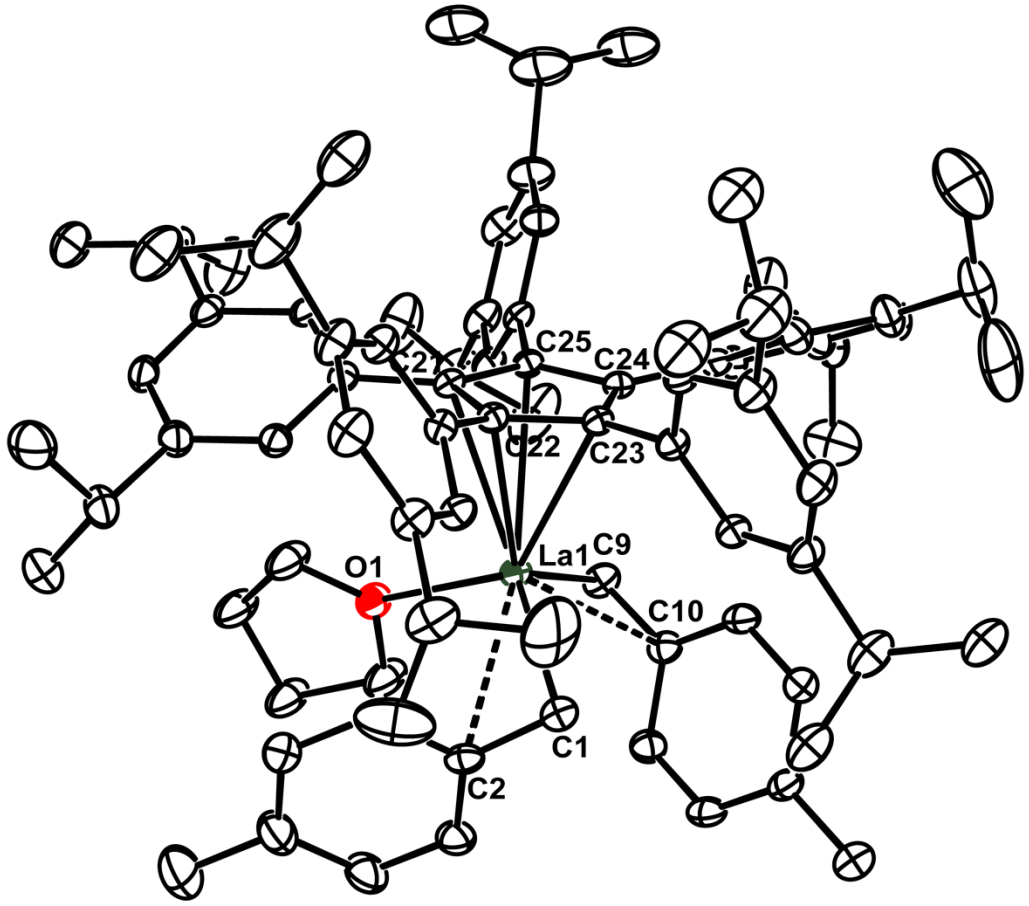


Figure S14. ORTEP plot (20% probability) of [(Cp^{Ar5})La(*p*-CH_2-C_6H_4-Me)$_2$(THF)] (**3**). All the hydrogen atoms are omitted for clarity. Selected interatomic distances [Å]: La1–C1 2.586(3), La1–C2 2.911(3), La1–C9 2.572(3), La1–C10 2.857(3), La1–O1 2.592(2), La1–C21 2.840(3), La1–C22 2.899(3), La1–C23 2.943(3), La1–C24 2.966(3), La1–C25 2.883(3), La1–Cent1 2.640.

- Cent1: Centre of the Cp^{Ar5} ring (C21~C25).

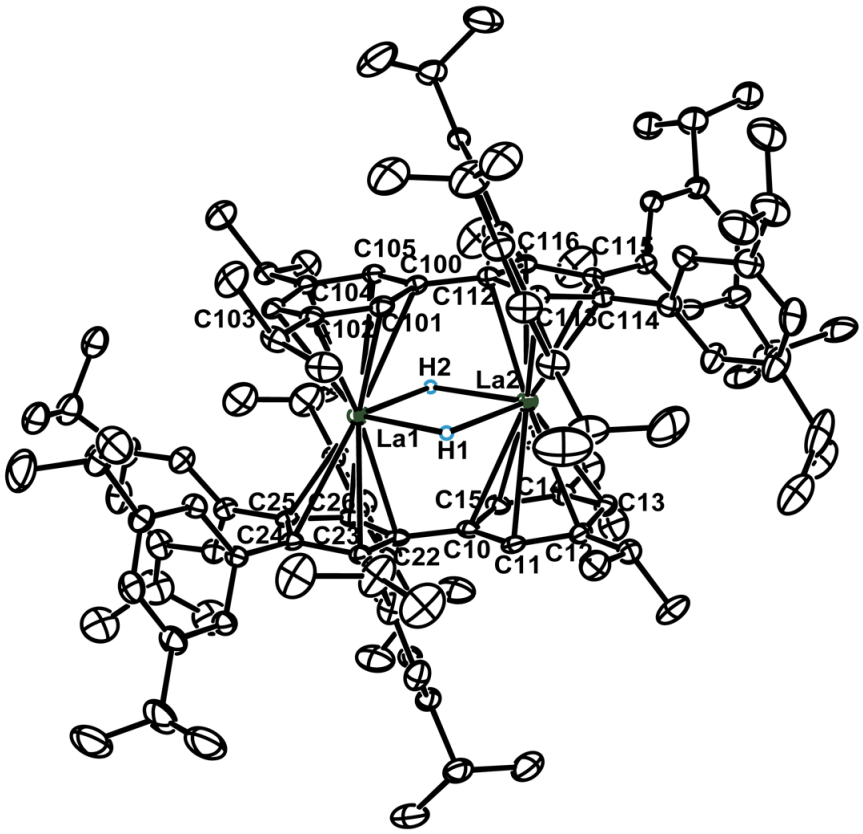


Figure S15. ORTEP plot (20% probability) of $[(Cp^{Ar5})La(\mu\text{-}H)]_2$ (**4**). All the hydrogen atoms, except the bridging hydrides (H1 and H2), are omitted for clarity. Selected interatomic distances [Å] and angles [º]: La1–H1 2.38(5), La1–H2 2.29(4), La2–H1 2.40(5), La2–H2 2.32(4), La1---La2 3.4266(4), La1–C22 2.752(4), La1–C23 2.813(4), La1–C24 2.856(4), La1–C25 2.863(4), La1–C26 2.800(4), La1–C100 2.929(4), La1–C101 2.894(5), La1–C102 2.881(4), La1–C103 2.818(5), La1–C104 2.867(4), La1–C105 2.898(4), La2–C10 2.942(4), La2–C11 2.904(5), La2–C12 2.880(5), La2–C13 2.828(5), La2–C14 2.906(5), La2–C15 2.910(5), La2–C112 2.753(4), La2–C113 2.817(4), La2–C114 2.861(5), La2–C115 2.845(4), La2–C116 2.805(4), C10–C11 1.432(6), C11–C12 1.389(7), C12–C13 1.415(7), C13–C14 1.411(7), C14–C15 1.382(7), C15–C10 1.431(6), C100–C101 1.441(6), C101–C102 1.382(7), C102–C103 1.422(7), C103–C104 1.416(6), C104–C105 1.389(7), C105–C100 1.428(6), C10–C22 1.464(6), C100–C112 1.458(6), La1–Cent1 2.540, La1–Cent4 2.509, La2–Cent2 2.537, La2–Cent3 2.531, La1–H1–La2 88.9(10), La1–H2–La2 92.0(10), Cent1–La1–Cent4 163.6, Cent2–La2–Cent3 164.2.

- Cent1: Centre of the Cp^{Ar5} ring (C22~C26); Cent2: Centre of the Cp^{Ar5} ring (C112~C116); Cent3: Centre of the anionic benzene (C10~C15); Cent4: Centre of the anionic benzene (C100~C105).

Computational details

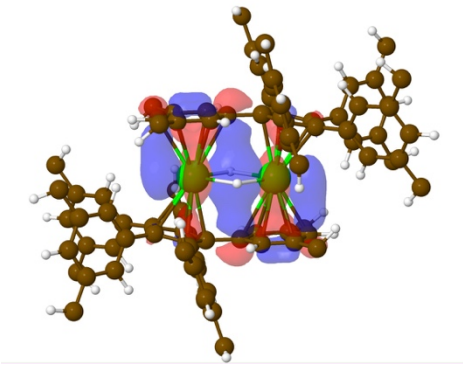
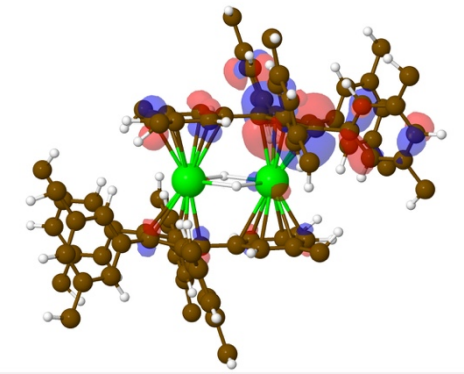
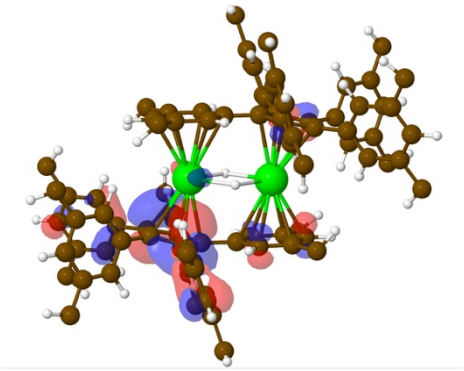
All calculations were carried out with the Gaussian 09 suite of programs.[12] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[13] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. CASSCF, CAS(2,4) calculations were performed to confirm the nature of the electronic ground state. Lanthanum atoms were treated with a small core effective core potential (28MWB), associated with its adapted basis set.[14] For the other elements (H and C), Pople's double-ζ basis set 6-31G(d,p) was used.[15] The electronic charges (at the DFT level) were computed using the natural population analysis (NPA) technique.[16]

Table S4. Selected bond lengths calculated for complex **4**

	Distances (Å)	WBI		Distances (Å)	WBI
M1 - M2	3.415	0.67			
M1 - H1	2.266	0.45	M2 - H1	2.274	0.44
M1 - H2	2.274	0.44	M2 - H2	2.267	0.45
M1 – C (Cp)	2.743	0.16	M2 – C (Cp)	2.746	0.16
	2.822	0.21		2.846	0.20
	2.890	0.17		2.878	0.18
	2.884	0.18		2.882	0.17
	2.824	0.20		2.824	0.20
M1 – C (aryl)	2.947	0.14	M2 – C (aryl)	2.943	0.15
	2.914	0.15		2.917	0.15
	2.898	0.13		2.910	0.13
	2.824	0.23		2.828	0.24
	2.913	0.13		2.904	0.13
	2.922	0.15		2.913	0.15
C (Cp) - C (Cp)	1.451	1.20	C (Cp) - C (Cp)	1.452	1.20
	1.427	1.28		1.427	1.28
	1.426	1.26		1.425	1.26
	1.425	1.28		1.426	1.28
	1.451	1.20		1.451	1.20
C (aryl) - C (aryl)	1.436	1.21	C (aryl) - C (aryl)	1.435	1.21
	1.392	1.43		1.392	1.43
	1.421	1.26		1.421	1.26
	1.420	1.26		1.421	1.26
	1.391	1.43		1.392	1.43
	1.435	1.21		1.435	1.21

Table S5. Natural charges of carbon, hydrogen and metal atoms of complex **4**

Metal atoms	
M1	0.78
M2	0.77
Carbon atoms	
Cp group	(-0.09)
	-0.11)
Aryl groups non-interacting with M	(-0.21) – (-0.24)
	(-0.02) – (-0.04)
Isopropyl of aryl groups non-interacting with M	(-0.27) – (-0.28)
	(-0.70)
Aryl groups interacting with M	(-0.04) – (-0.07) C12, C14, C10, C100, C102, C104
	(-0.24) C11, C15, C101, C105
	(-0.36) C13, C103
Isopropyl of aryl groups interacting with M	(-0.27)
	(-0.70) – (-0.71)
Hydrogen atoms	
Aryl groups non-interacting with M	(0.23) – (0.25)
Isopropyl of aryl groups non-interacting with M	(0.23) – (0.26)
H atoms between M atoms	-0.22
Aryl groups interacting with M	(0.26) – (0.28)
Isopropyl of aryl groups interacting with M	(0.24) – (0.26)

HOMO	
	**La**: 22.2% 5d (mixture of the $5d_{x2-y2}$, $5d_{z2}$ and $5d_{xz}$ orbitals) **μ–H:** 1.5 % **Aryl groups interacting with the La atoms:** 31.4 % aryl (24.0 % C(ring) + 7.4 % *i*Pr) **Cp groups:** 15.1% Cp carbons **other aryl groups:** 29.7 % aryl
HOMO-1	
	**La**: 13.3% 5p/5d mixture (mixture of the $5d_{xz}$, $5d_{z2}$ and $5d_{yz}$ orbitals) **μ–H:** 0.4 % **Aryl groups interacting with the La atoms:** 16.1 % aryl (12.8 % C(ring) + 3.3 % *i*Pr) **Cp groups:** 23.6% Cp carbons **other aryl groups:** 46.5 % aryl
HOMO-2	
	**La**: 12.5% 5d (mixture of the $5d_{x2-y2}$, $5d_{z2}$ and $5d_{xz}$ orbitals) **μ–H:** 0.5 % **Aryl groups interacting with the La atoms:** 14.2 % aryl (11.1 % C(ring) + 3.1 % *i*Pr) **Cp groups:** 23.4% Cp carbons **other aryl groups:** 49.4 % aryl
HOMO-3	

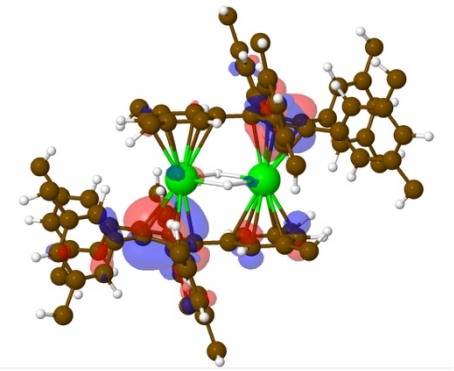
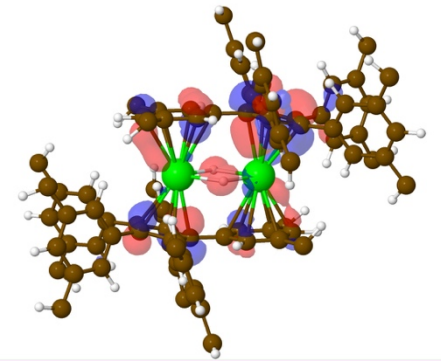
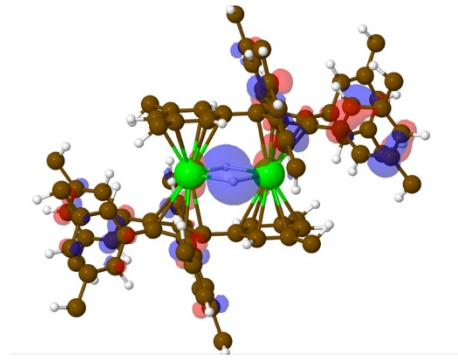
	**La**: 13.1% 5d (mixture of the $5d_{x2-y2}$ and $5d_{xy}$ orbitals) **μ–H:** 0.4 % **Aryl groups interacting with the La atoms:** 13.0 % aryl (10.3 % C(ring) + 2.8 % *i*Pr) **Cp groups:** 23.4% Cp carbons **other aryl groups:** 50.1 % aryl
HOMO-4	
	**La** : 13.9% 5d (mixture of the $5d_{x2-y2}$, $5d_{yz}$ and $5d_{xy}$ orbitals) **μ – H :** 1.9 % **Aryl groups interacting with the La atoms :** 17.7 % aryl (14.6 % C(ring) + 3.1 % *i*Pr) **Cp groups :** 21.9% Cp carbons **other aryl groups:** 40.7 % aryl
HOMO-5	
	**La**: 19.3% 5d (mixture of the $5d_{x2-y2}$, $5d_{xz}$ and $5d_{xy}$ orbitals) **μ–H:** 3.5 % **Aryl groups interacting with the La atoms:** 6.1 % aryl (4.7 % C(ring) + 1.4 % *i*Pr) **Cp groups:** 7.3% Cp carbons **other aryl groups:** 63.7 % aryl

Figure S16. Frontier orbitals of complex **4**. The methyl groups of the aryl ligands are omitted for clarity.

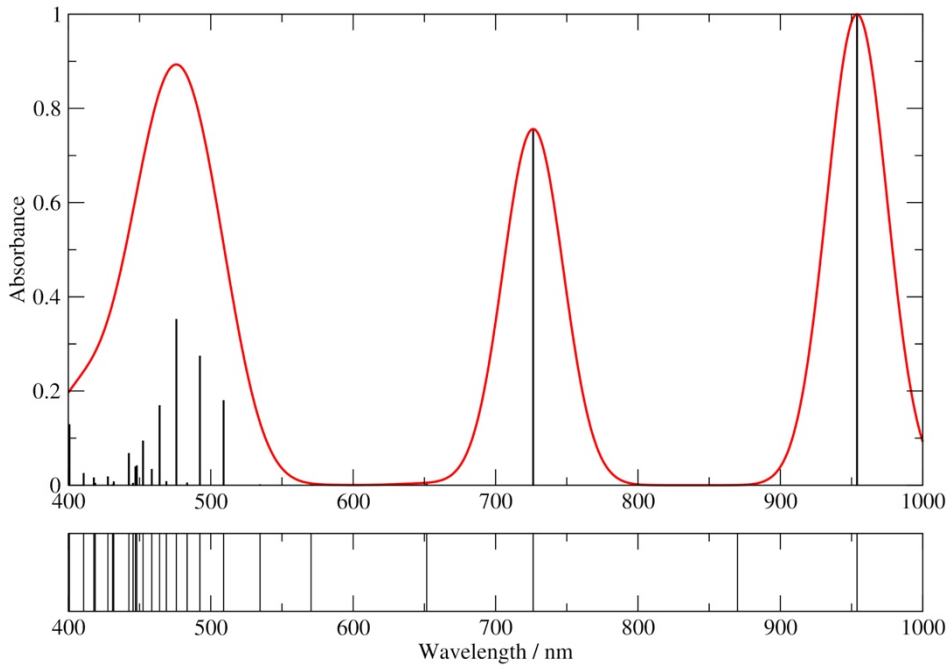


Figure S17. Electronic absorption spectra of complex **4**. The vertical lines show the positions and intensities of the vertical transitions used for the convolution of the theoretical spectrum.

Table S6. Orbitals involved on the transitions observed on the absorption spectrum of complex **4.**

Wavelength / nm	Orbitals involved
954	505 -> 506 / 0.71138
726	505 -> 508 / 0.69105
509	505 -> 512 / 0.64132 505 -> 515 / -0.12105 505 -> 516 / 0.10206 505 -> 518 / 0.10823
492	505 -> 509 / -0.12872 505 -> 513 / 0.61367 505 -> 514 / -0.12054 505 -> 515 / -0.12513 505 -> 516 / 0.15072 505 -> 519 / -0.14408

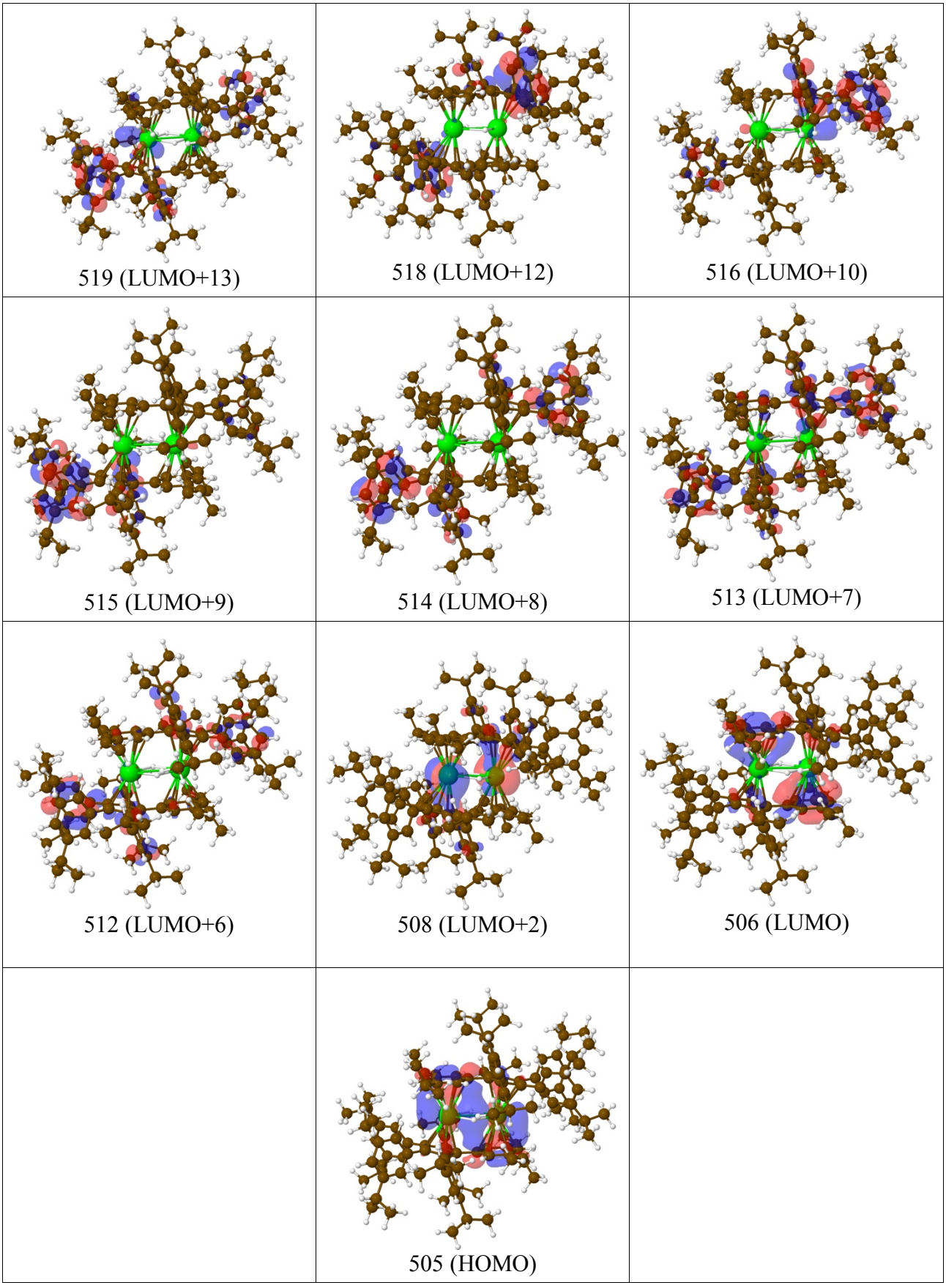


Figure S18. Highest occupied MOs and unoccupied MOs of complex **4**.

More details about the DFT calculation of complex 4:

The DFT study of complex **4** indicates (Figure S18 and Table S4-5) that HOMO displays a La-aryl interaction with a La-La bonding overlap. The HOMO is composed of 22.2% 5d (mixture of the $5d_{x2-y2}$, $5d_{z2}$ and $5d_{xz}$ orbitals) of La (La1 and La2) and 31.4% aryl and 15.1% Cp carbon (including C10, C13, C100 and C103) 2p contributions, which mainly reflects La1–La2, La–aryl and La–Cp ring interactions. The Wiberg bond index (WBI, Table S4) values of La–C (aryl) and La–C (Cp) locate in the ranges of 0.13–0.23 and 0.16–0.21 respectively. Furthermore, the WBI of the C–C bonds of aryl ring in complex **4** are lying in the narrower range (between 1.2 and 1.4). These data points in the direction of the formation of a benzenide anion of aryl ring coordinating with La. In addition, the shape of HOMO in combination with the WBI value (0.67) of La1---La2 bond confirm the existence of weak La1---La2 interaction originating from La 5d orbitals. TDDFT calculation was conducted on complex **4** (Figure S17) and compares well with the experimental one (Figure S11). In particular, an absorption in the green region (650-720 nm) is in line with the experimentally observed purple color. The transition corresponds to metal-metal transitions with excitation from the HOMO (displaying a bonding M-M overlap) to the M-M antibonding.

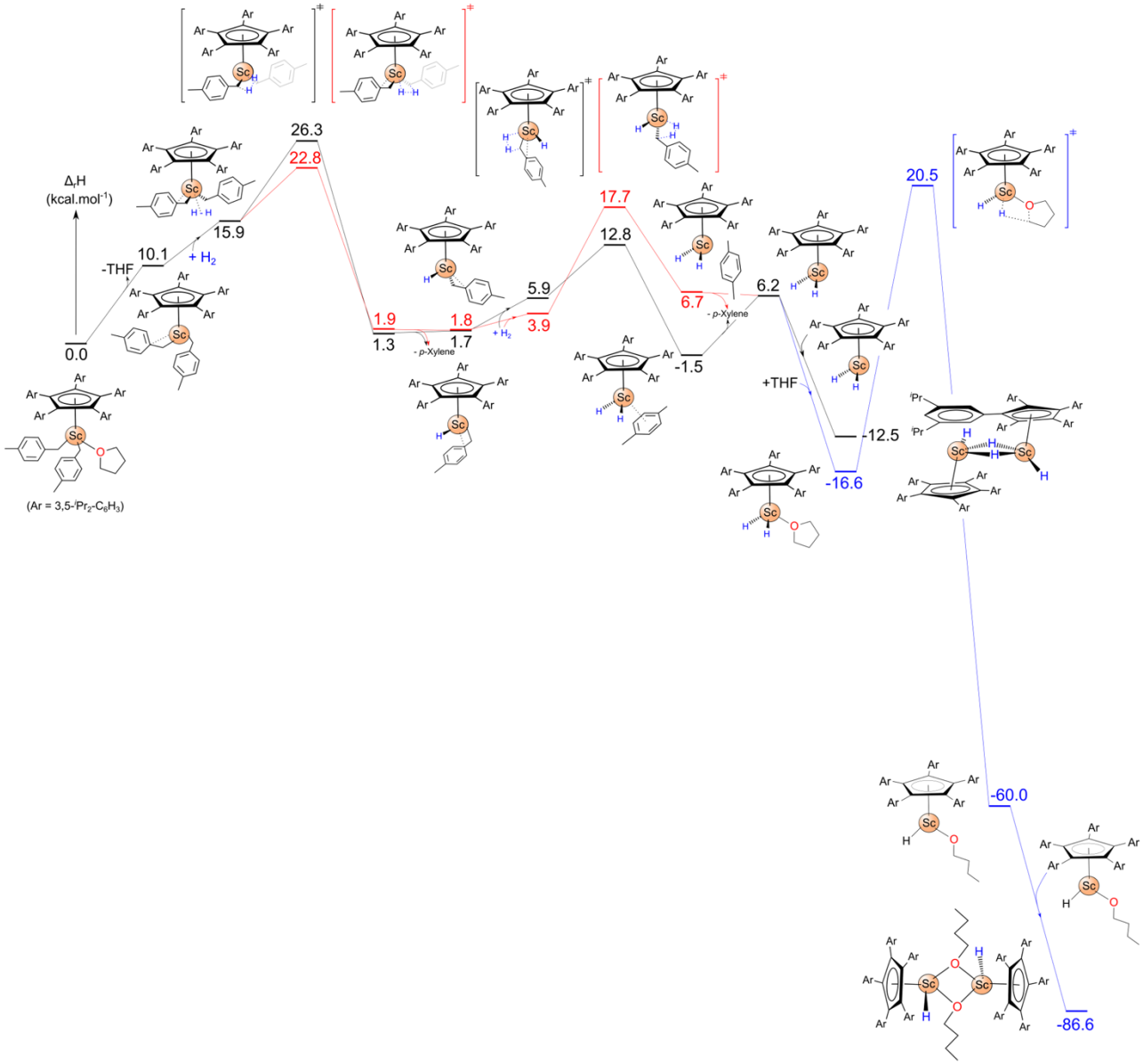


Figure S19. Computed reaction profiles for the reaction of complex **1** at room temperature

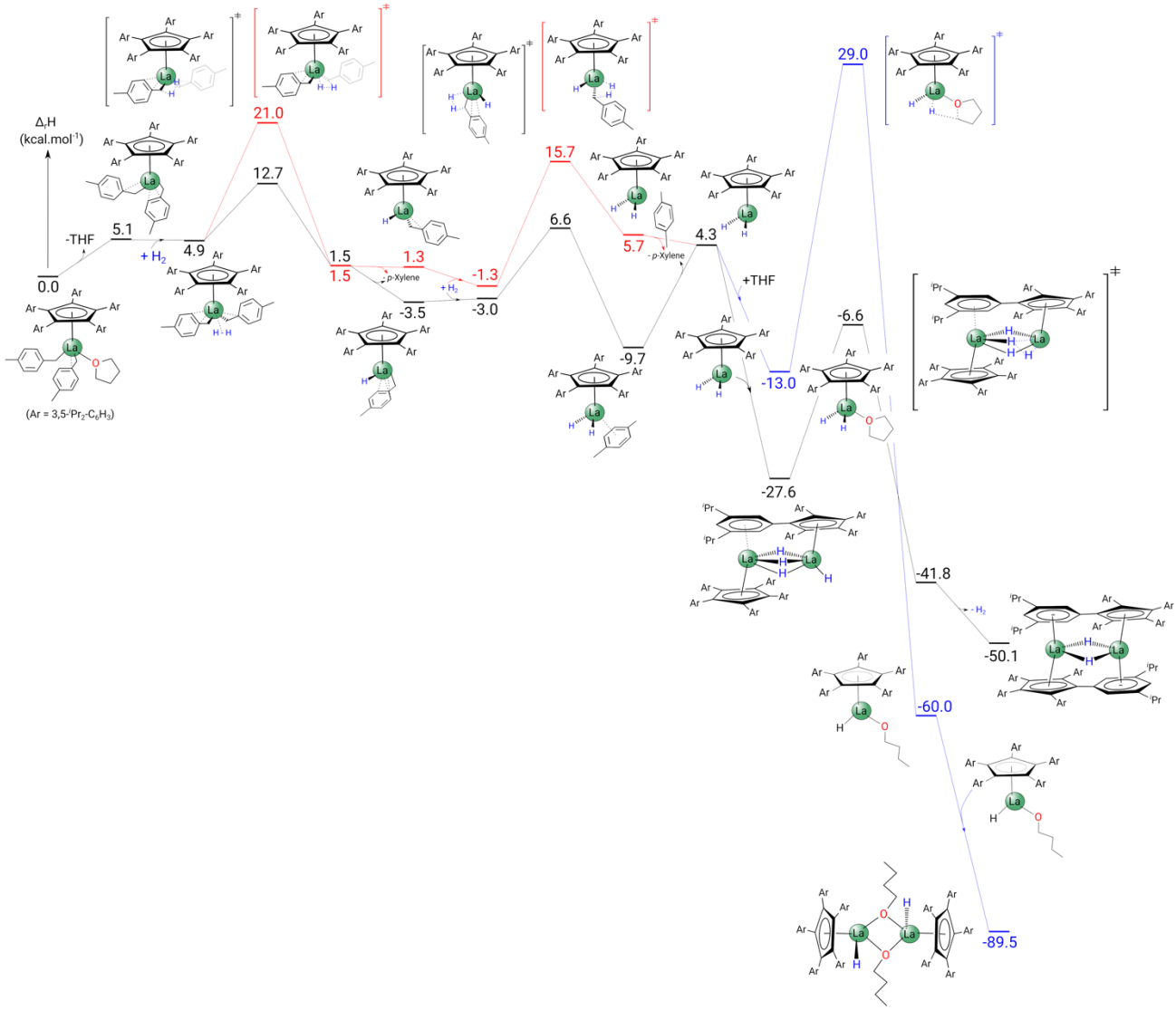


Figure S20. Computed reaction profiles for the reaction of complex **3** at room temperature

Cartesian Coordinates:

2

H2

H	0.854994	1.078161	-0.236297
H	0.252066	1.276669	-0.623233

18

p-xylene

C	-6.23817	0.87786	-1.13819
C	-6.60983	-0.58089	-1.19189
C	-5.64101	-1.56480	-1.42277
C	-5.98514	-2.91083	-1.49898
C	-7.31272	-3.32867	-1.34707
C	-8.27885	-2.34698	-1.11052
C	-7.93408	-0.99864	-1.03392
C	-7.68327	-4.78494	-1.45148
H	-6.20584	1.31668	-2.14335
H	-6.96167	1.45500	-0.55475
H	-8.70887	-0.25905	-0.84296
H	-9.31787	-2.64124	-0.97812
H	-4.59964	-1.27170	-1.53970
H	-5.20797	-3.65207	-1.67410
H	-7.70182	-5.11666	-2.49700
H	-8.67391	-4.97750	-1.02961
H	-6.96398	-5.42081	-0.92493
H	-5.25032	1.02424	-0.69018

13

THF

C	14.59870	14.86887	-0.18683
C	15.37348	13.54919	-0.17538
C	14.57542	12.74418	0.84878
H	15.32456	13.07067	-1.16026
H	16.42695	13.66057	0.09658
H	14.88849	15.48585	0.67153
H	14.75013	15.45947	-1.09474
H	14.62009	11.66217	0.67872
H	14.93817	12.94091	1.87024
C	13.15920	14.37663	-0.03063
H	12.70531	14.16871	-1.01199
H	12.51497	15.09395	0.49179
O	13.22238	13.17145	0.72756

198

Complex 1

Sc	11.02665	11.89659	1.89730
C	12.03148	11.57376	-0.06903
C	11.93256	10.56215	-1.14918
C	12.90191	9.55548	-1.31857
C	12.84128	8.65629	-2.37948

C	11.81123	8.70495	-3.32620
C	10.82400	9.67991	-3.14354
C	10.88083	10.58141	-2.08466
C	11.66428	16.37585	2.25645
C	12.34135	16.04104	0.92642
C	12.79611	14.61220	1.15739
C	12.36111	10.09780	3.13633
C	12.33463	11.24871	3.99103
C	10.98262	11.46445	4.41025
C	10.17335	10.43115	3.83643
C	11.02220	9.59826	3.03983
C	8.91058	12.21818	1.20275
C	8.52803	13.54405	0.66601
C	7.65527	14.39550	1.37564
C	7.31937	15.66513	0.91217
C	7.82619	16.16112	-0.29400
C	8.68293	15.32064	-1.01543
C	9.02389	14.05249	-0.55267
C	11.78497	7.77367	-4.50994
C	13.59376	9.48594	2.58047
C	14.63202	10.28151	2.06823
C	15.81067	9.72180	1.57140
C	15.95189	8.33083	1.61475
C	14.95389	7.50574	2.13796
C	13.77768	8.09640	2.61081
C	13.53784	11.89426	4.58409
C	13.81734	13.26338	4.48284
C	14.93559	13.83000	5.10008
C	15.77542	12.99859	5.84950
C	15.52168	11.63175	5.98786
C	14.40368	11.09437	5.34190
C	10.50553	12.48265	5.37813
C	9.34880	13.23688	5.12604
C	8.86070	14.16268	6.05200
C	9.54202	14.31650	7.26382
C	10.69378	13.57878	7.55422
C	11.16691	12.67345	6.60003
C	8.77984	10.09222	4.22290
C	7.80798	9.71061	3.29031
C	6.52131	9.32920	3.69011
C	6.22649	9.30122	5.05424
C	7.17826	9.65261	6.01917
C	8.44212	10.05380	5.58647
C	10.58986	8.28397	2.48751
C	10.24221	7.28309	3.40771
C	9.82956	6.01675	2.99144
C	9.75096	5.76595	1.61721
C	10.08814	6.73883	0.67112
C	10.51541	7.99543	1.12163
C	16.93353	10.58418	1.01666
C	16.44906	11.60264	-0.02204

C	15.15045	5.99992	2.18496
C	15.03977	5.44926	3.61295
C	15.23111	15.31366	4.95652
C	16.55309	15.56350	4.21750
C	16.41964	10.76632	6.85622
C	15.69218	10.32445	8.13469
C	7.60805	14.96853	5.74953
C	6.44292	14.56076	6.66136
C	11.39865	13.71151	8.89429
C	11.73050	15.16528	9.25092
C	5.45395	8.97492	2.66738
C	5.06031	10.19694	1.82507
C	6.87692	9.54840	7.50545
C	5.57606	10.25383	7.90576
C	9.46850	4.95155	4.01380
C	7.97594	4.59792	3.96345
C	9.97684	6.45115	-0.81684
C	8.51246	6.28818	-1.24808
C	7.42686	17.51527	-0.81910
C	17.71110	11.27857	2.14378
C	14.18508	5.27544	1.23756
C	15.21466	16.03703	6.30953
C	16.98453	9.55751	6.10084
C	7.85847	16.48065	5.82109
C	10.58267	13.04585	10.01248
C	5.86788	7.80151	1.77190
C	6.86278	8.08033	7.95814
C	10.33760	3.69531	3.87029
C	10.80658	5.23102	-1.23622
H	17.62992	9.90520	0.50581
H	17.29995	12.12736	-0.47029
H	15.88389	11.11984	-0.82480
H	15.80239	12.36163	0.43276
H	18.53508	11.87729	1.73862
H	17.05823	11.94326	2.71968
H	18.13428	10.54649	2.83837
H	15.74804	5.94355	4.28546
H	14.03325	5.59763	4.01891
H	15.24806	4.37370	3.62956
H	14.30154	5.63459	0.21033
H	14.37054	4.19534	1.24461
H	13.14312	5.44100	1.53083
H	14.42459	15.74266	4.34551
H	16.55986	15.07855	3.23623
H	16.71977	16.63648	4.07063
H	17.40345	15.17080	4.78532
H	14.26019	15.89163	6.82389
H	16.00740	15.66507	6.96759
H	15.37202	17.11324	6.17737
H	16.64729	13.42126	6.34588
H	17.26903	11.39300	7.16108

H	15.32250	11.18634	8.69920
H	14.83354	9.68627	7.89816
H	16.36309	9.75287	8.78563
H	17.52693	9.86829	5.20367
H	17.67287	8.99360	6.73991
H	16.18956	8.87371	5.78583
H	14.18337	10.03429	5.43073
H	8.81521	13.08976	4.18947
H	7.31718	14.73219	4.71784
H	6.22938	13.49202	6.56876
H	6.67221	14.76784	7.71269
H	5.53366	15.11462	6.40246
H	8.67144	16.78289	5.15335
H	6.95858	17.03471	5.53248
H	8.12709	16.79509	6.83550
H	9.16236	15.02170	8.00000
H	12.34918	13.16831	8.81004
H	12.31612	15.64566	8.46124
H	10.82407	15.76153	9.40330
H	12.30997	15.21035	10.17939
H	10.38141	11.99484	9.78327
H	11.11881	13.09059	10.96710
H	9.61787	13.54802	10.14591
H	12.05544	12.08812	6.81829
H	8.06265	9.70704	2.23555
H	5.23087	8.99181	5.36678
H	9.19289	10.32404	6.32417
H	10.29548	7.50454	4.47108
H	9.66974	5.37976	5.00502
H	7.35715	5.48531	4.12629
H	7.70255	4.16989	2.99253
H	7.72517	3.86052	4.73446
H	11.40224	3.93865	3.94049
H	10.10097	2.96952	4.65626
H	10.17242	3.20272	2.90571
H	9.41751	4.78859	1.27469
H	10.79951	8.75226	0.39510
H	14.51086	11.36052	2.06078
H	12.99021	7.47134	3.01884
H	16.86722	7.87937	1.23382
H	16.17232	5.80037	1.83424
H	10.38334	7.32094	-1.34526
H	11.85716	5.35397	-0.95828
H	10.75564	5.08827	-2.32117
H	10.44047	4.31061	-0.76700
H	8.44399	6.12313	-2.32926
H	7.92566	7.17925	-1.00527
H	8.04246	5.43255	-0.74968
H	6.05881	7.52548	7.46133
H	6.70332	8.00542	9.03994
H	7.80745	7.58324	7.71688

H	7.69929	10.04962	8.03340
H	5.58310	11.30524	7.60359
H	5.43593	10.21392	8.99155
H	4.70191	9.77952	7.44653
H	6.75833	8.04262	1.18275
H	5.06350	7.54980	1.07173
H	6.09749	6.91029	2.36273
H	4.56386	8.66287	3.23112
H	4.71780	11.02139	2.45849
H	4.25289	9.94382	1.12877
H	5.90889	10.56014	1.23547
H	8.18917	11.87682	1.95019
H	8.94729	11.45999	0.40156
H	9.68258	13.43338	-1.15668
H	9.08360	15.66056	-1.96938
H	7.21569	14.03663	2.30421
H	6.63525	16.27886	1.49606
H	6.53753	17.45172	-1.45937
H	8.22347	17.96525	-1.42058
H	7.18853	18.20815	-0.00571
H	13.72140	9.48686	-0.60776
H	10.09854	11.33187	-1.99197
H	13.62209	7.90425	-2.47924
H	9.99851	9.74407	-3.85044
H	12.25995	6.81504	-4.27877
H	12.32049	8.20022	-5.36826
H	10.76083	7.57057	-4.83907
H	11.61501	16.07657	0.10845
H	13.17658	16.70433	0.68667
H	12.41203	16.63863	3.01271
H	10.95391	17.20233	2.17841
H	13.08669	11.72923	0.20175
H	11.64783	12.53643	-0.45365
H	12.90692	14.02162	0.24782
H	13.72382	14.56295	1.73994
H	13.14497	13.89509	3.91138
C	10.96067	15.07278	2.61443
H	9.94551	15.02835	2.21332
H	10.94687	14.85296	3.68368
O	11.73239	14.01396	1.95034

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Complex 1 - THF

Sc	11.95266	12.79795	4.20956
C	11.58336	11.02294	5.55457
C	11.30588	10.33898	4.30265
C	10.36669	10.88719	3.38874
C	10.21299	10.37086	2.09038
C	10.98751	9.31143	1.63379
C	11.92080	8.76071	2.53690
C	12.08417	9.25605	3.81651

C	10.83611	8.75044	0.24562
C	13.65492	12.45886	2.81791
C	15.02539	12.22412	3.33687
C	16.00180	13.23968	3.34039
C	17.29272	13.00875	3.80850
C	17.68113	11.75962	4.30732
C	16.71040	10.75172	4.32720
C	15.42102	10.97528	3.85413
C	19.09330	11.49747	4.76162
C	10.02655	14.40778	4.62735
C	10.85230	14.96893	3.59595
C	12.12158	15.31738	4.16485
C	12.09342	14.91664	5.54258
C	10.79793	14.38095	5.83333
C	13.17744	16.12165	3.49779
C	13.49942	15.95664	2.14041
C	14.45853	16.75535	1.51278
C	15.08411	17.75598	2.26321
C	14.77266	17.97117	3.60723
C	13.82373	17.14204	4.21212
C	10.41341	15.30159	2.21367
C	10.15338	14.31573	1.25598
C	9.74448	14.64667	-0.04006
C	9.58220	15.99817	-0.35637
C	9.82221	17.01285	0.57837
C	10.24559	16.64737	1.85833
C	8.59378	14.03653	4.50810
C	8.06885	12.91298	5.16684
C	6.71913	12.56482	5.07284
C	5.87236	13.37960	4.31577
C	6.34952	14.52301	3.66754
C	7.70750	14.83465	3.76866
C	10.29773	14.08980	7.20132
C	10.96578	13.22461	8.07610
C	10.52057	13.02956	9.38774
C	9.39468	13.73498	9.82074
C	8.70465	14.61292	8.97746
C	9.16594	14.77435	7.67010
C	13.13525	15.15277	6.57817
C	12.84166	16.01527	7.64397
C	13.76938	16.26805	8.65581
C	15.00936	15.62240	8.59469
C	15.33685	14.75423	7.54820
C	14.39194	14.53755	6.53797
C	14.80516	16.58592	0.04166
C	13.73575	17.22935	-0.85330
C	15.45795	19.08239	4.38496
C	16.40919	18.52044	5.45012
C	9.49293	13.55975	-1.07121
C	8.02361	13.52242	-1.51294
C	9.57697	18.46104	0.18209

C	10.42804	19.47297	0.95266
C	6.20632	11.30699	5.75459
C	5.90111	10.20888	4.72510
C	5.41238	15.43135	2.88820
C	4.41036	16.12961	3.81841
C	11.19256	12.03838	10.32481
C	12.71948	12.01355	10.20764
C	7.50847	15.40864	9.47328
C	7.93973	16.49666	10.46746
C	13.42530	17.21365	9.79476
C	14.39843	18.39726	9.87491
C	16.68041	14.04580	7.51124
C	17.85038	15.03658	7.44981
C	15.04731	15.12653	-0.35967
C	14.45209	20.06158	5.00425
C	10.42940	13.68920	-2.28004
C	8.08340	18.80425	0.30531
C	4.99033	11.57250	6.65001
C	4.68795	14.68721	1.75922
C	10.60962	10.63021	10.12308
C	6.41777	14.51652	10.07864
C	13.34082	16.47615	11.13814
C	16.84120	13.08197	8.69512
H	15.74474	17.13078	-0.12447
H	15.39241	15.06959	-1.39788
H	15.80103	14.65298	0.27640
H	14.13047	14.53155	-0.28935
H	14.00755	17.14014	-1.91143
H	12.76469	16.74355	-0.70992
H	13.61518	18.29264	-0.62254
H	13.78328	20.47807	4.24441
H	13.83241	19.57028	5.76211
H	14.97327	20.89257	5.49238
H	17.16479	17.87087	4.99718
H	16.92795	19.33038	5.97551
H	15.86494	17.92930	6.19392
H	9.71703	12.60079	-0.58490
H	11.47914	13.68262	-1.97143
H	10.27415	12.86049	-2.97958
H	10.24802	14.62125	-2.82650
H	7.35588	13.38664	-0.65664
H	7.73643	14.45246	-2.01579
H	7.85034	12.69929	-2.21499
H	9.26480	16.27837	-1.35960
H	9.84565	18.54438	-0.88050
H	7.46525	18.11810	-0.28198
H	7.75840	18.73715	1.34974
H	7.88734	19.82418	-0.04384
H	11.49043	19.21433	0.92201
H	10.30620	20.47252	0.52272
H	10.12733	19.53656	2.00431

H	10.45807	17.40824	2.60271
H	8.72396	12.29819	5.77805
H	7.01605	10.93995	6.39910
H	5.20454	12.34794	7.39141
H	4.12263	11.89876	6.06616
H	4.70074	10.66091	7.18376
H	6.78223	9.97973	4.11781
H	5.58104	9.28654	5.22245
H	5.09844	10.51984	4.04678
H	4.81848	13.12274	4.23437
H	6.03305	16.20905	2.42441
H	5.40005	14.21696	1.07444
H	4.03355	13.90136	2.15246
H	4.06368	15.37676	1.18048
H	4.92418	16.69208	4.60420
H	3.77829	16.82703	3.25737
H	3.75223	15.40197	4.30632
H	8.08096	15.72481	3.27274
H	11.85037	12.70608	7.72203
H	9.05362	13.59373	10.84506
H	8.64903	15.45964	7.00286
H	11.86615	16.49360	7.68168
H	12.42784	17.62051	9.58118
H	12.60848	15.66443	11.09523
H	14.30883	16.04335	11.41436
H	13.04383	17.16258	11.93906
H	14.43519	18.94655	8.92912
H	14.09390	19.09480	10.66297
H	15.41604	18.06307	10.10517
H	15.73872	15.79944	9.38265
H	14.65252	13.88422	5.70704
H	12.98826	15.19190	1.56686
H	13.56874	17.29545	5.25531
H	15.83036	18.38867	1.78396
H	16.06498	19.64764	3.66446
H	16.70496	13.44880	6.59181
H	17.76074	15.70203	6.58632
H	18.80335	14.50171	7.37078
H	17.89651	15.66057	8.34957
H	17.79032	12.53944	8.62374
H	16.03116	12.34678	8.72056
H	16.83589	13.61828	9.65097
H	8.38433	16.05305	11.36533
H	7.08134	17.10070	10.78233
H	8.68363	17.16589	10.02418
H	7.07485	15.91143	8.59850
H	6.09881	13.74429	9.37231
H	5.54007	15.11250	10.35177
H	6.76780	14.01386	10.98695
H	13.04291	11.59845	9.24701
H	13.14931	11.38235	10.99278

H	13.14952	13.01505	10.29857
H	10.94416	12.35297	11.34815
H	9.52335	10.62644	10.25725
H	11.04510	9.92092	10.83606
H	10.82278	10.26651	9.11159
H	10.70339	11.32502	6.12729
H	12.34200	10.55870	6.18528
H	12.80670	8.79585	4.48555
H	12.52808	7.91610	2.21662
H	9.64199	11.62784	3.73715
H	9.45054	10.79784	1.44240
H	10.61619	7.67695	0.26972
H	11.75481	8.87739	-0.33898
H	10.02574	9.24395	-0.29807
H	15.74123	14.22266	2.95575
H	14.70333	10.15853	3.85825
H	18.01941	13.81888	3.77670
H	16.97311	9.76605	4.70827
H	19.57729	12.41222	5.11801
H	19.71164	11.10269	3.94476
H	19.12564	10.76253	5.57259
H	13.65545	13.25159	2.06291
H	13.26322	11.54457	2.34007
H	10.27976	13.26634	1.51665

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Complex 1 - THF + H2

Sc	-1.41359	-0.96918	0.21700
C	-3.00750	-0.12090	1.53734
C	-4.21414	0.50670	0.94334
C	-4.32935	1.90165	0.79199
C	-5.46000	2.48422	0.22252
C	-6.53366	1.71180	-0.23341
C	-6.42319	0.32327	-0.09321
C	-5.29945	-0.26275	0.48061
C	-7.77274	2.34439	-0.81111
C	-2.01580	-2.90526	-0.87669
C	-2.29372	-3.36843	0.46753
C	-1.29527	-3.30057	1.47403
C	-1.59447	-3.58426	2.81891
C	-2.87878	-3.91971	3.22628
C	-3.87721	-3.97707	2.22974
C	-3.60393	-3.70315	0.90500
C	-3.20680	-4.23987	4.65960
C	0.62290	-0.55920	-1.24869
C	-0.03332	0.70924	-1.10584
C	0.08154	1.11715	0.26411
C	0.78113	0.08634	0.96913
C	1.13940	-0.94162	0.03257
C	0.91903	-1.22192	-2.54613
C	-0.08878	-1.57394	-3.45509

C	0.21556	-2.12570	-4.70133
C	1.56277	-2.31046	-5.03300
C	2.59545	-1.96593	-4.15754
C	2.25599	-1.42732	-2.91224
C	-0.53259	1.55710	-2.22271
C	-1.78868	2.18293	-2.18177
C	-2.23308	2.99501	-3.22632
C	-1.37850	3.20754	-4.31484
C	-0.11095	2.62741	-4.37780
C	0.29458	1.79508	-3.32772
C	-0.20504	2.46555	0.81712
C	-0.75706	2.64777	2.09275
C	-0.95975	3.91911	2.63419
C	-0.56953	5.03304	1.88464
C	0.01020	4.89342	0.61996
C	0.17939	3.60790	0.09879
C	1.29700	0.24846	2.35817
C	0.82473	-0.47458	3.45570
C	1.35027	-0.26673	4.73998
C	2.37665	0.66558	4.89794
C	2.88280	1.40032	3.81817
C	2.32137	1.18796	2.56050
C	2.00509	-2.11863	0.30618
C	3.13040	-1.99715	1.13725
C	3.97385	-3.08008	1.39544
C	3.67977	-4.31680	0.81230
C	2.57823	-4.47798	-0.03230
C	1.76389	-3.36992	-0.28291
C	-0.86115	-2.56291	-5.68199
C	-2.12613	-1.70159	-5.64172
C	4.04629	-2.17689	-4.55801
C	4.68967	-3.31150	-3.74885
C	-3.61797	3.61793	-3.18424
C	-3.56210	5.15050	-3.22718
C	0.80201	2.89734	-5.56247
C	1.03925	1.63182	-6.39733
C	-1.60053	4.07479	4.00387
C	-2.94194	4.81635	3.92129
C	0.49605	6.10242	-0.16348
C	1.77940	6.67725	0.45465
C	0.84245	-1.04104	5.94510
C	1.33300	-2.49584	5.92119
C	4.01626	2.39536	4.00044
C	5.29801	1.70841	4.49218
C	5.20044	-2.89953	2.27449
C	6.49534	-3.02821	1.45933
C	2.21788	-5.82999	-0.62684
C	3.41759	-6.56926	-1.22904
C	-1.20587	-4.04671	-5.47405
C	4.87447	-0.88972	-4.45634
C	-4.51210	3.06887	-4.30499

C	2.13082	3.53166	-5.13004
C	-0.65788	4.75041	5.00814
C	-0.57493	7.19028	-0.30635
C	-0.68165	-0.96781	6.09613
C	3.62311	3.55424	4.92577
C	5.20656	-3.85941	3.47099
C	1.50577	-6.70505	0.41661
H	-0.42776	-2.46535	-6.68729
H	-1.93843	-4.38562	-6.21531
H	-0.31615	-4.67820	-5.56055
H	-1.63310	-4.20741	-4.47782
H	-2.79836	-1.97830	-6.46064
H	-2.68255	-1.84286	-4.70854
H	-1.89276	-0.63685	-5.73468
H	4.43376	-0.08497	-5.05293
H	4.94499	-0.53949	-3.42089
H	5.89531	-1.05951	-4.81583
H	4.13866	-4.24764	-3.88161
H	5.72518	-3.47767	-4.06654
H	4.69755	-3.07886	-2.67865
H	-4.07249	3.32622	-2.22954
H	-4.59044	1.97877	-4.24954
H	-5.52274	3.48563	-4.23273
H	-4.11551	3.32659	-5.29361
H	-2.95417	5.54665	-2.40830
H	-3.13001	5.51028	-4.16777
H	-4.56774	5.57688	-3.14151
H	-1.70430	3.84506	-5.13494
H	0.28538	3.62470	-6.20356
H	1.96450	4.44975	-4.55771
H	2.71370	2.84837	-4.50305
H	2.74248	3.78125	-6.00407
H	0.09464	1.22072	-6.76672
H	1.67531	1.85141	-7.26255
H	1.52985	0.85123	-5.80654
H	1.27380	1.32701	-3.35925
H	-1.02666	1.77931	2.68343
H	-1.80722	3.06273	4.37638
H	0.27569	4.18958	5.11108
H	-0.40533	5.76965	4.69509
H	-1.12705	4.81512	5.99629
H	-3.63421	4.30935	3.24241
H	-3.41406	4.87230	4.90848
H	-2.80766	5.84189	3.55931
H	-0.71384	6.02900	2.29806
H	0.74352	5.74985	-1.17351
H	-1.49122	6.79107	-0.75111
H	-0.83797	7.62857	0.66263
H	-0.21262	8.00372	-0.94440
H	2.56501	5.91759	0.51494
H	2.15891	7.51501	-0.14124

H	1.59329	7.04488	1.47009
H	0.63575	3.49128	-0.87983
H	0.02810	-1.19965	3.30837
H	2.78897	0.82238	5.89332
H	2.68321	1.75850	1.70832
H	3.36099	-1.03567	1.58304
H	5.15918	-1.87766	2.67387
H	4.29489	-3.75498	4.06678
H	5.27675	-4.90383	3.14772
H	6.06510	-3.65845	4.12109
H	6.51583	-2.31245	0.63155
H	7.37254	-2.84556	2.09011
H	6.59455	-4.03267	1.03280
H	4.32446	-5.16832	1.01633
H	0.92412	-3.48785	-0.96076
H	-1.12347	-1.40187	-3.17871
H	3.03752	-1.14438	-2.21238
H	1.81391	-2.72819	-6.00753
H	4.04394	-2.48356	-5.61287
H	1.50495	-5.64054	-1.44047
H	3.94374	-5.94976	-1.96101
H	3.08696	-7.48489	-1.73094
H	4.13896	-6.86580	-0.45964
H	1.19487	-7.65998	-0.02182
H	0.61628	-6.20581	0.81291
H	2.17154	-6.92223	1.25964
H	5.15651	1.26665	5.48477
H	6.12030	2.42881	4.56419
H	5.60634	0.90793	3.81234
H	4.22846	2.82220	3.01117
H	2.74160	4.07912	4.54650
H	4.44165	4.27785	5.00750
H	3.39451	3.19752	5.93621
H	0.95334	-3.02605	5.04110
H	0.99564	-3.03716	6.81221
H	2.42577	-2.54314	5.88680
H	1.28115	-0.56543	6.83280
H	-1.02555	0.07018	6.13961
H	-1.00036	-1.46992	7.01620
H	-1.19661	-1.45331	5.26057
H	-2.54204	0.54494	2.27086
H	-3.27635	-1.05220	2.06197
H	-5.26041	-1.34426	0.59192
H	-7.24007	-0.31317	-0.43041
H	-3.51855	2.53824	1.13939
H	-5.51213	3.56894	0.14134
H	-8.57021	2.42794	-0.06122
H	-8.17531	1.75633	-1.64274
H	-7.57144	3.35403	-1.18235
H	-0.24819	-3.18149	1.18988
H	-4.39750	-3.76698	0.16459

H	-0.78882	-3.57080	3.54884
H	-4.89100	-4.25190	2.51498
H	-3.96161	-3.55329	5.06014
H	-2.32145	-4.16942	5.29704
H	-3.61017	-5.25438	4.75965
H	-1.05577	-3.20936	-1.29801
H	-2.82661	-3.04360	-1.59189
H	-2.43157	2.04591	-1.31435
H	-2.69500	-0.82775	-1.49889
H	-2.69980	-0.07364	-1.38677

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Complex 1 - 1st xyl. hydro black path.

Sc	12.86146	11.32964	3.60200
C	11.48975	11.65354	5.33713
C	10.39720	12.23307	4.52840
C	10.34741	13.61195	4.22004
C	9.34377	14.14573	3.41744
C	8.34504	13.34188	2.85485
C	8.38711	11.97432	3.14862
C	9.38024	11.43450	3.95968
C	7.27641	13.91953	1.96506
C	12.14504	9.53387	2.04223
C	12.03947	8.80723	3.30860
C	13.15498	8.68581	4.16581
C	13.04191	8.05404	5.41574
C	11.83289	7.53739	5.86383
C	10.71879	7.65627	5.00768
C	10.81254	8.27549	3.77681
C	11.70582	6.84474	7.19385
C	15.00869	11.85430	2.43572
C	14.34121	13.12370	2.58358
C	14.30525	13.46221	3.97508
C	14.93638	12.40393	4.69741
C	15.41875	11.44079	3.75713
C	15.10577	11.07107	1.16893
C	14.31503	11.40583	0.05115
C	14.31836	10.64415	-1.11942
C	15.14115	9.51738	-1.18512
C	15.93731	9.14157	-0.10216
C	15.90639	9.91872	1.05969
C	14.03734	14.08805	1.48908
C	12.75861	14.60327	1.24111
C	12.54401	15.55652	0.24221
C	13.64258	16.01030	-0.49853
C	14.93461	15.53002	-0.26811
C	15.11266	14.56083	0.72471
C	13.94124	14.76953	4.57993
C	13.31616	14.84918	5.83423
C	13.04018	16.07283	6.44719
C	13.41841	17.24891	5.79334

C	14.05899	17.21381	4.55193
C	14.30963	15.97328	3.95904
C	15.34501	12.46882	6.12802
C	14.68415	11.77026	7.14143
C	15.09408	11.87044	8.47816
C	16.19659	12.67234	8.77741
C	16.89020	13.37631	7.78468
C	16.44550	13.26812	6.46757
C	16.52000	10.51365	4.14091
C	17.78820	10.73298	3.57685
C	18.91297	10.01239	3.98323
C	18.75648	9.04496	4.98184
C	17.51629	8.80704	5.57845
C	16.41210	9.55270	5.15166
C	13.43195	11.01159	-2.29873
C	13.83943	12.35182	-2.92426
C	16.83471	7.91909	-0.20087
C	16.57819	6.90627	0.92211
C	11.14470	16.08513	-0.02647
C	11.03744	17.58896	0.25956
C	16.11584	16.08137	-1.05012
C	16.90102	14.98780	-1.78455
C	12.33546	16.11280	7.79308
C	10.96483	16.79642	7.69407
C	14.52421	18.48979	3.86907
C	15.74693	19.08280	4.58504
C	14.34933	11.14605	9.58750
C	14.35814	9.62444	9.39478
C	18.09740	14.23386	8.12269
C	19.24373	13.39512	8.70476
C	20.27769	10.33713	3.39712
C	21.08376	9.09318	3.00597
C	17.36473	7.76731	6.67592
C	17.61853	6.34736	6.15097
C	11.94404	11.00850	-1.92370
C	18.31475	8.32348	-0.25039
C	10.67676	15.76267	-1.45212
C	17.04247	16.90589	-0.14458
C	13.20368	16.76699	8.87577
C	13.40947	19.53455	3.73735
C	12.91524	11.67113	9.74262
C	17.73317	15.39541	9.05699
C	21.08029	11.22480	4.36100
C	18.25586	8.07743	7.88613
H	13.57957	10.23351	-3.06032
H	11.32322	11.21543	-2.80266
H	11.64134	10.03887	-1.51560
H	11.72184	11.77333	-1.17187
H	13.22232	12.57351	-3.80244
H	13.71822	13.17479	-2.21208
H	14.88697	12.33384	-3.24134

H	18.50985	9.01361	-1.07726
H	18.61068	8.82318	0.67834
H	18.95652	7.44459	-0.38035
H	15.52607	6.60579	0.95237
H	17.18483	6.00581	0.77453
H	16.83831	7.32058	1.90196
H	10.47113	15.56684	0.66796
H	10.71802	14.68724	-1.64968
H	9.64514	16.09847	-1.60583
H	11.30211	16.26343	-2.19966
H	11.33222	17.81665	1.28826
H	11.68310	18.16906	-0.40918
H	10.00942	17.93864	0.11277
H	13.49502	16.76072	-1.27328
H	15.70691	16.76107	-1.81018
H	16.49795	17.71871	0.34608
H	17.48417	16.27946	0.63833
H	17.86261	17.34523	-0.72338
H	16.25464	14.42032	-2.45975
H	17.71108	15.42870	-2.37603
H	17.35308	14.27815	-1.08323
H	16.10528	14.16761	0.92908
H	13.04432	13.93649	6.35233
H	12.16305	15.07118	8.09436
H	14.16244	16.24970	8.97710
H	13.41182	17.81663	8.63970
H	12.69672	16.74145	9.84695
H	10.33133	16.30611	6.94851
H	10.44441	16.76391	8.65780
H	11.06613	17.84906	7.40684
H	13.21676	18.20899	6.26374
H	14.83615	18.21225	2.85359
H	12.53796	19.12401	3.21875
H	13.07585	19.89475	4.71674
H	13.76301	20.40453	3.17304
H	16.56310	18.35587	4.64229
H	16.11564	19.97074	4.05904
H	15.49444	19.38045	5.60910
H	14.82095	15.94596	3.00271
H	13.82563	11.15697	6.87886
H	16.51877	12.75046	9.81455
H	16.95914	13.81616	5.68131
H	17.89380	11.49825	2.81118
H	20.10183	10.91827	2.48179
H	20.53034	12.13754	4.60965
H	21.28549	10.69399	5.29752
H	22.04100	11.51265	3.91942
H	20.52139	8.44544	2.32700
H	22.01336	9.38452	2.50542
H	21.36189	8.49873	3.88327
H	19.62212	8.47628	5.31304

H 15.45604 9.40405 5.64156
H 13.65531 12.26215 0.10973
H 16.51915 9.61409 1.89743
H 15.15292 8.91538 -2.09267
H 16.59551 7.42438 -1.15218
H 16.32225 7.81261 7.01885
H 16.95424 6.10786 5.31481
H 17.45511 5.60589 6.94097
H 18.64994 6.23544 5.79874
H 18.07634 7.35800 8.69281
H 18.06223 9.08294 8.27144
H 19.31817 8.01926 7.62461
H 18.95888 12.94377 9.66173
H 20.12792 14.01738 8.88260
H 19.52655 12.58532 8.02523
H 18.45309 14.66938 7.17938
H 16.94555 16.01880 8.62309
H 18.60638 16.03020 9.24443
H 17.37607 15.02957 10.02614
H 13.82473 9.34012 8.48115
H 13.86430 9.12444 10.23543
H 15.38019 9.24024 9.32233
H 14.88255 11.36189 10.52339
H 12.90776 12.75039 9.92313
H 12.41087 11.18200 10.58361
H 12.32329 11.47864 8.84123
H 11.84892 12.32719 6.11556
H 11.22614 10.68318 5.77325
H 9.35477 10.37594 4.20062
H 7.61334 11.31988 2.75023
H 11.09545 14.27533 4.64613
H 9.33129 15.21865 3.23355
H 7.11225 14.98117 2.17419
H 6.32123 13.40041 2.09588
H 7.54591 13.83493 0.90443
H 14.14589 8.95766 3.79939
H 9.94029 8.33048 3.13083
H 13.92961 7.93507 6.03121
H 9.76439 7.23699 5.32014
H 12.66890 6.78562 7.70758
H 11.32571 5.82342 7.07642
H 11.00819 7.37337 7.85363
H 13.08261 9.36485 1.50738
H 11.29231 9.37616 1.37966
H 11.92001 14.24636 1.83341
H 11.99872 11.96926 2.04435
H 11.97874 10.97334 1.94826

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Complex 1 - 1st xyl. hydro black path. TS

Sc 12.86146 11.32964 3.60200

C	11.48975	11.65354	5.33713
C	10.39720	12.23307	4.52840
C	10.34741	13.61195	4.22004
C	9.34377	14.14573	3.41744
C	8.34504	13.34188	2.85485
C	8.38711	11.97432	3.14862
C	9.38024	11.43450	3.95968
C	7.27641	13.91953	1.96506
C	12.14504	9.53387	2.04223
C	12.03947	8.80723	3.30860
C	13.15498	8.68581	4.16581
C	13.04191	8.05404	5.41574
C	11.83289	7.53739	5.86383
C	10.71879	7.65627	5.00768
C	10.81254	8.27549	3.77681
C	11.70582	6.84474	7.19385
C	15.00869	11.85430	2.43572
C	14.34121	13.12370	2.58358
C	14.30525	13.46221	3.97508
C	14.93638	12.40393	4.69741
C	15.41875	11.44079	3.75713
C	15.10577	11.07107	1.16893
C	14.31503	11.40583	0.05115
C	14.31836	10.64415	-1.11942
C	15.14115	9.51738	-1.18512
C	15.93731	9.14157	-0.10216
C	15.90639	9.91872	1.05969
C	14.03734	14.08805	1.48908
C	12.75861	14.60327	1.24111
C	12.54401	15.55652	0.24221
C	13.64258	16.01030	-0.49853
C	14.93461	15.53002	-0.26811
C	15.11266	14.56083	0.72471
C	13.94124	14.76953	4.57993
C	13.31616	14.84918	5.83423
C	13.04018	16.07283	6.44719
C	13.41841	17.24891	5.79334
C	14.05899	17.21381	4.55193
C	14.30963	15.97328	3.95904
C	15.34501	12.46882	6.12802
C	14.68415	11.77026	7.14143
C	15.09408	11.87044	8.47816
C	16.19659	12.67234	8.77741
C	16.89020	13.37631	7.78468
C	16.44550	13.26812	6.46757
C	16.52000	10.51365	4.14091
C	17.78820	10.73298	3.57685
C	18.91297	10.01239	3.98323
C	18.75648	9.04496	4.98184
C	17.51629	8.80704	5.57845
C	16.41210	9.55270	5.15166

C	13.43195	11.01159	-2.29873
C	13.83943	12.35182	-2.92426
C	16.83471	7.91909	-0.20087
C	16.57819	6.90627	0.92211
C	11.14470	16.08513	-0.02647
C	11.03744	17.58896	0.25956
C	16.11584	16.08137	-1.05012
C	16.90102	14.98780	-1.78455
C	12.33546	16.11280	7.79308
C	10.96483	16.79642	7.69407
C	14.52421	18.48979	3.86907
C	15.74693	19.08280	4.58504
C	14.34933	11.14605	9.58750
C	14.35814	9.62444	9.39478
C	18.09740	14.23386	8.12269
C	19.24373	13.39512	8.70476
C	20.27769	10.33713	3.39712
C	21.08376	9.09318	3.00597
C	17.36473	7.76731	6.67592
C	17.61853	6.34736	6.15097
C	11.94404	11.00850	-1.92370
C	18.31475	8.32348	-0.25039
C	10.67676	15.76267	-1.45212
C	17.04247	16.90589	-0.14458
C	13.20368	16.76699	8.87577
C	13.40947	19.53455	3.73735
C	12.91524	11.67113	9.74262
C	17.73317	15.39541	9.05699
C	21.08029	11.22480	4.36100
C	18.25586	8.07743	7.88613
H	13.57957	10.23351	-3.06032
H	11.32322	11.21543	-2.80266
H	11.64134	10.03887	-1.51560
H	11.72184	11.77333	-1.17187
H	13.22232	12.57351	-3.80244
H	13.71822	13.17479	-2.21208
H	14.88697	12.33384	-3.24134
H	18.50985	9.01361	-1.07726
H	18.61068	8.82318	0.67834
H	18.95652	7.44459	-0.38035
H	15.52607	6.60579	0.95237
H	17.18483	6.00581	0.77453
H	16.83831	7.32058	1.90196
H	10.47113	15.56684	0.66796
H	10.71802	14.68724	-1.64968
H	9.64514	16.09847	-1.60583
H	11.30211	16.26343	-2.19966
H	11.33222	17.81665	1.28826
H	11.68310	18.16906	-0.40918
H	10.00942	17.93864	0.11277
H	13.49502	16.76072	-1.27328

H	15.70691	16.76107	-1.81018
H	16.49795	17.71871	0.34608
H	17.48417	16.27946	0.63833
H	17.86261	17.34523	-0.72338
H	16.25464	14.42032	-2.45975
H	17.71108	15.42870	-2.37603
H	17.35308	14.27815	-1.08323
H	16.10528	14.16761	0.92908
H	13.04432	13.93649	6.35233
H	12.16305	15.07118	8.09436
H	14.16244	16.24970	8.97710
H	13.41182	17.81663	8.63970
H	12.69672	16.74145	9.84695
H	10.33133	16.30611	6.94851
H	10.44441	16.76391	8.65780
H	11.06613	17.84906	7.40684
H	13.21676	18.20899	6.26374
H	14.83615	18.21225	2.85359
H	12.53796	19.12401	3.21875
H	13.07585	19.89475	4.71674
H	13.76301	20.40453	3.17304
H	16.56310	18.35587	4.64229
H	16.11564	19.97074	4.05904
H	15.49444	19.38045	5.60910
H	14.82095	15.94596	3.00271
H	13.82563	11.15697	6.87886
H	16.51877	12.75046	9.81455
H	16.95914	13.81616	5.68131
H	17.89380	11.49825	2.81118
H	20.10183	10.91827	2.48179
H	20.53034	12.13754	4.60965
H	21.28549	10.69399	5.29752
H	22.04100	11.51265	3.91942
H	20.52139	8.44544	2.32700
H	22.01336	9.38452	2.50542
H	21.36189	8.49873	3.88327
H	19.62212	8.47628	5.31304
H	15.45604	9.40405	5.64156
H	13.65531	12.26215	0.10973
H	16.51915	9.61409	1.89743
H	15.15292	8.91538	-2.09267
H	16.59551	7.42438	-1.15218
H	16.32225	7.81261	7.01885
H	16.95424	6.10786	5.31481
H	17.45511	5.60589	6.94097
H	18.64994	6.23544	5.79874
H	18.07634	7.35800	8.69281
H	18.06223	9.08294	8.27144
H	19.31817	8.01926	7.62461
H	18.95888	12.94377	9.66173
H	20.12792	14.01738	8.88260

H	19.52655	12.58532	8.02523
H	18.45309	14.66938	7.17938
H	16.94555	16.01880	8.62309
H	18.60638	16.03020	9.24443
H	17.37607	15.02957	10.02614
H	13.82473	9.34012	8.48115
H	13.86430	9.12444	10.23543
H	15.38019	9.24024	9.32233
H	14.88255	11.36189	10.52339
H	12.90776	12.75039	9.92313
H	12.41087	11.18200	10.58361
H	12.32329	11.47864	8.84123
H	11.84892	12.32719	6.11556
H	11.22614	10.68318	5.77325
H	9.35477	10.37594	4.20062
H	7.61334	11.31988	2.75023
H	11.09545	14.27533	4.64613
H	9.33129	15.21865	3.23355
H	7.11225	14.98117	2.17419
H	6.32123	13.40041	2.09588
H	7.54591	13.83493	0.90443
H	14.14589	8.95766	3.79939
H	9.94029	8.33048	3.13083
H	13.92961	7.93507	6.03121
H	9.76439	7.23699	5.32014
H	12.66890	6.78562	7.70758
H	11.32571	5.82342	7.07642
H	11.00819	7.37337	7.85363
H	13.08261	9.36485	1.50738
H	11.29231	9.37616	1.37966
H	11.92001	14.24636	1.83341
H	11.99872	11.96926	2.04435
H	11.97874	10.97334	1.94826

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Complex 1 - 1st xyl. hydro black path. prod

Sc	-0.99835	-0.25755	0.33424
C	-1.80817	-0.67290	2.39884
C	-3.04023	-0.44122	1.66582
C	-3.28721	0.83081	1.07895
C	-4.35905	1.03847	0.19550
C	-5.20178	-0.00196	-0.18268
C	-4.93422	-1.27561	0.35639
C	-3.88619	-1.49643	1.23266
C	-6.35471	0.20827	-1.12653
C	-3.05430	-5.25411	-0.91563
C	-4.26197	-5.41344	-0.03064
C	-4.12540	-5.66195	1.34153
C	-5.23901	-5.78089	2.16817
C	-6.53735	-5.66215	1.65742
C	-6.67478	-5.41716	0.28833

C	-5.55896	-5.29704	-0.53988
C	-7.73962	-5.82143	2.55080
C	1.02100	0.00534	-1.11913
C	0.39523	1.28711	-1.02054
C	0.49033	1.72954	0.34144
C	1.17378	0.71065	1.08612
C	1.48754	-0.35400	0.18267
C	1.31153	-0.72363	-2.38097
C	0.30352	-1.13522	-3.25946
C	0.60891	-1.77267	-4.46482
C	1.95372	-1.98329	-4.78441
C	2.98751	-1.58422	-3.93223
C	2.64885	-0.95568	-2.73020
C	-0.14932	2.05475	-2.17027
C	-1.48405	2.48219	-2.22101
C	-1.97618	3.21037	-3.30595
C	-1.09535	3.52901	-4.34623
C	0.24268	3.13042	-4.32582
C	0.69829	2.38289	-3.23446
C	0.06323	3.04743	0.87117
C	-0.55993	3.16931	2.12315
C	-0.94786	4.41057	2.63324
C	-0.68216	5.55513	1.87508
C	-0.04424	5.47718	0.63316
C	0.31584	4.21912	0.14314
C	1.68163	0.82233	2.47792
C	1.43382	-0.15814	3.44608
C	1.99197	-0.07331	4.72517
C	2.82195	1.01292	5.01937
C	3.09434	2.00976	4.07683
C	2.51138	1.90224	2.81237
C	2.23624	-1.59232	0.50937
C	3.49628	-1.51707	1.11802
C	4.23476	-2.66775	1.40335
C	3.68233	-3.91211	1.07904
C	2.42663	-4.02314	0.47360
C	1.71749	-2.85329	0.18656
C	-0.49038	-2.25906	-5.39425
C	-1.41329	-1.12212	-5.85016
C	4.43788	-1.84515	-4.30293
C	5.07513	-2.88486	-3.37070
C	-3.43295	3.63904	-3.35569
C	-3.58255	5.16521	-3.40132
C	1.17829	3.50616	-5.46260
C	1.65575	2.27022	-6.23692
C	-1.65529	4.50249	3.97536
C	-3.10483	4.98229	3.81418
C	0.29755	6.72929	-0.15761
C	1.44023	7.50759	0.51134
C	1.68625	-1.09349	5.81123
C	1.46656	-2.51530	5.28734

C	4.03344	3.16176	4.39326
C	5.48067	2.67384	4.55266
C	5.60710	-2.55873	2.04795
C	6.70818	-3.15295	1.15925
C	1.83623	-5.38010	0.12747
C	2.68610	-6.12473	-0.91087
C	-1.29692	-3.39661	-4.75133
C	5.27002	-0.55655	-4.33994
C	-4.17644	2.97715	-4.52422
C	2.36654	4.34381	-4.97094
C	-0.89305	5.38350	4.97321
C	-0.91921	7.63327	-0.38991
C	0.48492	-0.63523	6.65418
C	3.58647	3.96191	5.62296
C	5.63108	-3.18811	3.44755
C	1.61278	-6.24064	1.37836
H	0.00148	-2.66531	-6.28881
H	-2.05763	-3.77483	-5.44402
H	-0.64689	-4.23061	-4.46890
H	-1.80636	-3.05110	-3.84522
H	-2.16116	-1.49221	-6.56049
H	-1.94837	-0.68110	-5.00269
H	-0.84707	-0.32205	-6.33603
H	4.83634	0.17737	-5.02644
H	5.33151	-0.09280	-3.34930
H	6.29372	-0.76685	-4.66915
H	4.51770	-3.82618	-3.39014
H	6.10909	-3.09393	-3.66805
H	5.08617	-2.53085	-2.33443
H	-3.90173	3.28909	-2.42617
H	-4.10199	1.88658	-4.47417
H	-5.23777	3.24925	-4.51367
H	-3.76200	3.29474	-5.48730
H	-3.08386	5.63691	-2.54944
H	-3.14499	5.58055	-4.31570
H	-4.63968	5.45247	-3.38030
H	-1.45687	4.10422	-5.19688
H	0.60148	4.13076	-6.15842
H	2.02827	5.24085	-4.44271
H	3.00122	3.77157	-4.28574
H	2.99127	4.65967	-5.81374
H	0.81013	1.71504	-6.65369
H	2.31279	2.56138	-7.06410
H	2.21142	1.58449	-5.58901
H	1.73164	2.05015	-3.19730
H	-0.73409	2.27837	2.72101
H	-1.68727	3.48661	4.39110
H	0.13172	5.02676	5.11213
H	-0.84215	6.42342	4.63217
H	-1.39043	5.38054	5.94926
H	-3.66677	4.32927	3.13906

H	-3.61938	4.99488	4.78135
H	-3.14135	5.99749	3.40363
H	-0.97155	6.52888	2.26383
H	0.65405	6.39784	-1.14182
H	-1.73469	7.08569	-0.87183
H	-1.30270	8.04349	0.55084
H	-0.65256	8.48049	-1.03102
H	2.32513	6.87697	0.64173
H	1.72629	8.37697	-0.09135
H	1.14117	7.87022	1.50123
H	0.81552	4.14789	-0.81862
H	0.80015	-0.99803	3.18239
H	3.26831	1.07420	6.01086
H	2.71854	2.66180	2.06237
H	3.90759	-0.54239	1.36743
H	5.82022	-1.48793	2.16588
H	4.88379	-2.72648	4.09984
H	5.42052	-4.26246	3.40304
H	6.61475	-3.06167	3.91370
H	6.71423	-2.68686	0.16917
H	7.69452	-3.00355	1.61251
H	6.56902	-4.23053	1.01855
H	4.24624	-4.81584	1.30137
H	0.74313	-2.91477	-0.29570
H	-0.73108	-0.98126	-2.96867
H	3.43053	-0.63694	-2.04532
H	2.20303	-2.47821	-5.72243
H	4.43813	-2.26571	-5.31791
H	0.85377	-5.19204	-0.32480
H	2.81271	-5.52600	-1.81775
H	2.21386	-7.07324	-1.19033
H	3.68342	-6.35406	-0.51902
H	1.13329	-7.19033	1.11575
H	0.97626	-5.72573	2.10484
H	2.56094	-6.47526	1.87481
H	5.57516	1.99255	5.40565
H	6.15971	3.51705	4.72211
H	5.81843	2.13796	3.66015
H	4.00691	3.84123	3.53088
H	2.56401	4.33258	5.50412
H	4.24454	4.82304	5.78288
H	3.61710	3.35122	6.53193
H	0.53584	-2.59504	4.71511
H	1.39198	-3.21890	6.12324
H	2.28531	-2.83988	4.63843
H	2.56190	-1.11747	6.47534
H	0.65344	0.35853	7.08074
H	0.29607	-1.33347	7.47749
H	-0.42038	-0.58548	6.03873
H	-1.50111	0.11995	3.08317
H	-1.69959	-1.66723	2.83409

H	-3.71649	-2.49769	1.61841
H	-5.56498	-2.11661	0.07657
H	-2.70383	1.69306	1.40845
H	-4.53925	2.04150	-0.18546
H	-6.44394	1.25729	-1.42196
H	-7.30428	-0.09180	-0.66867
H	-6.23697	-0.38658	-2.03975
H	-3.12958	-5.76694	1.76760
H	-5.69960	-5.11205	-1.60284
H	-5.09798	-5.97398	3.22979
H	-7.67072	-5.32456	-0.14022
H	-7.92956	-6.87772	2.77808
H	-8.64284	-5.42050	2.08183
H	-7.60000	-5.30648	3.50694
H	-2.26069	-5.95431	-0.63555
H	-3.30315	-5.43088	-1.96605
H	-2.15590	2.24616	-1.39770
H	-1.27420	-1.70328	-0.74868
H	-2.63681	-4.24215	-0.84207

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Complex 1 - 1st xyl. hydro black path. prod - p-xyl.

C	-1.63341	-2.32679	0.89516
C	-1.84569	-1.01749	1.34742
C	-2.30555	-0.06440	0.42721
C	-2.54148	-0.39147	-0.90973
C	-2.29313	-1.70295	-1.32968
C	-1.83999	-2.68304	-0.44152
C	-1.64339	-0.62063	2.76462
C	-2.29201	-1.20622	3.89887
C	-1.96052	-0.43222	5.05249
C	-1.09938	0.63309	4.63395
C	-0.90648	0.52574	3.22016
Sc	0.15390	-1.48633	4.24962
C	2.32697	-0.90538	3.96027
C	2.37866	-2.31926	3.65113
C	2.91710	-3.28504	4.54422
C	2.75258	-4.64149	4.33453
C	2.01238	-5.14900	3.24729
C	1.44182	-4.22254	2.38227
C	1.59999	-2.84017	2.58004
C	1.85549	-6.63173	3.04530
C	-3.20173	-2.37878	3.89765
C	-2.97992	-3.45171	4.77131
C	-3.85460	-4.54209	4.81267
C	-4.97346	-4.52626	3.97544
C	-5.23117	-3.46635	3.09925
C	-4.32601	-2.40217	3.06066
C	-2.56695	-0.57613	6.40150
C	-1.79642	-0.73481	7.56102
C	-2.39011	-0.81788	8.82064

C	-3.78496	-0.72417	8.90854
C	-4.58350	-0.56066	7.77557
C	-3.95816	-0.49247	6.52492
C	-0.59944	1.72405	5.50923
C	0.76498	2.01545	5.62636
C	1.22042	3.05450	6.44275
C	0.27774	3.82347	7.13198
C	-1.09399	3.56968	7.02757
C	-1.51584	2.51039	6.22082
C	-0.21017	1.51122	2.35637
C	0.68665	1.12236	1.35104
C	1.29503	2.05844	0.51103
C	0.97355	3.40898	0.67941
C	0.07872	3.83612	1.66463
C	-0.49898	2.87597	2.49838
C	-3.60535	-5.71242	5.74837
C	-2.28991	-6.43203	5.41891
C	-6.46774	-3.48587	2.21620
C	-7.34539	-2.24321	2.41375
C	-1.53597	-1.02342	10.06066
C	-1.84492	-2.36131	10.74660
C	-6.09423	-0.45799	7.90213
C	-6.62323	0.88142	7.37123
C	2.71031	3.31585	6.59075
C	3.09601	4.74686	6.19622
C	-2.11322	4.43715	7.74774
C	-1.89314	4.46071	9.26537
C	2.32247	1.66596	-0.53999
C	3.74623	1.82886	0.01721
C	-0.28874	5.30307	1.81357
C	0.93611	6.18318	2.09233
C	-3.07014	0.65697	-1.87453
C	-2.08686	0.93275	-3.01982
C	-1.54382	-4.09684	-0.91542
C	-0.29800	-4.12883	-1.81351
C	-3.64211	-5.28390	7.22129
C	-6.10081	-3.67229	0.73781
C	-1.66406	0.14355	11.04845
C	-6.80344	-1.63818	7.22464
C	3.19461	2.98715	8.01043
C	-2.13926	5.86065	7.17308
C	2.12847	0.26126	-1.11637
C	-1.06643	5.81225	0.59160
C	-4.45571	0.27888	-2.41650
C	-2.73964	-4.74823	-1.62041
H	-4.42266	-6.42959	5.59013
H	-2.15817	-7.30909	6.06252
H	-2.27296	-6.76785	4.37702
H	-1.42974	-5.77189	5.57447
H	-3.50591	-6.14995	7.87881
H	-2.84702	-4.56491	7.44409

H	-4.59613	-4.81103	7.47270
H	-7.62770	-2.11985	3.46383
H	-6.82673	-1.33176	2.09727
H	-8.26378	-2.32139	1.82136
H	-5.53549	-4.59773	0.59023
H	-7.00105	-3.72086	0.11479
H	-5.48369	-2.84318	0.37545
H	-0.49111	-1.05873	9.72510
H	-1.71565	-3.19902	10.05462
H	-1.18068	-2.52008	11.60356
H	-2.87609	-2.38950	11.11615
H	-1.39547	1.09239	10.57443
H	-2.68828	0.23569	11.42692
H	-1.00460	-0.00443	11.91100
H	-4.26705	-0.78374	9.88309
H	-6.32978	-0.50209	8.97438
H	-6.14123	1.72539	7.87471
H	-6.43800	0.98385	6.29626
H	-7.70453	0.96200	7.52965
H	-6.46497	-2.59239	7.63945
H	-7.88867	-1.57091	7.36240
H	-6.60132	-1.65685	6.14850
H	-4.55576	-0.37050	5.62508
H	1.48314	1.41520	5.07371
H	3.22454	2.63424	5.90010
H	2.78230	4.97333	5.17279
H	2.63193	5.48466	6.85996
H	4.18109	4.88496	6.25835
H	2.95615	1.95376	8.28096
H	4.27908	3.12077	8.09302
H	2.72033	3.64199	8.74998
H	0.61911	4.63989	7.76506
H	-3.09899	3.98877	7.56594
H	-1.90954	3.44959	9.68218
H	-0.93043	4.91515	9.52442
H	-2.67656	5.04574	9.75972
H	-2.33654	5.84949	6.09654
H	-2.91744	6.46187	7.65649
H	-1.18056	6.36778	7.32990
H	-2.57730	2.29199	6.13708
H	0.90319	0.06769	1.21672
H	1.43379	4.14062	0.01691
H	-1.19987	3.19056	3.26665
H	-2.48622	0.95167	0.76759
H	-3.18113	1.58885	-1.30459
H	-1.11390	1.25377	-2.63607
H	-1.92840	0.03855	-3.63283
H	-2.46988	1.72089	-3.67749
H	-5.16821	0.11244	-1.60265
H	-4.85087	1.07365	-3.05877
H	-4.41166	-0.63883	-3.01337

H	-2.46154	-1.96728	-2.37153
H	-1.30743	-3.09017	1.59850
H	-2.11226	-3.41517	5.42774
H	-4.49484	-1.56587	2.38751
H	-5.67093	-5.36250	4.00954
H	-7.06219	-4.35816	2.52067
H	-1.32598	-4.69507	-0.01992
H	-3.62908	-4.73804	-0.98467
H	-2.51402	-5.78899	-1.87742
H	-2.98791	-4.22788	-2.55191
H	-0.05623	-5.15575	-2.10957
H	0.57352	-3.70580	-1.30405
H	-0.46088	-3.54726	-2.72768
H	-0.45290	5.76437	-0.31501
H	-1.37280	6.85487	0.73187
H	-1.96554	5.21321	0.41640
H	-0.95336	5.37891	2.68433
H	1.47396	5.84122	2.98149
H	0.63480	7.22378	2.25545
H	1.63789	6.17124	1.25112
H	2.36174	-0.51401	-0.37780
H	2.80283	0.10567	-1.96489
H	1.10260	0.10024	-1.46085
H	2.21136	2.38019	-1.36827
H	3.91749	2.84604	0.38265
H	4.49502	1.61111	-0.75274
H	3.91249	1.14176	0.85454
H	2.94111	-0.58314	4.80148
H	2.37186	-0.22091	3.11106
H	1.20875	-2.15792	1.82176
H	0.87131	-4.56934	1.52386
H	3.48530	-2.93700	5.40263
H	3.20470	-5.34041	5.03557
H	2.82785	-7.12362	2.92534
H	1.25939	-6.85202	2.15548
H	1.36039	-7.10192	3.90262
H	-0.71821	-0.82721	7.46677
H	-0.02254	-2.41313	5.80869

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Complex 1 - 2nd xyl. hydro black path.

C	-0.57597	-1.88823	-3.16840
C	-0.52949	-0.55703	-2.73043
C	-0.78412	0.45651	-3.66498
C	-1.06393	0.16396	-5.00275
C	-1.08038	-1.17487	-5.40588
C	-0.83826	-2.21342	-4.50053
C	-0.28664	-0.22590	-1.30325
C	-0.95905	-0.84673	-0.20147
C	-0.56599	-0.17022	0.99245
C	0.34061	0.88233	0.63359

C	0.51653	0.84626	-0.78992
Sc	1.50874	-1.24607	0.12496
C	3.65598	-0.71789	-0.50909
C	3.88931	-1.59657	0.61824
C	3.47977	-1.20941	1.92433
C	3.50315	-2.11016	2.99869
C	3.88878	-3.43720	2.83200
C	4.25478	-3.83979	1.53483
C	4.24069	-2.96441	0.46208
C	3.90417	-4.41261	3.97740
C	-2.06700	-1.83595	-0.30954
C	-2.00875	-3.11245	0.25788
C	-3.09243	-3.99215	0.16819
C	-4.25002	-3.56168	-0.48678
C	-4.34625	-2.28865	-1.05836
C	-3.24024	-1.43894	-0.96745
C	-1.09005	-0.46169	2.35091
C	-0.23883	-0.74386	3.42911
C	-0.73828	-0.99307	4.70814
C	-2.12314	-0.93650	4.90257
C	-3.00202	-0.65315	3.85563
C	-2.47041	-0.42670	2.58113
C	0.88479	1.91638	1.54869
C	2.21442	2.35681	1.46798
C	2.71323	3.34848	2.31648
C	1.84620	3.92585	3.24923
C	0.50844	3.53026	3.34565
C	0.04610	2.52222	2.49574
C	1.20091	1.87739	-1.61277
C	2.17679	1.55253	-2.56241
C	2.73848	2.52854	-3.39089
C	2.29772	3.84871	-3.25888
C	1.32747	4.21204	-2.31909
C	0.79289	3.21477	-1.50044
C	-3.00718	-5.39558	0.74365
C	-1.95058	-6.23548	0.01150
C	-5.62217	-1.85060	-1.75898
C	-6.24283	-0.60992	-1.10304
C	0.19913	-1.32643	5.85600
C	-0.03509	-2.75007	6.38013
C	-4.50035	-0.59930	4.10346
C	-5.10775	0.74853	3.69285
C	4.17010	3.77270	2.22854
C	4.32154	5.26863	1.92491
C	-0.44778	4.20534	4.31544
C	0.09095	4.25122	5.75001
C	3.83505	2.20350	-4.39333
C	5.22042	2.37084	-3.74861
C	0.82762	5.64335	-2.21261
C	1.96245	6.64175	-1.95154
C	-1.37455	1.28667	-5.97975

C	-0.47608	1.25367	-7.22240
C	-0.85002	-3.66643	-4.94611
C	0.24405	-3.95079	-5.98444
C	-2.74920	-5.38894	2.25584
C	-5.39921	-1.62315	-3.26008
C	0.10792	-0.29929	6.99197
C	-5.22538	-1.76505	3.41726
C	4.94446	3.38827	3.49733
C	-0.82185	5.61221	3.82514
C	3.69938	0.81902	-5.03327
C	0.01949	6.04520	-3.45490
C	-2.85796	1.28298	-6.37712
C	-2.22822	-4.09717	-5.46440
H	-3.98310	-5.87221	0.57644
H	-1.93458	-7.26141	0.39665
H	-2.15425	-6.27782	-1.06318
H	-0.94991	-5.81056	0.14618
H	-2.74317	-6.41121	2.65069
H	-1.78085	-4.93485	2.49106
H	-3.51986	-4.82235	2.78687
H	-6.44082	-0.77915	-0.04008
H	-5.57898	0.25757	-1.18632
H	-7.18990	-0.34866	-1.58818
H	-5.01088	-2.52461	-3.74314
H	-6.33799	-1.34878	-3.75454
H	-4.67881	-0.81770	-3.43760
H	1.22140	-1.28540	5.45668
H	0.06059	-3.48805	5.57790
H	0.68809	-2.99930	7.16484
H	-1.03802	-2.85281	6.80886
H	0.31641	0.71131	6.62827
H	-0.89057	-0.29258	7.44255
H	0.82731	-0.53227	7.78486
H	-2.53332	-1.11925	5.89431
H	-4.64820	-0.70891	5.18657
H	-4.60502	1.58082	4.19560
H	-5.02636	0.91160	2.61288
H	-6.17154	0.78645	3.95203
H	-4.84513	-2.72745	3.77294
H	-6.30147	-1.72731	3.62149
H	-5.08441	-1.73634	2.33175
H	-3.13332	-0.21318	1.74792
H	2.87170	1.92935	0.71635
H	4.61532	3.22060	1.39015
H	3.79617	5.53963	1.00440
H	3.91709	5.88507	2.73531
H	5.37779	5.53328	1.80490
H	4.87788	2.31343	3.69279
H	6.00356	3.65152	3.40013
H	4.55011	3.91192	4.37537
H	2.22032	4.70529	3.90910

H	-1.36621	3.60368	4.32802
H	0.35470	3.25177	6.10861
H	0.98437	4.88069	5.82630
H	-0.66064	4.66887	6.42862
H	-1.25394	5.57916	2.82014
H	-1.55248	6.07816	4.49585
H	0.06034	6.26124	3.78655
H	-0.99204	2.20928	2.56099
H	2.49116	0.51806	-2.64999
H	2.72346	4.60860	-3.91257
H	0.02900	3.47437	-0.77158
H	-0.77358	1.49302	-3.34098
H	-1.17402	2.23008	-5.45500
H	0.58277	1.28047	-6.94835
H	-0.64527	0.34961	-7.81751
H	-0.68226	2.11421	-7.86828
H	-3.50407	1.35935	-5.49707
H	-3.08604	2.12391	-7.04185
H	-3.12201	0.35913	-6.90394
H	-1.29167	-1.41498	-6.44586
H	-0.41488	-2.68797	-2.45046
H	-1.08528	-3.41249	0.74471
H	-3.28024	-0.44566	-1.40779
H	-5.10118	-4.23802	-0.55793
H	-6.34275	-2.67312	-1.65293
H	-0.62796	-4.27426	-4.05887
H	-3.00014	-3.93765	-4.70590
H	-2.22724	-5.15959	-5.73260
H	-2.51307	-3.53008	-6.35758
H	0.26475	-5.01493	-6.24469
H	1.23245	-3.67305	-5.60486
H	0.07238	-3.38707	-6.90815
H	0.64544	6.02860	-4.35408
H	-0.38329	7.05854	-3.34702
H	-0.81864	5.36101	-3.62007
H	0.14926	5.68158	-1.34987
H	2.52545	6.37612	-1.05189
H	1.56374	7.65327	-1.81718
H	2.66743	6.67448	-2.78939
H	3.90195	0.01911	-4.31264
H	4.42048	0.70594	-5.84972
H	2.69544	0.65712	-5.43679
H	3.75530	2.94799	-5.19802
H	5.34929	3.37746	-3.33881
H	6.01708	2.19477	-4.48034
H	5.35130	1.65709	-2.92746
H	3.80424	0.34641	-0.32363
H	4.09864	-1.03551	-1.45262
H	4.53709	-3.31658	-0.52300
H	4.55629	-4.87197	1.36739
H	3.25042	-0.15997	2.11902

H	3.22734	-1.75435	3.98887
H	3.13522	-5.18439	3.85293
H	3.71751	-3.91135	4.93107
H	4.86853	-4.92743	4.05293
H	0.83670	-0.77120	3.26888
H	0.93385	-2.96211	0.38271
H	2.10257	-2.27869	-1.77150
H	1.73097	-2.81602	-1.36997

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Complex 1 - 2nd xyl. hydro black path. TS

C	-1.79773	-2.27282	0.55424
C	-1.90866	-0.97998	1.08068
C	-2.35093	0.04746	0.23654
C	-2.66568	-0.19270	-1.10377
C	-2.52353	-1.49285	-1.59976
C	-2.09138	-2.54436	-0.78410
C	-1.63447	-0.69156	2.51218
C	-2.29131	-1.32325	3.61351
C	-1.89547	-0.65313	4.80982
C	-0.99631	0.40862	4.45515
C	-0.83407	0.37943	3.02725
Sc	0.17540	-1.72326	3.92172
C	2.49325	-1.28459	3.27412
C	2.60130	-1.97614	4.56361
C	2.15940	-1.37218	5.76309
C	2.13724	-2.09049	6.96707
C	2.51609	-3.42871	7.02504
C	2.91586	-4.04174	5.82492
C	2.94545	-3.34840	4.62660
C	2.48892	-4.20617	8.31264
C	-3.36242	-2.35020	3.51439
C	-3.28740	-3.57790	4.18035
C	-4.33521	-4.50133	4.10895
C	-5.47095	-4.16683	3.36699
C	-5.58093	-2.94699	2.69164
C	-4.51238	-2.05000	2.76965
C	-2.47260	-0.93921	6.15061
C	-1.71557	-1.46095	7.20706
C	-2.28509	-1.69884	8.45968
C	-3.63923	-1.39661	8.64443
C	-4.42722	-0.88519	7.61153
C	-3.82831	-0.66604	6.36588
C	-0.41423	1.41645	5.37620
C	0.88093	1.92801	5.18749
C	1.43020	2.88612	6.04266
C	0.65243	3.35456	7.10603
C	-0.64923	2.88962	7.31502
C	-1.16553	1.92325	6.44749
C	-0.15337	1.39190	2.18028
C	0.74563	1.02458	1.17048

C	1.31075	1.97651	0.31648
C	0.95019	3.31697	0.48333
C	0.05504	3.72181	1.47897
C	-0.48342	2.74761	2.32233
C	-4.24084	-5.84321	4.81499
C	-3.07275	-6.68310	4.27995
C	-6.82407	-2.62922	1.87711
C	-7.45526	-1.28524	2.26181
C	-1.45083	-2.27544	9.59133
C	-2.01227	-3.61010	10.09951
C	-5.89888	-0.58458	7.83979
C	-6.22693	0.89644	7.60741
C	2.84943	3.38488	5.82523
C	2.91763	4.91152	5.69474
C	-1.51295	3.44635	8.43510
C	-0.83579	3.34723	9.80734
C	2.32388	1.60438	-0.75516
C	3.75438	1.69962	-0.20061
C	-0.37413	5.17336	1.61528
C	0.81276	6.14001	1.70308
C	-3.15918	0.93963	-1.98971
C	-2.21008	1.20461	-3.16613
C	-1.91456	-3.94940	-1.33588
C	-0.77097	-4.00859	-2.35852
C	-4.14876	-5.67961	6.33779
C	-6.53154	-2.68824	0.37121
C	-1.28661	-1.27373	10.74259
C	-6.79858	-1.49019	6.98797
C	3.79208	2.88629	6.93025
C	-1.93931	4.89112	8.13592
C	2.07969	0.23411	-1.39339
C	-1.32377	5.57464	0.47650
C	-4.59160	0.69383	-2.48312
C	-3.21232	-4.51156	-1.92964
H	-5.16942	-6.38845	4.59557
H	-3.05296	-7.66932	4.75777
H	-3.15484	-6.83006	3.19834
H	-2.11267	-6.19471	4.47853
H	-4.13529	-6.65706	6.83356
H	-3.23548	-5.14594	6.62097
H	-4.99876	-5.11076	6.72689
H	-7.68710	-1.24640	3.33075
H	-6.78718	-0.44778	2.03319
H	-8.38568	-1.12310	1.70625
H	-6.15612	-3.67493	0.08328
H	-7.43717	-2.48534	-0.21197
H	-5.77262	-1.95118	0.08823
H	-0.45248	-2.47512	9.18010
H	-2.10476	-4.33615	9.28637
H	-1.35842	-4.03736	10.86806
H	-3.00447	-3.48137	10.54567

H	-0.84430	-0.33646	10.39115
H	-2.25303	-1.03415	11.19972
H	-0.64095	-1.68366	11.52750
H	-4.09977	-1.57136	9.61520
H	-6.11067	-0.80578	8.89493
H	-5.60770	1.54376	8.23659
H	-6.05769	1.18357	6.56382
H	-7.27804	1.10066	7.83958
H	-6.60396	-2.54682	7.19412
H	-7.85626	-1.28989	7.19315
H	-6.62569	-1.32750	5.91907
H	-4.41724	-0.27704	5.53945
H	1.47138	1.58507	4.34186
H	3.19783	2.95757	4.87528
H	2.25190	5.27169	4.90488
H	2.62720	5.40730	6.62743
H	3.93722	5.23310	5.45608
H	3.78633	1.79364	6.99513
H	4.82127	3.21015	6.73950
H	3.49382	3.27948	7.90853
H	1.06591	4.10364	7.77769
H	-2.42243	2.83256	8.47198
H	-0.54367	2.31728	10.03306
H	0.06474	3.96912	9.85877
H	-1.51459	3.68881	10.59634
H	-2.46666	4.95782	7.17927
H	-2.60385	5.27211	8.91946
H	-1.06882	5.55473	8.08303
H	-2.17834	1.56552	6.60170
H	0.98243	-0.02650	1.04166
H	1.37493	4.05877	-0.19099
H	-1.19001	3.04041	3.09486
H	-2.45443	1.05345	0.63480
H	-3.17444	1.84616	-1.37009
H	-1.19870	1.42839	-2.81386
H	-2.14909	0.33647	-3.83181
H	-2.55900	2.05506	-3.76266
H	-5.27902	0.54343	-1.64496
H	-4.95181	1.54567	-3.07087
H	-4.64527	-0.19555	-3.12066
H	-2.75560	-1.69110	-2.64426
H	-1.46532	-3.07977	1.20224
H	-2.38082	-3.80254	4.73547
H	-4.56336	-1.09732	2.24910
H	-6.29449	-4.87808	3.31010
H	-7.56088	-3.41279	2.10163
H	-1.63468	-4.59045	-0.48946
H	-4.02168	-4.49660	-1.19410
H	-3.06886	-5.54645	-2.25973
H	-3.53947	-3.93109	-2.79948
H	-0.61739	-5.03445	-2.71203

H	0.16817	-3.65318	-1.92311
H	-0.99001	-3.38432	-3.23214
H	-0.81946	5.51166	-0.49439
H	-1.67572	6.60435	0.60560
H	-2.19802	4.91726	0.44008
H	-0.93399	5.25302	2.55670
H	1.49310	5.86322	2.51406
H	0.46295	7.16192	1.88556
H	1.39136	6.15458	0.77288
H	2.27784	-0.58189	-0.68978
H	2.74878	0.09081	-2.24841
H	1.04861	0.12812	-1.74269
H	2.23106	2.35874	-1.54913
H	3.95745	2.69420	0.20859
H	4.49279	1.49463	-0.98403
H	3.90543	0.97097	0.60407
H	2.49623	-0.19399	3.32807
H	3.21029	-1.62850	2.52598
H	3.26644	-3.85320	3.71888
H	3.20811	-5.08950	5.83634
H	1.92992	-0.30746	5.78054
H	1.83465	-1.57704	7.87660
H	1.69559	-4.96259	8.29833
H	2.30976	-3.55285	9.17075
H	3.43463	-4.73232	8.48199
H	-0.67007	-1.70796	7.04081
H	-0.32575	-3.29556	4.68354
H	1.42316	-1.86501	2.46495
H	0.60515	-2.34851	2.15464

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Complex 1 - 2nd xyl. hydro black path. prod

C	-0.33769	-1.93146	-3.09302
C	-0.50274	-0.62619	-2.61417
C	-0.95670	0.36180	-3.49739
C	-1.23941	0.06790	-4.83432
C	-1.05401	-1.24446	-5.28229
C	-0.60246	-2.25484	-4.42564
C	-0.25080	-0.30576	-1.18889
C	-0.87756	-0.95839	-0.08604
C	-0.43819	-0.31634	1.11571
C	0.45358	0.75156	0.74945
C	0.56353	0.75270	-0.68036
Sc	1.60094	-1.41478	0.10649
C	5.15137	-0.24667	-0.51942
C	4.36802	-1.17466	0.36129
C	3.84168	-0.76220	1.58657
C	3.11850	-1.65195	2.40704
C	2.89499	-2.97556	2.02073
C	3.36409	-3.36994	0.74917
C	4.08492	-2.49192	-0.06051

C	2.15616	-3.95288	2.88678
C	-1.98923	-1.94134	-0.17835
C	-1.99324	-3.14579	0.53278
C	-3.08567	-4.01554	0.48385
C	-4.19160	-3.65453	-0.29094
C	-4.22437	-2.46033	-1.01710
C	-3.11332	-1.61455	-0.95077
C	-1.06193	-0.55146	2.44723
C	-0.34505	-0.94361	3.58476
C	-0.96448	-1.11727	4.82408
C	-2.34014	-0.87863	4.91784
C	-3.09160	-0.48343	3.80937
C	-2.43924	-0.33150	2.58100
C	1.04283	1.76853	1.65617
C	2.32829	2.29341	1.43646
C	2.87858	3.27321	2.26544
C	2.11548	3.74879	3.33708
C	0.82517	3.27012	3.57746
C	0.30545	2.28475	2.73251
C	1.19839	1.79607	-1.52814
C	2.08432	1.47616	-2.56616
C	2.57677	2.46283	-3.42573
C	2.16198	3.78518	-3.23441
C	1.28089	4.14025	-2.20867
C	0.81223	3.13358	-1.36084
C	-3.06507	-5.34103	1.22657
C	-2.01162	-6.29081	0.63873
C	-5.42998	-2.11806	-1.87670
C	-5.98430	-0.71658	-1.59263
C	-0.16209	-1.56223	6.03551
C	-0.60925	-2.94257	6.53661
C	-4.58392	-0.22964	3.94054
C	-4.96813	1.19073	3.50474
C	4.27996	3.80415	2.00833
C	4.28320	5.31554	1.74505
C	-0.02839	3.83404	4.70187
C	0.69220	3.82829	6.05546
C	3.55861	2.15410	-4.54730
C	4.99594	2.48963	-4.11750
C	0.78080	5.56680	-2.04865
C	1.91191	6.60138	-2.02598
C	-1.74521	1.15540	-5.76854
C	-0.78424	1.39935	-6.93977
C	-0.38096	-3.67218	-4.92760
C	0.76518	-3.73361	-5.94697
C	-2.86333	-5.16015	2.73600
C	-5.10959	-2.29046	-3.36845
C	-0.20567	-0.52887	7.16879
C	-5.40294	-1.28137	3.17960
C	5.24077	3.44767	3.15161
C	-0.53010	5.24394	4.35587

C	3.47302	0.72090	-5.07644
C	-0.24987	5.91056	-3.13469
C	-3.16371	0.85899	-6.27423
C	-1.66157	-4.29227	-5.50142
H	-4.04897	-5.80773	1.07956
H	-2.03093	-7.26093	1.14877
H	-2.18622	-6.46144	-0.42813
H	-1.00446	-5.87259	0.74448
H	-2.91154	-6.12566	3.25244
H	-1.88841	-4.71214	2.95581
H	-3.62873	-4.50520	3.16261
H	-6.22832	-0.59178	-0.53290
H	-5.26462	0.06308	-1.86489
H	-6.89530	-0.53804	-2.17462
H	-4.79143	-3.31472	-3.58585
H	-5.98770	-2.06835	-3.98586
H	-4.29875	-1.62167	-3.67573
H	0.88536	-1.64973	5.71316
H	-0.55029	-3.69363	5.74283
H	0.01697	-3.27545	7.37198
H	-1.64616	-2.91607	6.88879
H	0.13852	0.45084	6.82484
H	-1.22328	-0.40717	7.55568
H	0.43022	-0.84203	8.00428
H	-2.84482	-1.00342	5.87436
H	-4.83230	-0.32402	5.00675
H	-4.40134	1.94436	4.06059
H	-4.77567	1.34701	2.43790
H	-6.03491	1.37099	3.67708
H	-5.18408	-2.29022	3.54231
H	-6.47668	-1.10033	3.30361
H	-5.17708	-1.26206	2.10850
H	-3.00262	-0.02885	1.70320
H	2.90358	1.94214	0.58381
H	4.64803	3.31279	1.09723
H	3.61884	5.57134	0.91491
H	3.94701	5.87387	2.62562
H	5.29172	5.66453	1.49711
H	5.27711	2.36677	3.32353
H	6.25728	3.79033	2.92838
H	4.92939	3.91960	4.08995
H	2.53153	4.51481	3.98766
H	-0.90663	3.18166	4.79324
H	1.05576	2.82796	6.31002
H	1.55329	4.50586	6.05823
H	0.01620	4.15782	6.85193
H	-1.08565	5.24586	3.41304
H	-1.18936	5.62868	5.14216
H	0.30836	5.94154	4.24961
H	-0.70284	1.92319	2.90688
H	2.35654	0.43248	-2.69411

H	2.52989	4.55076	-3.91594
H	0.11243	3.38660	-0.56796
H	-1.09320	1.37744	-3.13438
H	-1.79095	2.08355	-5.18328
H	0.21630	1.65805	-6.58059
H	-0.69332	0.50894	-7.57177
H	-1.14228	2.21944	-7.57256
H	-3.86174	0.72926	-5.44140
H	-3.53198	1.67717	-6.90358
H	-3.18789	-0.05789	-6.87345
H	-1.26646	-1.48442	-6.32248
H	0.01856	-2.69869	-2.40908
H	-1.10662	-3.40682	1.10127
H	-3.10868	-0.68104	-1.50645
H	-5.04924	-4.32508	-0.33611
H	-6.21831	-2.83986	-1.62174
H	-0.08339	-4.27356	-4.05856
H	-2.47119	-4.27646	-4.76587
H	-1.48862	-5.33296	-5.79817
H	-2.00525	-3.74933	-6.38896
H	0.95152	-4.76653	-6.26286
H	1.69127	-3.33265	-5.52350
H	0.52824	-3.14899	-6.84316
H	0.20512	5.86982	-4.13075
H	-0.65080	6.92017	-2.98925
H	-1.08710	5.20586	-3.12287
H	0.26864	5.61788	-1.07841
H	2.65063	6.36858	-1.25318
H	1.51307	7.60176	-1.82525
H	2.43729	6.64697	-2.98626
H	3.81469	-0.00689	-4.33224
H	4.10989	0.60575	-5.96004
H	2.44956	0.45252	-5.35382
H	3.30491	2.82811	-5.37835
H	5.08097	3.52769	-3.78108
H	5.69767	2.34005	-4.94599
H	5.31107	1.84483	-3.28919
H	5.41276	0.67719	0.00154
H	6.07600	-0.72256	-0.86139
H	4.43607	-2.82550	-1.03063
H	3.15805	-4.37478	0.39714
H	3.99919	0.25525	1.92847
H	2.76750	-1.30237	3.37250
H	1.30027	-4.36179	2.34037
H	1.79112	-3.48692	3.80435
H	2.80743	-4.78934	3.16370
H	0.72323	-1.11078	3.49997
H	0.87110	-3.08504	0.03092
H	4.56077	0.00978	-1.40590
H	2.33756	-1.37307	-1.56172

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Complex 1 - 2nd xyl. hydro black path. prod - p-xyl.

C	11.58728	11.35250	2.44859
C	12.85218	11.00356	1.96019
C	13.18094	9.64620	1.85886
C	12.27854	8.65007	2.23923
C	11.01775	9.03556	2.70690
C	10.65205	10.38120	2.81422
C	13.84384	12.03409	1.56887
C	14.47603	12.14571	0.29389
C	15.37888	13.25884	0.34903
C	15.33957	13.80503	1.67391
C	14.37401	13.06119	2.41892
Sc	13.15728	14.18729	0.59290
C	14.31340	11.21804	-0.85475
C	15.44415	10.55021	-1.34379
C	15.34723	9.64265	-2.40165
C	14.09005	9.42623	-2.97453
C	12.94280	10.08028	-2.51531
C	13.06774	10.96972	-1.44364
C	16.13564	13.79924	-0.80435
C	15.47689	14.01688	-2.02709
C	16.14140	14.55773	-3.12889
C	17.50154	14.85881	-2.99422
C	18.19308	14.64004	-1.79978
C	17.49342	14.12005	-0.70532
C	16.22925	14.85778	2.22857
C	16.26048	16.16448	1.73651
C	17.13538	17.12202	2.26399
C	17.99370	16.74040	3.29795
C	17.99315	15.43656	3.81110
C	17.10505	14.50846	3.26761
C	14.00956	13.29441	3.83760
C	13.61236	14.56203	4.27799
C	13.26959	14.78619	5.61732
C	13.35604	13.71891	6.51293
C	13.76389	12.44116	6.10728
C	14.07634	12.24213	4.76286
C	16.56958	8.89994	-2.91414
C	17.64143	9.85755	-3.45130
C	11.60055	9.85169	-3.18925
C	10.54297	9.32118	-2.21310
C	15.40394	14.79778	-4.43462
C	15.97659	13.94705	-5.57633
C	19.67320	14.96845	-1.69829
C	19.92442	16.14760	-0.74823
C	17.08051	18.54413	1.72571
C	15.92179	19.31830	2.37503
C	18.93598	15.03350	4.93270
C	20.40801	15.18076	4.52394
C	12.82380	16.15861	6.09160

C	13.96570	17.18123	6.01089
C	13.88685	11.30077	7.10363
C	14.99794	11.57033	8.12841
C	12.67374	7.18488	2.15632
C	12.70123	6.52928	3.54399
C	9.27020	10.78813	3.29742
C	8.98298	10.28603	4.71815
C	17.15293	7.96554	-1.84482
C	11.10784	11.12442	-3.89339
C	15.38224	16.28591	-4.80977
C	20.50825	13.74613	-1.29472
C	18.39324	19.31823	1.86637
C	18.64333	15.80445	6.22704
C	11.58510	16.65439	5.33293
C	12.55632	10.99452	7.80297
C	11.77543	6.39955	1.19204
C	8.17736	10.33435	2.31941
H	13.17321	15.92756	1.17896
H	11.71678	13.70387	-0.45445
H	16.23542	8.27333	-3.75226
H	18.49122	9.29786	-3.85779
H	17.24155	10.49511	-4.24545
H	18.02169	10.51323	-2.66066
H	17.99366	7.39073	-2.24883
H	17.52227	8.53256	-0.98311
H	16.39973	7.25937	-1.48167
H	10.87332	8.39443	-1.73443
H	10.33236	10.04799	-1.42186
H	9.60259	9.11774	-2.73723
H	11.84274	11.48382	-4.62078
H	10.16811	10.93450	-4.42402
H	10.92848	11.92886	-3.17179
H	14.36393	14.48195	-4.27799
H	15.95335	12.88244	-5.32504
H	15.39779	14.09380	-6.49479
H	17.01590	14.21824	-5.79253
H	14.94173	16.89034	-4.01067
H	16.39324	16.66483	-4.99628
H	14.79511	16.44530	-5.72070
H	18.04488	15.26987	-3.84318
H	20.00155	15.27500	-2.70069
H	19.37841	17.03860	-1.07326
H	19.59971	15.91226	0.27074
H	20.99131	16.39517	-0.71384
H	20.35136	12.91164	-1.98523
H	21.57565	13.99241	-1.29475
H	20.24989	13.40092	-0.28778
H	18.00499	13.95210	0.23764
H	15.57101	16.44945	0.94586
H	16.85874	18.46413	0.65236
H	14.96731	18.80546	2.22288

H	16.08226	19.41750	3.45460
H	15.83959	20.32545	1.95096
H	19.23699	18.76607	1.44070
H	18.32111	20.28005	1.34810
H	18.62574	19.53623	2.91492
H	18.68136	17.47091	3.71589
H	18.75481	13.96948	5.13585
H	20.62955	14.60251	3.62141
H	20.66103	16.22689	4.31952
H	21.06937	14.83063	5.32420
H	17.60466	15.66589	6.54183
H	19.29544	15.46204	7.03829
H	18.81288	16.87892	6.09621
H	17.08993	13.49149	3.65240
H	13.57176	15.37765	3.55860
H	13.10004	13.89293	7.55671
H	14.38692	11.25700	4.42429
H	14.16148	9.36590	1.48258
H	13.69516	7.15204	1.75453
H	13.36933	7.06723	4.22375
H	11.70383	6.51854	3.99714
H	13.04633	5.49166	3.47624
H	11.79457	6.83840	0.19015
H	12.10768	5.35837	1.11516
H	10.73464	6.39067	1.53394
H	10.30217	8.26817	2.99522
H	11.31577	12.40257	2.54571
H	16.40766	10.74508	-0.87995
H	12.19982	11.50694	-1.07061
H	14.00274	8.72869	-3.80673
H	11.75542	9.08466	-3.96060
H	9.25124	11.88584	3.32560
H	8.36311	10.71930	1.31211
H	7.19397	10.69071	2.64532
H	8.13103	9.24142	2.25643
H	8.00346	10.63656	5.06143
H	9.73839	10.64346	5.42430
H	8.97548	9.19132	4.76132
H	12.21631	11.84369	8.40586
H	12.66108	10.13458	8.47364
H	11.77156	10.76485	7.07615
H	14.17242	10.40711	6.53278
H	15.95684	11.75519	7.63434
H	15.12018	10.71561	8.80295
H	14.76472	12.44777	8.74168
H	11.80149	16.80134	4.26924
H	11.24453	17.61433	5.73652
H	10.75920	15.94021	5.41239
H	12.54460	16.05642	7.14929
H	14.83243	16.85369	6.59318
H	13.64177	18.15374	6.39819

H	14.29551	17.32456	4.97678
H	14.43081	13.72759	-2.13677

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Complex 1 - 1st xyl. hydro red path. TS

Sc	13.04323	11.35114	4.02332
C	11.19169	12.44475	4.97523
C	9.89392	13.14059	4.75883
C	9.83827	14.53191	4.57443
C	8.62961	15.17582	4.32272
C	7.42685	14.46492	4.24158
C	7.48379	13.07843	4.41880
C	8.68832	12.42855	4.67231
C	6.11722	15.16994	4.00455
C	12.48450	9.36260	3.05316
C	12.03605	9.05134	4.38964
C	12.93892	9.13355	5.48632
C	12.49385	8.98922	6.81312
C	11.15193	8.80192	7.11871
C	10.24680	8.75097	6.03580
C	10.66317	8.88150	4.72565
C	10.66714	8.63791	8.53395
C	15.07323	11.76778	2.62330
C	14.40880	13.03275	2.75387
C	14.50019	13.43977	4.12608
C	15.20443	12.41573	4.84131
C	15.57874	11.39059	3.91032
C	15.35317	11.09590	1.32855
C	14.32635	10.76885	0.43423
C	14.60564	10.20807	-0.81543
C	15.94289	9.98533	-1.15852
C	16.99416	10.30218	-0.29257
C	16.68198	10.85440	0.95281
C	13.95243	13.87787	1.61548
C	12.66407	14.42545	1.53961
C	12.28444	15.25473	0.48373
C	13.23043	15.55122	-0.50516
C	14.52752	15.03839	-0.45625
C	14.87175	14.19724	0.60870
C	14.12638	14.75613	4.70176
C	13.59421	14.86988	5.99650
C	13.27867	16.10741	6.56150
C	13.53028	17.26335	5.81621
C	14.08212	17.19581	4.53338
C	14.36833	15.94044	3.98963
C	15.73228	12.58350	6.22505
C	15.33986	11.80101	7.31322
C	15.88999	12.00276	8.58816
C	16.86115	12.99173	8.74752
C	17.28744	13.78858	7.67698
C	16.70239	13.57912	6.42970

C	16.45214	10.22337	4.20215
C	17.59769	10.37961	4.99912
C	18.45359	9.31033	5.27268
C	18.14920	8.05245	4.74238
C	17.02723	7.85727	3.93262
C	16.20176	8.95268	3.66310
C	13.49590	9.81652	-1.77691
C	12.47794	10.94033	-2.00254
C	18.43317	10.03495	-0.70256
C	19.02307	8.85347	0.08041
C	10.86629	15.79484	0.40424
C	10.82812	17.32608	0.32106
C	15.53805	15.39151	-1.53494
C	15.92922	14.16494	-2.37010
C	12.66747	16.18252	7.95136
C	11.26779	16.81175	7.92359
C	14.41114	18.45541	3.74868
C	15.65315	19.15130	4.32502
C	15.44633	11.17412	9.78220
C	15.82601	9.69552	9.62668
C	18.36722	14.84223	7.85553
C	19.70612	14.21430	8.26753
C	19.70489	9.52817	6.10787
C	20.97323	9.41263	5.24995
C	16.66126	6.48374	3.39345
C	17.84712	5.74068	2.76866
C	12.79760	8.52834	-1.31578
C	19.32375	11.27720	-0.57651
C	10.09549	15.16364	-0.76423
C	16.77947	16.08208	-0.95446
C	13.58244	16.91479	8.94147
C	13.22942	19.42879	3.66352
C	13.94817	11.34096	10.06915
C	17.94732	15.93938	8.84239
C	19.77313	8.58718	7.31701
C	16.00057	5.63213	4.48888
H	13.97350	9.60370	-2.74331
H	12.03541	8.21705	-2.03917
H	13.51342	7.70835	-1.20008
H	12.30328	8.67794	-0.34967
H	11.74934	10.64860	-2.76693
H	11.92113	11.16772	-1.08753
H	12.96704	11.86255	-2.32921
H	18.92225	12.11518	-1.15465
H	19.41468	11.60190	0.46567
H	20.33413	11.06476	-0.94300
H	18.42248	7.95011	-0.06464
H	20.04652	8.63966	-0.24804
H	19.04994	9.06681	1.15443
H	10.35819	15.50039	1.33152
H	10.08000	14.07252	-0.68338

H	9.05908	15.51906	-0.78286
H	10.55489	15.42116	-1.72537
H	11.35792	17.78241	1.16265
H	11.29270	17.69033	-0.60199
H	9.79368	17.68687	0.33254
H	12.95447	16.19928	-1.33513
H	15.04899	16.10848	-2.20865
H	16.50585	16.97232	-0.37934
H	17.33368	15.41156	-0.28866
H	17.46121	16.38965	-1.75529
H	15.05155	13.71234	-2.84144
H	16.63524	14.44278	-3.16098
H	16.40155	13.39658	-1.74925
H	15.87436	13.78310	0.66676
H	13.43495	13.97527	6.59230
H	12.55691	15.14962	8.30774
H	14.56005	16.42847	9.00804
H	13.74419	17.95539	8.63904
H	13.13868	16.92646	9.94327
H	10.59999	16.26579	7.25047
H	10.82212	16.80627	8.92455
H	11.30749	17.85307	7.58495
H	13.29858	18.23497	6.24718
H	14.65197	18.13948	2.72521
H	12.33748	18.93854	3.26190
H	12.97112	19.83747	4.64666
H	13.47485	20.27546	3.01327
H	16.51269	18.47406	4.34447
H	15.92331	20.02931	3.72740
H	15.47111	19.48753	5.35209
H	14.80320	15.88417	2.99656
H	14.59139	11.02670	7.16450
H	17.29417	13.14283	9.73480
H	17.00738	14.19264	5.58523
H	17.83389	11.35768	5.40497
H	19.65659	10.55515	6.49322
H	18.87857	8.67748	7.94035
H	19.85962	7.53990	7.00731
H	20.64649	8.81903	7.93639
H	20.95001	10.11587	4.41166
H	21.86821	9.62195	5.84659
H	21.07691	8.40385	4.83486
H	18.80267	7.21076	4.95898
H	15.35006	8.81171	3.00617
H	13.30012	10.96233	0.73459
H	17.47665	11.11669	1.64594
H	16.17350	9.55546	-2.13269
H	18.41416	9.75105	-1.76367
H	15.91574	6.64016	2.60234
H	18.33404	6.34197	1.99563
H	17.51083	4.80398	2.31128

H	18.60272	5.48097	3.51829
H	15.68639	4.66055	4.09131
H	15.11933	6.13181	4.90289
H	16.69965	5.44876	5.31285
H	19.63310	13.73006	9.24762
H	20.48847	14.97850	8.33261
H	20.02922	13.45809	7.54529
H	18.51289	15.31840	6.87685
H	17.02287	16.42696	8.51973
H	18.72607	16.70589	8.92212
H	17.78066	15.53173	9.84567
H	15.33980	9.24646	8.75402
H	15.52562	9.12107	10.50997
H	16.90594	9.57800	9.49582
H	15.99016	11.55945	10.65522
H	13.69051	12.39333	10.22350
H	13.66177	10.78542	10.96911
H	13.33753	10.96888	9.23956
H	11.90063	13.10498	5.49002
H	11.05161	11.52077	5.55815
H	8.69842	11.35017	4.81148
H	6.56675	12.49523	4.35996
H	10.75465	15.11439	4.63556
H	8.62149	16.25588	4.18957
H	5.65311	15.47998	4.94959
H	5.40066	14.52276	3.48932
H	6.25144	16.07195	3.39942
H	14.01406	9.15175	5.29182
H	9.93702	8.82618	3.91844
H	13.22594	8.99857	7.61724
H	9.18945	8.59268	6.24107
H	9.95774	9.42700	8.80985
H	11.49581	8.67317	9.24628
H	10.15080	7.68049	8.67073
H	13.43785	8.92682	2.75588
H	11.73437	9.29911	2.26796
H	11.94029	14.19627	2.31529
H	11.84804	11.94707	2.67396
H	11.46194	12.22431	3.53596

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Complex 1 - 1st xyl. hydro red path. prod

Sc	-0.93276	-0.61121	0.22885
C	-5.67706	1.84350	1.44928
C	-6.71429	0.82398	1.05939
C	-6.89027	0.45303	-0.28109
C	-7.83235	-0.50299	-0.64753
C	-8.64292	-1.12736	0.30958
C	-8.46997	-0.75689	1.64523
C	-7.52525	0.20213	2.01283
C	-9.67957	-2.14220	-0.09578

C	-2.05061	-2.13370	-0.99774
C	-2.53947	-2.46184	0.33053
C	-1.63373	-2.91638	1.32810
C	-2.02919	-3.06728	2.66749
C	-3.31388	-2.73621	3.08743
C	-4.19937	-2.23125	2.11523
C	-3.82713	-2.08052	0.79132
C	-3.75532	-2.90478	4.51613
C	1.03258	-0.45564	-1.30300
C	0.50775	0.86810	-1.16228
C	0.69446	1.28667	0.19144
C	1.31254	0.20986	0.89986
C	1.52541	-0.87016	-0.02055
C	1.25230	-1.15308	-2.59658
C	0.20905	-1.41785	-3.49481
C	0.45534	-2.00167	-4.73885
C	1.77955	-2.30329	-5.08068
C	2.84519	-2.04438	-4.21630
C	2.56317	-1.47514	-2.96991
C	-0.07225	1.70779	-2.23917
C	-1.33333	2.30220	-2.07947
C	-1.88024	3.11645	-3.07243
C	-1.12992	3.34794	-4.23189
C	0.13342	2.78161	-4.41744
C	0.64707	1.95229	-3.41398
C	0.47804	2.65720	0.71979
C	-0.29343	2.91178	1.85893
C	-0.43335	4.20482	2.36838
C	0.22540	5.25495	1.72002
C	1.00536	5.03699	0.58003
C	1.12011	3.73288	0.09210
C	1.78184	0.28775	2.30804
C	1.30037	-0.55070	3.31776
C	1.77845	-0.45379	4.63193
C	2.76508	0.49213	4.91261
C	3.27469	1.34538	3.92560
C	2.76554	1.23524	2.63261
C	2.21236	-2.15254	0.26957
C	3.38350	-2.17407	1.04029
C	4.06262	-3.36610	1.30657
C	3.54434	-4.56101	0.79761
C	2.38075	-4.58114	0.02146
C	1.73662	-3.37008	-0.24264
C	-0.66163	-2.35526	-5.70825
C	-1.87630	-1.42721	-5.62597
C	4.27322	-2.35259	-4.63472
C	4.91111	-3.42741	-3.74503
C	-3.25364	3.73845	-2.88563
C	-3.18075	5.26981	-2.81610
C	0.93218	3.07345	-5.67721
C	1.14381	1.81265	-6.52597

C	-1.29840	4.45492	3.59283
C	-2.47807	5.38456	3.27774
C	1.72324	6.18201	-0.11521
C	2.77284	6.83270	0.79610
C	1.23487	-1.34064	5.73928
C	1.48816	-2.82869	5.46649
C	4.35964	2.35971	4.24505
C	5.65376	1.67687	4.70859
C	5.35822	-3.34111	2.10105
C	6.56858	-3.59181	1.18917
C	1.81147	-5.88548	-0.51200
C	2.79569	-6.61326	-1.43656
C	-1.08725	-3.82114	-5.52382
C	5.14070	-1.08694	-4.67650
C	-4.23985	3.28122	-3.96897
C	2.27005	3.75487	-5.35856
C	-0.47773	4.98781	4.77483
C	0.74113	7.22843	-0.65895
C	-0.25222	-1.06658	6.00168
C	3.88620	3.40092	5.26767
C	5.35113	-4.31932	3.28188
C	1.34609	-6.80393	0.62653
H	-0.24145	-2.26116	-6.71965
H	-1.84812	-4.10316	-6.26046
H	-0.23660	-4.50082	-5.63497
H	-1.51001	-3.97546	-4.52468
H	-2.57497	-1.64618	-6.44027
H	-2.42372	-1.56278	-4.68676
H	-1.58684	-0.37445	-5.69538
H	4.70573	-0.32921	-5.33569
H	5.24461	-0.64326	-3.68022
H	6.14717	-1.31932	-5.04199
H	4.32571	-4.35158	-3.76310
H	5.92616	-3.66104	-4.08542
H	4.97482	-3.09599	-2.70325
H	-3.63464	3.38250	-1.91941
H	-4.31551	2.18971	-4.00084
H	-5.23955	3.68827	-3.78043
H	-3.92633	3.62149	-4.96218
H	-2.50927	5.59557	-2.01609
H	-2.81238	5.69350	-3.75720
H	-4.17141	5.69765	-2.62538
H	-1.53294	3.99001	-5.01352
H	0.33911	3.77883	-6.27534
H	2.11981	4.67032	-4.77781
H	2.92434	3.09502	-4.77840
H	2.79957	4.01828	-6.28092
H	0.18726	1.36709	-6.81583
H	1.69898	2.04999	-7.44071
H	1.70891	1.05224	-5.97691
H	1.62517	1.49515	-3.53498

H	-0.81864	2.08740	2.33267
H	-1.71491	3.48382	3.89139
H	0.33114	4.29867	5.03589
H	-0.02807	5.95932	4.54075
H	-1.11092	5.12071	5.65937
H	-3.08356	4.98994	2.45619
H	-3.12506	5.50082	4.15452
H	-2.13184	6.38286	2.98757
H	0.12443	6.26656	2.10883
H	2.25383	5.75172	-0.97513
H	0.01566	6.77217	-1.33909
H	0.18301	7.70932	0.15215
H	1.27411	8.01452	-1.20556
H	3.49344	6.09410	1.16093
H	3.32522	7.61231	0.25942
H	2.30466	7.30009	1.66956
H	1.72197	3.54605	-0.79401
H	0.54052	-1.29261	3.07833
H	3.14292	0.56448	5.93102
H	3.13725	1.89313	1.85122
H	3.77876	-1.24068	1.43018
H	5.45849	-2.32879	2.51426
H	4.49400	-4.14316	3.93851
H	5.30542	-5.36047	2.94416
H	6.26470	-4.20916	3.87608
H	6.60633	-2.86531	0.37149
H	7.50476	-3.51831	1.75398
H	6.52342	-4.59208	0.74398
H	4.06008	-5.49568	1.00674
H	0.85100	-3.37212	-0.87303
H	-0.80115	-1.14973	-3.20609
H	3.37161	-1.25545	-2.27765
H	1.98516	-2.74580	-6.05500
H	4.22777	-2.75324	-5.65663
H	0.92764	-5.62781	-1.11075
H	3.10017	-5.97464	-2.27068
H	2.33877	-7.51932	-1.84953
H	3.70097	-6.91600	-0.89881
H	0.88408	-7.71334	0.22680
H	0.61257	-6.30351	1.26638
H	2.18757	-7.10847	1.25872
H	5.50345	1.13779	5.65053
H	6.44517	2.41649	4.87275
H	6.00975	0.95607	3.96580
H	4.58298	2.89306	3.31153
H	2.99069	3.92025	4.91424
H	4.66607	4.14917	5.44765
H	3.64657	2.93435	6.22968
H	0.97404	-3.16216	4.55863
H	1.12744	-3.44280	6.29906
H	2.55537	-3.02897	5.33253

H	1.78313	-1.07826	6.65419
H	-0.42299	-0.01170	6.23788
H	-0.61540	-1.66760	6.84296
H	-0.86193	-1.31314	5.12582
H	-5.76299	2.75040	0.84060
H	-5.77976	2.13491	2.49855
H	-7.41846	0.47285	3.06127
H	-9.08603	-1.22166	2.41236
H	-6.27866	0.92317	-1.04844
H	-7.94360	-0.76882	-1.69695
H	-10.55995	-1.65800	-0.53616
H	-10.02301	-2.72788	0.76181
H	-9.28792	-2.83939	-0.84387
H	-0.64597	-3.27452	1.03019
H	-4.54389	-1.68342	0.07809
H	-1.31855	-3.47377	3.38381
H	-5.20784	-1.94730	2.40795
H	-3.98928	-1.93907	4.97948
H	-2.98090	-3.38450	5.12076
H	-4.66004	-3.51968	4.58213
H	-1.34716	-2.84376	-1.43658
H	-2.81023	-1.80488	-1.70832
H	-1.88699	2.12363	-1.15870
H	-2.06854	0.70787	0.78746
H	-4.66155	1.45370	1.30831

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Complex 1 - 1st xyl. hydro red path. prod - p-xyl.

Sc	-0.88049	-0.68786	0.30419
C	-2.02117	-2.20225	-0.92054
C	-2.49766	-2.53530	0.40990
C	-1.58560	-3.00338	1.39533
C	-1.96744	-3.15988	2.73766
C	-3.24531	-2.82350	3.17403
C	-4.13710	-2.30713	2.21387
C	-3.77808	-2.14925	0.88748
C	-3.67232	-2.99679	4.60649
C	1.05422	-0.47784	-1.25151
C	0.50440	0.83351	-1.09199
C	0.70282	1.24519	0.26233
C	1.35330	0.17573	0.95236
C	1.57352	-0.89266	0.02053
C	1.26801	-1.16254	-2.55287
C	0.21687	-1.44344	-3.43697
C	0.45613	-2.01655	-4.68730
C	1.78087	-2.29014	-5.05010
C	2.85400	-2.01392	-4.20055
C	2.57927	-1.45641	-2.94722
C	-0.11781	1.66617	-2.15035
C	-1.38978	2.22734	-1.95896
C	-1.97976	3.03206	-2.93488

C	-1.26111	3.28870	-4.10920
C	0.01231	2.75701	-4.32561
C	0.56920	1.93561	-3.33891
C	0.46762	2.60779	0.80331
C	-0.29591	2.84129	1.95216
C	-0.45515	4.12871	2.46992
C	0.17631	5.19476	1.82039
C	0.94711	4.99801	0.67040
C	1.08137	3.69895	0.17404
C	1.83543	0.24863	2.35625
C	1.37655	-0.60671	3.36232
C	1.86482	-0.51455	4.67299
C	2.83839	0.44487	4.95373
C	3.32492	1.31566	3.97040
C	2.80635	1.20907	2.68083
C	2.28044	-2.16797	0.29225
C	3.45972	-2.18319	1.05053
C	4.15424	-3.37023	1.29900
C	3.64359	-4.56616	0.78463
C	2.47241	-4.59222	0.02011
C	1.81234	-3.38601	-0.22573
C	-0.66737	-2.38745	-5.64263
C	-1.90204	-1.48935	-5.53342
C	4.28136	-2.29116	-4.64232
C	4.95605	-3.35477	-3.76642
C	-3.36424	3.61753	-2.71452
C	-3.32996	5.15027	-2.64660
C	0.77609	3.07963	-5.59948
C	1.00904	1.83134	-6.46094
C	-1.31533	4.35593	3.70230
C	-2.52527	5.24841	3.39475
C	1.63397	6.16042	-0.02720
C	2.68295	6.82545	0.87448
C	1.34555	-1.42063	5.77643
C	1.61459	-2.90214	5.48397
C	4.39462	2.34594	4.29043
C	5.70414	1.68205	4.73793
C	5.45751	-3.33888	2.08066
C	6.66088	-3.57413	1.15559
C	1.91368	-5.89751	-0.52202
C	2.89724	-6.60129	-1.46570
C	-1.05526	-3.86480	-5.46639
C	5.12137	-1.00745	-4.69410
C	-4.36399	3.13343	-3.77345
C	2.09878	3.79968	-5.30293
C	-0.50057	4.91627	4.87558
C	0.62508	7.19116	-0.55152
C	-0.14189	-1.16901	6.05868
C	3.91072	3.36948	5.32593
C	5.46984	-4.32426	3.25550
C	1.47259	-6.83540	0.61030

H	-0.26512	-2.27416	-6.65939
H	-1.82051	-4.15770	-6.19418
H	-0.19064	-4.52298	-5.59736
H	-1.45890	-4.03911	-4.46264
H	-2.60753	-1.71722	-6.33934
H	-2.43236	-1.64594	-4.58765
H	-1.63850	-0.42949	-5.59707
H	4.65996	-0.25704	-5.34362
H	5.23225	-0.56465	-3.69817
H	6.12633	-1.21773	-5.07668
H	4.38935	-4.29064	-3.77661
H	5.96952	-3.56714	-4.12495
H	5.03133	-3.02437	-2.72509
H	-3.71302	3.25223	-1.73962
H	-4.41288	2.04035	-3.80146
H	-5.36892	3.51461	-3.56046
H	-4.08376	3.48012	-4.77443
H	-2.64627	5.49406	-1.86465
H	-2.99859	5.58350	-3.59707
H	-4.32618	5.55145	-2.42893
H	-1.69765	3.92413	-4.87810
H	0.15005	3.77027	-6.18098
H	1.93262	4.70501	-4.71077
H	2.78539	3.15555	-4.74267
H	2.60024	4.08735	-6.23370
H	0.06103	1.35797	-6.73426
H	1.53736	2.09173	-7.38528
H	1.60921	1.08561	-5.92918
H	1.55614	1.50527	-3.48412
H	-0.80138	2.00458	2.42564
H	-1.70010	3.37362	4.00663
H	0.33082	4.25234	5.13138
H	-0.08194	5.90013	4.63557
H	-1.12968	5.03265	5.76533
H	-3.12675	4.83088	2.58156
H	-3.16676	5.34983	4.27741
H	-2.21171	6.25487	3.09568
H	0.06024	6.20224	2.21565
H	2.16134	5.74520	-0.89646
H	-0.10124	6.72490	-1.22395
H	0.06939	7.65697	0.26996
H	1.13536	7.99014	-1.10115
H	3.42180	6.09834	1.22570
H	3.21382	7.61844	0.33569
H	2.21720	7.27869	1.75665
H	1.67562	3.52867	-0.72054
H	0.62573	-1.35800	3.12306
H	3.22403	0.51418	5.96943
H	3.16019	1.88029	1.90248
H	3.84879	-1.24900	1.44477
H	5.55354	-2.32824	2.49896

H	4.61821	-4.15874	3.92200
H	5.42846	-5.36363	2.91180
H	6.38857	-4.21079	3.84109
H	6.68495	-2.84207	0.34238
H	7.60179	-3.49679	1.71193
H	6.61941	-4.57183	0.70436
H	4.17200	-5.49688	0.97946
H	0.92087	-3.39071	-0.84788
H	-0.79396	-1.19656	-3.13205
H	3.39326	-1.22390	-2.26572
H	1.98067	-2.72361	-6.02969
H	4.22791	-2.68992	-5.66458
H	1.02015	-5.64434	-1.10819
H	3.18500	-5.94841	-2.29471
H	2.44757	-7.50787	-1.88545
H	3.81166	-6.89907	-0.94082
H	1.01808	-7.74596	0.20467
H	0.73961	-6.35229	1.26400
H	2.32454	-7.13653	1.22998
H	5.57022	1.13059	5.67515
H	6.48309	2.43425	4.90446
H	6.06799	0.97559	3.98523
H	4.60114	2.89137	3.36005
H	3.00320	3.87558	4.98413
H	4.67843	4.13009	5.50633
H	3.68717	2.89024	6.28555
H	1.09218	-3.23272	4.57975
H	1.27381	-3.53001	6.31466
H	2.68233	-3.08674	5.33290
H	1.90085	-1.16131	6.68795
H	-0.32364	-0.11973	6.31091
H	-0.48810	-1.78585	6.89567
H	-0.75792	-1.41149	5.18605
H	-0.60306	-3.36483	1.08402
H	-4.49526	-1.74247	0.17958
H	-1.25158	-3.57419	3.44416
H	-5.14045	-2.02292	2.52494
H	-3.89683	-2.03231	5.07692
H	-2.89319	-3.48236	5.20015
H	-4.57843	-3.60888	4.68016
H	-1.32412	-2.91272	-1.36884
H	-2.78504	-1.86607	-1.62298
H	-1.91795	2.03038	-1.02691
H	-2.01020	0.60416	0.91670

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Complex 1 - 2nd xyl. hydro red path.

C	1.25437	-3.30761	-0.17827
C	1.53334	-2.06606	0.41469
C	2.63821	-1.97898	1.27301
C	3.44192	-3.08932	1.54861

C	3.11758	-4.31374	0.95685
C	2.02569	-4.44044	0.09125
C	0.72429	-0.86038	0.10860
C	0.33106	-0.43676	-1.20424
C	-0.32579	0.82820	-1.07834
C	-0.32973	1.19761	0.30075
C	0.30995	0.15210	1.04041
Sc	-1.76207	-0.84770	0.09862
C	-2.49973	-2.50595	-1.21412
C	-3.06528	-2.94587	0.05345
C	-2.24277	-3.51476	1.06209
C	-2.74354	-3.81995	2.33315
C	-4.06155	-3.53291	2.68898
C	-4.86216	-2.90138	1.72180
C	-4.38339	-2.60065	0.45503
C	-4.61505	-3.88096	4.04457
C	0.73564	-1.05154	-2.49529
C	-0.19668	-1.37097	-3.49063
C	0.20795	-1.86650	-4.73270
C	1.57782	-2.02083	-4.97073
C	2.53804	-1.70522	-4.00534
C	2.09935	-1.23011	-2.76545
C	-0.81213	1.68115	-2.19310
C	-2.13178	2.15476	-2.22576
C	-2.57346	2.99397	-3.24987
C	-1.66119	3.37246	-4.24245
C	-0.33825	2.92455	-4.23625
C	0.07068	2.06813	-3.20783
C	-0.75659	2.51778	0.83165
C	-1.73624	2.65853	1.81970
C	-2.10110	3.91406	2.31202
C	-1.45045	5.04472	1.80762
C	-0.45620	4.94159	0.82943
C	-0.12486	3.67215	0.34975
C	0.62484	0.20568	2.49204
C	0.27507	-0.81477	3.38411
C	0.60906	-0.74171	4.74252
C	1.31971	0.37121	5.19465
C	1.69703	1.40629	4.33094
C	1.33758	1.30967	2.98705
C	-0.79820	-2.27497	-5.79654
C	-1.36043	-3.67432	-5.50098
C	4.01859	-1.86123	-4.31146
C	4.77487	-0.53187	-4.18593
C	-4.01118	3.48555	-3.27257
C	-4.74860	3.04170	-4.54306
C	0.63146	3.36980	-5.31867
C	1.83709	4.11801	-4.73386
C	-3.20287	4.03716	3.35135
C	-2.71494	4.71090	4.64032
C	0.25126	6.17337	0.28948

C	-0.70938	7.08507	-0.48616
C	0.20353	-1.83537	5.71618
C	-1.32182	-1.94013	5.84673
C	2.48864	2.60189	4.83336
C	1.71965	3.39131	5.90066
C	4.67060	-2.93050	2.42990
C	4.82283	-4.04751	3.46832
C	1.66860	-5.77973	-0.53312
C	1.20771	-6.78928	0.52774
C	-1.93120	-1.26068	-5.98383
C	4.66861	-2.94779	-3.44508
C	-4.09471	5.00713	-3.08991
C	1.08504	2.19633	-6.19738
C	-4.43190	4.76046	2.78270
C	0.97807	6.95063	1.39489
C	0.82564	-3.19005	5.35528
C	3.87515	2.18711	5.34547
C	5.94003	-2.80734	1.57280
C	2.81650	-6.35417	-1.37306
H	-0.24837	-2.33570	-6.74602
H	-2.04345	-3.99701	-6.29500
H	-0.55843	-4.41465	-5.41841
H	-1.91624	-3.67700	-4.55671
H	-2.56191	-1.54652	-6.83265
H	-2.57779	-1.21015	-5.10136
H	-1.54304	-0.25487	-6.16760
H	4.33265	0.23819	-4.82560
H	4.75954	-0.16003	-3.15563
H	5.82407	-0.65484	-4.47681
H	4.17633	-3.91387	-3.59200
H	5.72843	-3.06484	-3.69797
H	4.60235	-2.69969	-2.38058
H	-4.51886	3.02218	-2.41648
H	-4.71804	1.95388	-4.65952
H	-5.79898	3.35216	-4.50939
H	-4.30136	3.48564	-5.43954
H	-3.60924	5.31922	-2.16037
H	-3.60603	5.53386	-3.91737
H	-5.13910	5.33738	-3.05731
H	-1.98302	4.03624	-5.04328
H	0.08914	4.07552	-5.96275
H	1.51740	4.96915	-4.12456
H	2.44324	3.46193	-4.09963
H	2.48451	4.49389	-5.53398
H	0.23089	1.71102	-6.67942
H	1.76790	2.54038	-6.98264
H	1.60575	1.43567	-5.60648
H	1.09332	1.70199	-3.18065
H	-2.24526	1.77491	2.19185
H	-3.51276	3.01574	3.61004
H	-1.86594	4.17223	5.07218

H	-2.39749	5.74307	4.45569
H	-3.51488	4.74081	5.38855
H	-4.80425	4.25827	1.88459
H	-5.24195	4.78954	3.52019
H	-4.19192	5.79468	2.51133
H	-1.72644	6.02818	2.18325
H	1.01192	5.81954	-0.41928
H	-1.19448	6.54191	-1.30257
H	-1.49523	7.47986	0.16751
H	-0.17348	7.93966	-0.91441
H	1.68707	6.31072	1.92949
H	1.53239	7.79647	0.97318
H	0.27235	7.35241	2.13046
H	0.63941	3.57413	-0.41740
H	-0.26321	-1.68516	3.01332
H	1.58416	0.42808	6.24912
H	1.61761	2.10396	2.30068
H	2.88398	-1.02240	1.72522
H	4.54847	-1.98641	2.97727
H	3.91732	-4.15933	4.07210
H	5.03262	-5.01391	2.99693
H	5.65783	-3.82925	4.14260
H	5.86140	-1.97653	0.86474
H	6.82153	-2.63787	2.20145
H	6.10948	-3.72282	0.99480
H	3.72990	-5.18723	1.16790
H	0.42486	-3.38781	-0.87555
H	-1.25083	-1.22330	-3.27969
H	2.82148	-0.97386	-1.99468
H	1.90652	-2.39349	-5.94030
H	4.09512	-2.18397	-5.35879
H	0.82258	-5.60262	-1.21054
H	3.12380	-5.65214	-2.15324
H	2.51111	-7.28931	-1.85513
H	3.69458	-6.57278	-0.75532
H	0.90549	-7.73283	0.06003
H	0.35623	-6.40621	1.09892
H	2.01214	-7.01168	1.23759
H	3.79544	1.52712	6.21645
H	4.45591	3.06573	5.64725
H	4.43983	1.65391	4.57426
H	2.63846	3.26903	3.97431
H	0.74891	3.72360	5.52136
H	2.28622	4.27652	6.21002
H	1.54093	2.78366	6.79465
H	0.48660	-3.53916	4.37391
H	0.55273	-3.95170	6.09422
H	1.91714	-3.12394	5.32144
H	0.59668	-1.54607	6.70020
H	-1.75987	-0.98173	6.14253
H	-1.59652	-2.68744	6.59972

H	-1.78105	-2.23798	4.89784
H	-1.22131	-3.80067	0.81527
H	-5.03833	-2.11798	-0.26538
H	-2.08851	-4.30515	3.05374
H	-5.89071	-2.64595	1.96930
H	-3.84896	-4.32327	4.68705
H	-5.43806	-4.60096	3.96495
H	-5.01081	-2.99675	4.55699
H	-1.71535	-3.13857	-1.62976
H	-3.23250	-2.20166	-1.96445
H	-2.81507	1.85329	-1.43432
H	-3.13733	0.35975	0.17272
H	-2.43276	-0.89991	2.31667
H	-2.88775	-0.42608	1.92827

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Complex 1 - 2nd xyl. hydro red path. TS

C	1.88774	-3.42560	-0.58880
C	2.20457	-2.18615	-0.01109
C	3.29539	-2.12656	0.86754
C	4.04709	-3.26249	1.17806
C	3.68321	-4.48470	0.60352
C	2.60626	-4.58488	-0.28306
C	1.43905	-0.95550	-0.33199
C	1.03889	-0.52597	-1.64250
C	0.38042	0.73654	-1.51898
C	0.35598	1.08438	-0.13115
C	1.01206	0.04464	0.60223
Sc	-1.01479	-0.97576	-0.36636
C	-1.78234	-2.96290	0.37734
C	-2.52770	-3.85588	1.29543
C	-1.86513	-4.65560	2.23891
C	-2.57564	-5.46053	3.12484
C	-3.97373	-5.50107	3.11061
C	-4.63457	-4.70605	2.16689
C	-3.93105	-3.89912	1.27900
C	-4.74081	-6.34975	4.08977
C	1.31426	-1.21297	-2.92955
C	0.27321	-1.51320	-3.81794
C	0.52852	-2.13312	-5.04544
C	1.85452	-2.42468	-5.37739
C	2.91932	-2.12251	-4.52133
C	2.63139	-1.52728	-3.29029
C	-0.04300	1.61846	-2.63638
C	-1.35015	2.11256	-2.73962
C	-1.71842	2.98230	-3.76575
C	-0.74313	3.36783	-4.69450
C	0.56879	2.89686	-4.62164
C	0.90396	2.01663	-3.58591
C	-0.12619	2.37174	0.43115
C	-1.10276	2.42998	1.43229

C	-1.52690	3.65007	1.96615
C	-0.93986	4.82645	1.49009
C	0.04874	4.80470	0.50050
C	0.43797	3.57060	-0.02468
C	1.30004	0.09740	2.05965
C	0.81903	-0.85296	2.96536
C	1.10856	-0.76298	4.33318
C	1.90917	0.29159	4.77545
C	2.41771	1.25509	3.89595
C	2.09777	1.14591	2.54313
C	-0.60014	-2.46885	-6.00489
C	-1.62239	-3.42578	-5.37630
C	4.34779	-2.44250	-4.92962
C	5.25359	-1.20482	-4.89348
C	-3.14800	3.48694	-3.86855
C	-3.80979	3.06668	-5.18789
C	1.60275	3.32853	-5.64840
C	2.81023	4.01614	-4.99730
C	-2.60907	3.68458	3.03251
C	-2.10285	4.29487	4.34604
C	0.69800	6.08720	0.00678
C	-0.30617	6.99281	-0.71894
C	0.56468	-1.77596	5.32666
C	-0.96961	-1.80579	5.33819
C	3.29349	2.39263	4.39242
C	2.54033	3.30844	5.36660
C	5.26006	-3.14775	2.08635
C	5.23237	-4.15014	3.24647
C	2.19330	-5.92095	-0.87995
C	1.49798	-6.80150	0.16937
C	-1.28671	-1.20288	-6.53569
C	4.93417	-3.57961	-4.08201
C	-3.23306	5.00607	-3.66873
C	2.04632	2.15291	-6.52982
C	-3.86851	4.40840	2.53622
C	1.40320	6.84347	1.14072
C	1.14501	-3.17614	5.08881
C	4.59842	1.87716	5.01453
C	6.56163	-3.27743	1.28090
C	3.36337	-6.67121	-1.52728
H	-0.14764	-2.98559	-6.86243
H	-2.39022	-3.70333	-6.10684
H	-1.14238	-4.34377	-5.02225
H	-2.12986	-2.96013	-4.52443
H	-2.06761	-1.46158	-7.25959
H	-1.75511	-0.63700	-5.72369
H	-0.56856	-0.54131	-7.02931
H	4.85503	-0.40233	-5.52183
H	5.35630	-0.81338	-3.87553
H	6.25821	-1.45196	-5.25397
H	4.32103	-4.48251	-4.16177

H	5.94970	-3.82695	-4.41104
H	4.98132	-3.30061	-3.02394
H	-3.71143	3.01495	-3.05287
H	-3.78001	1.98049	-5.31701
H	-4.85802	3.38497	-5.21330
H	-3.30570	3.51952	-6.04898
H	-2.81121	5.30027	-2.70300
H	-2.68481	5.54148	-4.45203
H	-4.27484	5.34407	-3.70290
H	-1.00974	4.04921	-5.50071
H	1.11682	4.06671	-6.30098
H	2.49922	4.87175	-4.38971
H	3.35889	3.32610	-4.34686
H	3.50899	4.37535	-5.76095
H	1.19205	1.70259	-7.04429
H	2.76611	2.48373	-7.28722
H	2.52189	1.36830	-5.93182
H	1.91790	1.63344	-3.50675
H	-1.54289	1.50534	1.79972
H	-2.88722	2.64251	3.23888
H	-1.23080	3.75230	4.72352
H	-1.81378	5.34323	4.21248
H	-2.88345	4.26235	5.11421
H	-4.25132	3.95245	1.61785
H	-4.66073	4.37121	3.29221
H	-3.66197	5.46320	2.32323
H	-1.25749	5.78283	1.90078
H	1.46476	5.79624	-0.72348
H	-0.77042	6.47079	-1.56071
H	-1.10556	7.32045	-0.04489
H	0.18990	7.89004	-1.10577
H	2.14137	6.20950	1.64170
H	1.91968	7.72862	0.75324
H	0.68765	7.18311	1.89768
H	1.19860	3.53578	-0.80053
H	0.19815	-1.66840	2.60157
H	2.13677	0.36217	5.83770
H	2.46978	1.88924	1.84254
H	3.56798	-1.17217	1.30866
H	5.23800	-2.14005	2.52179
H	4.31105	-4.05859	3.82914
H	5.30116	-5.18355	2.88927
H	6.08014	-3.98066	3.91906
H	6.60946	-2.53172	0.48122
H	7.43578	-3.14110	1.92741
H	6.63830	-4.26759	0.81769
H	4.25651	-5.37666	0.84537
H	1.07254	-3.49121	-1.30650
H	-0.74385	-1.24470	-3.53730
H	3.43469	-1.28787	-2.59856
H	2.06677	-2.89591	-6.33636

H	4.31128	-2.79191	-5.97045
H	1.46124	-5.70595	-1.66990
H	3.87211	-6.05181	-2.27113
H	3.00620	-7.57944	-2.02446
H	4.10565	-6.97854	-0.78267
H	1.17417	-7.75051	-0.27224
H	0.61668	-6.30586	0.58785
H	2.17821	-7.03109	0.99727
H	4.40340	1.27946	5.91191
H	5.24467	2.71210	5.30707
H	5.15231	1.24866	4.31011
H	3.56229	2.99567	3.51478
H	1.63193	3.70973	4.90759
H	3.17011	4.15163	5.67154
H	2.24761	2.76859	6.27402
H	0.86022	-3.56013	4.10371
H	0.77654	-3.88184	5.84155
H	2.23811	-3.16371	5.13860
H	0.89406	-1.44944	6.32254
H	-1.38262	-0.80932	5.52341
H	-1.33557	-2.47767	6.12238
H	-1.37252	-2.16519	4.38562
H	-0.77788	-4.65590	2.26972
H	-4.47527	-3.29986	0.55220
H	-2.03050	-6.07508	3.83818
H	-5.72156	-4.72240	2.12244
H	-4.16027	-7.22188	4.40560
H	-5.68105	-6.70852	3.65975
H	-4.99391	-5.78266	4.99456
H	-0.74449	-3.31240	0.22718
H	-2.28212	-2.89549	-0.61202
H	-2.09521	1.78541	-2.01989
H	-2.18951	-0.67423	-1.73429
H	-1.95971	-1.63719	1.13257
H	-1.95233	-0.69664	1.33359

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Complex 1 - 2nd xyl. hydro red path. prod

C	1.02430	-3.07531	-0.43130
C	1.39160	-1.91087	0.26408
C	2.38095	-2.01282	1.25265
C	2.99565	-3.23303	1.54449
C	2.60334	-4.37105	0.83134
C	1.61895	-4.31036	-0.16049
C	0.75800	-0.61022	-0.05972
C	0.43153	-0.15907	-1.38325
C	-0.19177	1.12146	-1.26664
C	-0.22734	1.48041	0.11814
C	0.35265	0.40848	0.86476
Sc	-1.69495	-0.50054	-0.18159
C	-2.41410	-2.62879	1.11547

C	-2.93948	-3.79586	1.91198
C	-2.07396	-4.71783	2.50304
C	-2.57524	-5.79498	3.23449
C	-3.94934	-5.98267	3.39733
C	-4.81189	-5.05359	2.79928
C	-4.31878	-3.97830	2.06996
C	-4.49557	-7.13703	4.19501
C	0.87247	-0.80469	-2.65072
C	-0.01574	-1.30532	-3.60855
C	0.45409	-1.88464	-4.79198
C	1.83452	-1.93562	-5.00907
C	2.74967	-1.43451	-4.07765
C	2.25077	-0.87723	-2.89726
C	-0.72130	1.96019	-2.36693
C	-2.02090	2.48405	-2.28319
C	-2.54224	3.29665	-3.28948
C	-1.72389	3.60253	-4.38403
C	-0.42262	3.10760	-4.49400
C	0.06400	2.27336	-3.48078
C	-0.58429	2.81502	0.66330
C	-1.51401	2.98756	1.69409
C	-1.77474	4.25091	2.23074
C	-1.08307	5.35312	1.71769
C	-0.14836	5.21679	0.68614
C	0.08846	3.94104	0.16945
C	0.62672	0.47691	2.32636
C	-0.05154	-0.28733	3.27891
C	0.22537	-0.15982	4.64703
C	1.21370	0.74208	5.04314
C	1.92099	1.51867	4.11686
C	1.61017	1.37725	2.76523
C	-0.50720	-2.48046	-5.80657
C	-1.21928	-3.71631	-5.23722
C	4.24351	-1.48755	-4.35251
C	4.84830	-0.08107	-4.46401
C	-3.96029	3.83148	-3.18891
C	-4.84525	3.30604	-4.32751
C	0.44452	3.48243	-5.68438
C	1.71984	4.21868	-5.25197
C	-2.79420	4.41110	3.34621
C	-2.13719	4.88791	4.64891
C	0.60614	6.41807	0.14113
C	-0.33781	7.46114	-0.47116
C	-0.53086	-0.96954	5.68708
C	-2.04035	-0.69659	5.64481
C	2.98754	2.50340	4.56449
C	2.38585	3.64666	5.39345
C	4.08645	-3.30553	2.60018
C	3.73974	-4.29020	3.72441
C	1.21675	-5.54408	-0.95210
C	0.71110	-6.67842	-0.05140

C	-1.52418	-1.45476	-6.32284
C	4.99284	-2.32571	-3.30827
C	-3.99184	5.36423	-3.12505
C	0.77819	2.26358	-6.55460
C	-3.95078	5.33436	2.94066
C	1.51112	7.05145	1.20714
C	-0.23788	-2.47103	5.56920
C	4.12800	1.81081	5.32209
C	5.44966	-3.63843	1.97756
C	2.36239	-6.02565	-1.85348
H	0.09550	-2.81118	-6.66374
H	-1.86371	-4.17651	-5.99478
H	-0.49900	-4.46859	-4.90010
H	-1.84886	-3.44565	-4.38253
H	-2.16736	-1.90315	-7.08825
H	-2.17000	-1.09337	-5.51583
H	-1.02353	-0.58746	-6.76271
H	4.34341	0.50761	-5.23620
H	4.75925	0.46309	-3.51728
H	5.91293	-0.13451	-4.71764
H	4.59641	-3.34419	-3.25757
H	6.05905	-2.38636	-3.55365
H	4.90577	-1.88690	-2.30855
H	-4.37699	3.45356	-2.24595
H	-4.85100	2.21194	-4.35058
H	-5.87811	3.65109	-4.20594
H	-4.49002	3.65875	-5.30224
H	-3.39307	5.73669	-2.28838
H	-3.59768	5.81007	-4.04515
H	-5.01854	5.72462	-2.99641
H	-2.10489	4.24636	-5.17514
H	-0.14245	4.17735	-6.30033
H	1.48329	5.10294	-4.65176
H	2.36872	3.57143	-4.65195
H	2.29454	4.54375	-6.12640
H	-0.13379	1.78256	-6.92097
H	1.37973	2.55843	-7.42190
H	1.34398	1.51445	-5.99075
H	1.07019	1.86923	-3.54513
H	-2.05879	2.12100	2.05737
H	-3.21823	3.41614	3.53481
H	-1.34312	4.20372	4.96321
H	-1.69346	5.88262	4.52766
H	-2.87473	4.95017	5.45716
H	-4.43785	4.97907	2.02740
H	-4.70501	5.38164	3.73407
H	-3.60052	6.35616	2.75659
H	-1.27955	6.34154	2.12901
H	1.25462	6.04945	-0.66501
H	-0.95518	7.01939	-1.25901
H	-1.01003	7.88281	0.28437

H	0.23120	8.29008	-0.90685
H	2.21184	6.31808	1.61832
H	2.09157	7.87839	0.78289
H	0.92261	7.45211	2.03998
H	0.81297	3.81512	-0.63159
H	-0.82288	-0.98288	2.95833
H	1.43113	0.84298	6.10501
H	2.13320	1.98244	2.02877
H	2.68489	-1.12205	1.79421
H	4.16247	-2.30660	3.04944
H	2.77929	-4.04209	4.18606
H	3.67548	-5.31813	3.35063
H	4.50874	-4.27118	4.50438
H	5.71793	-2.91542	1.20112
H	6.23723	-3.62966	2.73928
H	5.44243	-4.63304	1.51793
H	3.08061	-5.32456	1.04742
H	0.27525	-3.01311	-1.21815
H	-1.08031	-1.25789	-3.39597
H	2.93488	-0.48351	-2.14953
H	2.20900	-2.38137	-5.92992
H	4.37220	-1.97983	-5.32608
H	0.38695	-5.24732	-1.60699
H	2.69463	-5.22920	-2.52590
H	2.04311	-6.87748	-2.46422
H	3.22539	-6.34680	-1.25951
H	0.38428	-7.53205	-0.65520
H	-0.13622	-6.35510	0.56110
H	1.49752	-7.03490	0.62328
H	3.77176	1.36101	6.25537
H	4.91251	2.53033	5.58058
H	4.57952	1.01594	4.72016
H	3.41555	2.94545	3.65491
H	1.60347	4.16913	4.83513
H	3.15710	4.37579	5.66567
H	1.94146	3.27095	6.32189
H	-0.59912	-2.87306	4.61673
H	-0.73690	-3.02657	6.37085
H	0.83635	-2.67029	5.63348
H	-0.16586	-0.64021	6.66940
H	-2.25376	0.37116	5.75299
H	-2.55155	-1.23145	6.45272
H	-2.48113	-1.03155	4.69964
H	-0.99897	-4.59795	2.39110
H	-5.01099	-3.27208	1.61694
H	-1.88134	-6.49995	3.68616
H	-5.88739	-5.17488	2.90802
H	-3.70058	-7.81879	4.50883
H	-5.22304	-7.71453	3.61416
H	-5.00967	-6.78731	5.09787
H	-1.31353	-2.61501	1.15993

H	-2.72267	-2.71078	0.05660
H	-2.63231	2.25833	-1.41017
H	-2.36885	-1.27254	-1.70398
H	-2.82862	-1.68616	1.52407
H	-2.95861	0.45231	0.74319

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Complex 1 - 2nd xyl. + THF

Sc	1.20795	-1.66163	0.15093
C	-0.55811	-0.29962	-0.93395
C	-0.04432	0.20936	1.26421
C	0.95053	0.81014	0.43257
C	0.63639	0.49217	-0.92684
C	1.39831	0.97793	-2.10227
C	0.74342	1.64230	-3.14828
C	1.45764	2.18004	-4.22249
C	2.84600	2.01481	-4.24696
C	3.53174	1.34922	-3.22646
C	2.79365	0.84242	-2.15241
C	-0.97790	-0.47196	0.42599
O	1.64854	-3.17031	-1.37305
C	0.87233	-4.40388	-1.48927
C	1.80727	-5.40924	-2.15902
C	3.20031	-4.86416	-1.82846
C	2.98302	-3.36519	-1.91971
C	-1.31493	-0.74447	-2.13267
C	-0.72735	-1.50616	-3.15546
C	-1.45394	-1.90763	-4.27833
C	-2.79076	-1.50529	-4.38490
C	-3.40477	-0.73141	-3.39788
C	-2.65662	-0.36925	-2.27211
C	-2.23391	-1.11664	0.88327
C	-2.54127	-2.44978	0.58986
C	-3.73474	-3.03656	1.01604
C	-4.64003	-2.25502	1.74170
C	-4.37087	-0.91713	2.04825
C	-3.16387	-0.36395	1.61257
C	-0.14256	0.34157	2.74018
C	-0.14761	-0.78038	3.57417
C	-0.26491	-0.64641	4.96331
C	-0.39665	0.63472	5.50181
C	-0.40467	1.77872	4.69301
C	-0.26709	1.61554	3.31476
C	1.99198	1.76418	0.89504
C	1.93371	3.09444	0.45818
C	2.84226	4.05286	0.91440
C	3.83214	3.65417	1.81840
C	3.92311	2.33331	2.27003
C	2.99237	1.40129	1.80343
C	0.75586	2.94946	-5.32956
C	-0.00049	4.16889	-4.78508

C	5.04601	1.22989	-3.27257
C	5.52955	-0.21481	-3.09740
C	-0.80946	-2.77590	-5.34668
C	-1.48876	-4.14928	-5.44387
C	-4.85105	-0.29199	-3.55078
C	-4.98513	1.23679	-3.56315
C	-4.01986	-4.49900	0.71609
C	-5.28212	-4.67952	-0.13703
C	-5.35661	-0.07760	2.84429
C	-5.54609	-0.62215	4.26656
C	-0.23972	-1.86666	5.86758
C	1.10680	-2.59999	5.78592
C	-0.57213	3.16564	5.29083
C	0.58219	3.52959	6.23370
C	2.73680	5.49520	0.44662
C	3.99108	5.94968	-0.31128
C	5.01003	1.90662	3.24311
C	6.41440	2.11779	2.66162
C	-0.17202	2.04778	-6.15370
C	5.70510	2.15653	-2.24073
C	-0.77816	-2.08602	-6.71645
C	-5.75184	-0.91695	-2.47736
C	-4.09785	-5.33579	2.00028
C	-6.70453	0.06369	2.12449
C	-1.40331	-2.82257	5.57281
C	-1.92782	3.32099	5.99352
C	2.42326	6.44580	1.61056
C	4.86565	2.60563	4.60160
H	0.53664	-2.95056	1.28558
H	2.99711	-1.36745	0.49423
H	1.53838	3.32265	-6.00430
H	-0.65182	2.61501	-6.95926
H	0.38617	1.22255	-6.60650
H	-0.96154	1.61426	-5.53070
H	-0.44309	4.74715	-5.60378
H	-0.81333	3.86683	-4.11591
H	0.66628	4.82962	-4.22242
H	5.41733	3.19876	-2.40823
H	5.40262	1.88992	-1.22270
H	6.79753	2.09100	-2.29952
H	5.07560	-0.87765	-3.84161
H	6.61783	-0.27336	-3.20960
H	5.28120	-0.59753	-2.10169
H	0.23252	-2.94077	-5.03854
H	-0.26264	-1.12348	-6.66147
H	-0.26120	-2.71060	-7.45356
H	-1.79053	-1.90111	-7.09178
H	-1.49345	-4.66397	-4.47750
H	-2.53038	-4.05195	-5.76870
H	-0.97388	-4.78835	-6.17002
H	-3.37312	-1.79893	-5.25662

H	-5.19549	-0.65935	-4.52730
H	-5.70818	-2.00957	-2.51340
H	-5.44754	-0.60853	-1.47180
H	-6.79466	-0.61311	-2.62223
H	-4.36241	1.68399	-4.34431
H	-6.02453	1.53132	-3.74518
H	-4.68207	1.67111	-2.60434
H	-3.11411	0.22287	-1.48488
H	-1.81730	-3.05089	0.04616
H	-3.16998	-4.87512	0.13034
H	-3.18318	-5.23609	2.59234
H	-4.93778	-5.01962	2.62876
H	-4.24091	-6.39647	1.76474
H	-5.21000	-4.11767	-1.07310
H	-5.43686	-5.73607	-0.38344
H	-6.17471	-4.33015	0.39355
H	-5.57242	-2.70067	2.08302
H	-4.92233	0.92718	2.93248
H	-6.57836	0.49069	1.12466
H	-7.19904	-0.90750	2.01162
H	-7.38001	0.71525	2.69004
H	-4.58974	-0.68488	4.79401
H	-6.21416	0.02588	4.84493
H	-5.98723	-1.62507	4.25144
H	-2.93479	0.67218	1.84889
H	-0.05190	-1.76427	3.11939
H	-0.49488	0.73986	6.58127
H	-0.26326	2.49032	2.66912
H	1.15745	3.38659	-0.24538
H	1.89325	5.54279	-0.25511
H	1.50889	6.14560	2.13172
H	3.23661	6.45373	2.34458
H	2.29043	7.47228	1.25057
H	4.19197	5.29819	-1.16689
H	3.87114	6.97399	-0.68188
H	4.87518	5.93292	0.33561
H	4.54926	4.38939	2.17845
H	3.05807	0.36587	2.12615
H	-0.33591	1.75670	-3.10019
H	3.29557	0.34624	-1.32394
H	3.41188	2.42899	-5.08079
H	5.36295	1.56475	-4.26990
H	4.88125	0.82936	3.41101
H	6.53064	1.59262	1.70860
H	7.17995	1.74579	3.35180
H	6.61716	3.17998	2.48434
H	5.62756	2.25042	5.30467
H	3.88197	2.41330	5.04027
H	4.98371	3.69086	4.50489
H	0.62095	2.85410	7.09555
H	0.46341	4.54933	6.61705

H	1.54511	3.46982	5.71803
H	-0.55009	3.87784	4.45501
H	-2.75486	3.09596	5.31288
H	-2.05866	4.34392	6.36410
H	-2.01005	2.64449	6.85144
H	1.27740	-2.99823	4.77980
H	1.13389	-3.44124	6.48796
H	1.93784	-1.92896	6.02513
H	-0.35872	-1.50577	6.89868
H	-2.36826	-2.31598	5.67134
H	-1.39138	-3.67232	6.26487
H	-1.33942	-3.21881	4.55403
H	3.49537	-5.13951	-0.81051
H	3.97228	-5.21268	-2.51935
H	1.65076	-5.42006	-3.24284
H	1.64376	-6.42280	-1.78451
H	3.66288	-2.76091	-1.31611
H	2.98476	-3.00803	-2.95609
H	0.31876	-1.79040	-3.07209
H	0.58772	-4.69090	-0.47352
H	-0.02308	-4.17874	-2.07423

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Complex 1 - 2nd xyl. + THF RO TS

Sc	11.08335	12.88403	3.70027
C	9.31690	14.30909	2.71613
C	9.87408	14.75574	4.91923
C	10.85986	15.36714	4.08286
C	10.51365	15.09392	2.72164
C	11.22688	15.62068	1.53251
C	10.53477	16.39556	0.59200
C	11.19046	16.96112	-0.50466
C	12.55791	16.71303	-0.65998
C	13.27735	15.93398	0.25095
C	12.59896	15.40291	1.35188
C	8.92581	14.09782	4.07878
O	11.63533	11.52224	2.36954
C	11.24873	10.25429	1.93052
C	12.47725	9.34635	2.02881
C	13.10236	9.69859	3.36306
C	13.44816	11.13895	3.49299
C	8.56480	13.87318	1.51265
C	9.18541	13.16953	0.46802
C	8.47723	12.77801	-0.66915
C	7.12333	13.12325	-0.76203
C	6.47534	13.83341	0.25082
C	7.20785	14.19347	1.38765
C	7.69767	13.40428	4.53868
C	7.44419	12.06341	4.22706
C	6.28156	11.41936	4.65678
C	5.35131	12.15171	5.40173

C	5.56676	13.49523	5.72649
C	6.74607	14.10496	5.29083
C	9.77375	14.90292	6.39427
C	9.78284	13.80066	7.25359
C	9.65479	13.96436	8.63862
C	9.50266	15.25461	9.14924
C	9.48263	16.38006	8.31529
C	9.62585	16.18710	6.94142
C	11.94717	16.26201	4.55147
C	12.01356	17.57964	4.08016
C	12.98615	18.47156	4.53962
C	13.91408	18.01852	5.48259
C	13.88206	16.70786	5.97036
C	12.88862	15.84564	5.50065
C	10.44908	17.84054	-1.49773
C	9.84420	19.07830	-0.82104
C	14.75672	15.66472	0.03231
C	15.01451	14.18228	-0.27309
C	9.16286	11.98476	-1.76932
C	8.54500	10.58863	-1.92937
C	5.00887	14.20667	0.11362
C	4.79862	15.72642	0.15333
C	6.05259	9.95216	4.33350
C	4.79969	9.73993	3.47370
C	4.54951	14.28348	6.53503
C	4.36527	13.70155	7.94288
C	9.69241	12.76458	9.56975
C	11.04152	12.03539	9.49600
C	9.30017	17.77825	8.88176
C	10.45313	18.17542	9.81306
C	13.01319	19.90476	4.03421
C	14.32364	20.23720	3.30898
C	14.90070	16.22090	6.98781
C	16.33625	16.31789	6.45436
C	9.37973	17.05726	-2.27020
C	15.61725	16.14037	1.20951
C	9.17037	12.73714	-3.10634
C	4.14221	13.50144	1.16528
C	6.00211	9.09304	5.60415
C	3.20389	14.39808	5.80583
C	8.53212	11.79650	9.30297
C	7.94484	17.93498	9.58473
C	12.73975	20.90724	5.16436
C	14.75983	16.95270	8.32942
H	10.73268	11.71001	5.08763
H	12.93768	13.11150	3.86268
H	11.19055	18.19451	-2.22710
H	8.87430	17.70344	-2.99678
H	9.82332	16.21779	-2.81400
H	8.61901	16.64955	-1.59608
H	9.37361	19.73364	-1.56243

H	9.07566	18.79686	-0.09300
H	10.60970	19.65489	-0.29241
H	15.46594	17.20564	1.40627
H	15.37176	15.59809	2.12874
H	16.68085	15.97924	1.00032
H	14.43029	13.84790	-1.13624
H	16.07480	14.00616	-0.48755
H	14.73572	13.55515	0.58112
H	10.20932	11.85231	-1.46203
H	9.65014	13.71468	-3.00494
H	9.71256	12.16731	-3.86928
H	8.15243	12.90128	-3.47658
H	8.56022	10.03584	-0.98453
H	7.50156	10.65277	-2.25716
H	9.09190	10.00415	-2.67781
H	6.55416	12.83471	-1.64422
H	4.68086	13.85611	-0.87465
H	4.24215	12.41427	1.09288
H	4.43177	13.79177	2.18061
H	3.08475	13.75550	1.03055
H	5.39576	16.22961	-0.61360
H	3.74532	15.97577	-0.01660
H	5.08379	16.14296	1.12547
H	6.72613	14.74048	2.19302
H	8.17858	11.50043	3.65479
H	6.91693	9.61719	3.74404
H	6.91067	9.21748	6.20105
H	5.14893	9.36733	6.23438
H	5.89981	8.03167	5.35131
H	4.85445	10.31882	2.54696
H	4.68385	8.68253	3.21020
H	3.89397	10.04899	4.00712
H	4.44070	11.66266	5.74229
H	4.95088	15.29922	6.64929
H	3.32541	14.85111	4.81697
H	2.74240	13.41416	5.66650
H	2.50278	15.01486	6.37919
H	5.31893	13.65497	8.47683
H	3.67410	14.31680	8.52980
H	3.95363	12.68685	7.90268
H	6.93457	15.14594	5.54125
H	9.90943	12.81149	6.81986
H	9.39963	15.38201	10.22589
H	9.61745	17.04728	6.27613
H	11.28476	17.91568	3.34670
H	12.19941	20.00110	3.30313
H	11.79024	20.69144	5.66395
H	13.52959	20.87351	5.92297
H	12.69665	21.93072	4.77509
H	14.49552	19.55266	2.47295
H	14.30025	21.25909	2.91400

H	15.18303	20.16288	3.98453
H	14.67941	18.70179	5.84558
H	12.85073	14.82431	5.87130
H	9.47161	16.56607	0.73931
H	13.13281	14.80979	2.09138
H	13.07936	17.14401	-1.51393
H	15.05958	16.23984	-0.85343
H	14.68726	15.15888	7.16887
H	16.44460	15.77773	5.50863
H	17.04712	15.89556	7.17349
H	16.62590	17.35955	6.27712
H	15.47001	16.55811	9.06493
H	13.75032	16.83839	8.73525
H	14.95733	18.02489	8.21910
H	10.50014	17.51972	10.68964
H	10.32537	19.20237	10.17367
H	11.41552	18.11311	9.29647
H	9.31228	18.47162	8.03003
H	7.11854	17.68679	8.91129
H	7.80423	18.96431	9.93338
H	7.87167	17.27644	10.45731
H	11.20816	11.61961	8.49625
H	11.07534	11.20734	10.21336
H	11.87068	12.71434	9.71942
H	9.57790	13.14701	10.59356
H	7.56542	12.30006	9.39941
H	8.55360	10.96047	10.01138
H	8.59017	11.38159	8.29133
H	12.46707	9.38890	4.20007
H	14.07493	9.19030	3.49461
H	13.17400	9.56785	1.21173
H	12.20170	8.28938	1.96569
H	13.66642	11.45744	4.50424
H	14.06884	11.59517	2.72960
H	10.24151	12.92214	0.54942
H	10.43417	9.84989	2.54943
H	10.89598	10.32051	0.89287

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Complex 1 - 2nd xyl. + THF RO prod

Sc	0.95638	-1.55393	0.12120
C	-0.73804	-0.14767	-0.94341
C	-0.21715	0.34628	1.26456
C	0.78506	0.92783	0.43274
C	0.47150	0.61855	-0.93113
C	1.22437	1.08860	-2.12071
C	0.57545	1.85702	-3.09582
C	1.26737	2.36035	-4.20065
C	2.62665	2.05846	-4.32634
C	3.30585	1.28325	-3.38185
C	2.58976	0.81377	-2.27684

C	-1.15075	-0.33418	0.41599
O	1.26387	-3.04010	-0.95101
C	1.35841	-4.19689	-1.73091
C	2.77296	-4.50020	-2.22605
C	3.76077	-5.03859	-1.18458
C	4.24601	-4.02875	-0.14506
C	-1.49396	-0.57193	-2.14877
C	-0.91524	-1.35732	-3.15647
C	-1.63668	-1.72865	-4.29204
C	-2.95795	-1.28096	-4.41711
C	-3.56366	-0.49009	-3.43841
C	-2.81882	-0.14896	-2.30377
C	-2.32676	-1.11992	0.86123
C	-2.53750	-2.42260	0.38506
C	-3.63086	-3.18638	0.80131
C	-4.53574	-2.61369	1.70018
C	-4.36541	-1.31262	2.18606
C	-3.25172	-0.58168	1.76530
C	-0.34860	0.56178	2.73013
C	-0.22680	-0.47111	3.66190
C	-0.36812	-0.22919	5.03366
C	-0.65030	1.07115	5.45657
C	-0.78440	2.12981	4.54935
C	-0.62710	1.85797	3.19012
C	1.91740	1.75737	0.90984
C	2.11065	3.04620	0.39554
C	3.13862	3.86738	0.86365
C	3.99256	3.36781	1.85337
C	3.83416	2.08247	2.38111
C	2.78592	1.28972	1.90502
C	0.57070	3.22270	-5.23997
C	-0.05599	4.47743	-4.61736
C	4.77652	0.95367	-3.57460
C	4.97800	-0.53706	-3.88264
C	-1.00299	-2.61239	-5.35346
C	-1.72528	-3.96173	-5.47073
C	-4.99462	-0.00890	-3.61002
C	-5.07722	1.52247	-3.67106
C	-3.81662	-4.60447	0.28857
C	-5.13058	-4.76811	-0.48665
C	-5.37410	-0.69191	3.13845
C	-5.51230	-1.49388	4.43892
C	-0.18046	-1.34705	6.04573
C	1.26842	-1.85590	6.04960
C	-1.09182	3.54032	5.02277
C	0.01679	4.09344	5.92829
C	3.29836	5.27936	0.32452
C	4.66807	5.50035	-0.32969
C	4.76543	1.55151	3.45827
C	6.22493	1.50716	2.98680
C	-0.46919	2.42228	-6.03539

C	5.64014	1.39037	-2.38491
C	-0.92379	-1.91179	-6.71608
C	-5.92030	-0.56759	-2.52128
C	-3.71126	-5.63418	1.42177
C	-6.73971	-0.49887	2.46415
C	-1.16763	-2.50060	5.82891
C	-2.46071	3.62383	5.71172
C	3.03301	6.32891	1.41336
C	4.62993	2.34563	4.76484
H	1.71984	-1.89848	1.75223
H	3.43193	-3.67108	0.49081
H	1.34236	3.55668	-5.94684
H	-0.94523	3.05209	-6.79527
H	-0.00601	1.57061	-6.54275
H	-1.25520	2.03025	-5.38128
H	-0.49301	5.11578	-5.39298
H	-0.85520	4.21696	-3.91511
H	0.68959	5.06473	-4.07232
H	5.52429	2.45846	-2.17990
H	5.37252	0.84806	-1.47182
H	6.69881	1.19385	-2.58664
H	4.39050	-0.84547	-4.75309
H	6.03246	-0.75296	-4.08751
H	4.66986	-1.15820	-3.03432
H	0.02602	-2.81473	-5.02720
H	-0.37684	-0.96740	-6.64279
H	-0.41313	-2.54675	-7.44857
H	-1.92217	-1.69030	-7.10920
H	-1.75555	-4.48141	-4.50790
H	-2.75877	-3.82973	-5.80975
H	-1.21941	-4.61114	-6.19380
H	-3.53642	-1.55546	-5.29765
H	-5.34853	-0.39577	-4.57543
H	-5.90034	-1.66142	-2.50810
H	-5.62078	-0.22013	-1.52693
H	-6.95436	-0.24708	-2.69050
H	-4.44315	1.92296	-4.46822
H	-6.10659	1.84728	-3.85883
H	-4.75438	1.97561	-2.72732
H	-3.26545	0.46027	-1.52253
H	-1.84229	-2.85068	-0.33634
H	-2.99429	-4.80079	-0.41260
H	-2.75825	-5.54346	1.95223
H	-4.51416	-5.50137	2.15541
H	-3.78732	-6.65344	1.02719
H	-5.18838	-4.06175	-1.32023
H	-5.21668	-5.78228	-0.89215
H	-5.99859	-4.59549	0.15921
H	-5.39503	-3.19409	2.02972
H	-4.99222	0.30257	3.40448
H	-6.65270	0.10552	1.55592

H	-7.18125	-1.46136	2.18255
H	-7.43967	0.00242	3.14186
H	-4.54559	-1.60581	4.93829
H	-6.19800	-0.99205	5.13048
H	-5.90975	-2.49725	4.25038
H	-3.09984	0.42611	2.14164
H	0.02319	-1.46595	3.30523
H	-0.76041	1.26103	6.52313
H	-0.71875	2.66612	2.46781
H	1.43729	3.41714	-0.37317
H	2.53593	5.41160	-0.45477
H	2.04225	6.19568	1.85871
H	3.77211	6.25777	2.21902
H	3.08879	7.34185	0.99918
H	4.84238	4.77985	-1.13436
H	4.73642	6.50816	-0.75417
H	5.48023	5.39251	0.39758
H	4.79822	3.99745	2.22626
H	2.63499	0.29066	2.30987
H	-0.48262	2.07019	-2.97165
H	3.10694	0.23366	-1.51442
H	3.17529	2.44261	-5.18536
H	5.11534	1.51900	-4.45335
H	4.45479	0.51939	3.66656
H	6.32820	0.91377	2.07296
H	6.86617	1.06238	3.75581
H	6.60894	2.51184	2.77729
H	5.26227	1.91353	5.54854
H	3.59551	2.34423	5.12145
H	4.93626	3.38910	4.62952
H	0.10536	3.50809	6.85025
H	-0.19568	5.13000	6.21315
H	0.98700	4.07006	5.42295
H	-1.13346	4.17573	4.12780
H	-3.25741	3.26025	5.05514
H	-2.69330	4.65767	5.99058
H	-2.48242	3.02083	6.62618
H	1.53568	-2.29291	5.08132
H	1.40742	-2.62638	6.81641
H	1.97148	-1.04195	6.25234
H	-0.38431	-0.91971	7.03730
H	-2.20288	-2.14760	5.85953
H	-1.04537	-3.26493	6.60448
H	-1.00929	-2.98396	4.85904
H	3.30265	-5.89775	-0.67444
H	4.63145	-5.44014	-1.71979
H	3.17867	-3.59707	-2.70215
H	2.67124	-5.24845	-3.02462
H	5.00724	-4.47467	0.50442
H	4.70023	-3.15605	-0.63001
H	0.11132	-1.69546	-3.04017

H	0.98751	-5.05762	-1.15143
H	0.69489	-4.09182	-2.60348

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Complex 2

C	3.31126	0.79523	0.84328
C	2.03756	1.20347	0.43772
C	1.81112	2.57086	0.21921
C	2.81033	3.52320	0.42489
C	4.06631	3.08105	0.85556
C	4.33635	1.72514	1.06068
C	0.87556	0.28977	0.23112
C	0.30977	0.00753	-1.06073
C	-0.96964	-0.59635	-0.84911
C	-1.20378	-0.67125	0.55684
C	-0.06682	-0.12398	1.23437
Sc	0.81385	-2.19628	0.07338
O	1.97663	-3.33457	-1.23147
C	1.51756	-3.90411	-2.46792
C	1.68261	-2.95053	-3.63990
C	1.08415	-3.48456	-4.94598
C	1.67343	-4.80426	-5.44324
C	0.90960	0.43936	-2.34814
C	0.10720	0.96609	-3.36839
C	0.66270	1.42811	-4.56768
C	2.04622	1.36850	-4.72661
C	2.88528	0.86424	-3.72437
C	2.30187	0.39277	-2.54947
C	-2.02829	-0.88609	-1.85794
C	-2.03350	-2.02783	-2.66644
C	-3.06347	-2.26920	-3.58082
C	-4.09305	-1.32806	-3.68562
C	-4.12656	-0.17924	-2.89194
C	-3.08886	0.02247	-1.97573
C	-2.52990	-0.98608	1.15277
C	-3.17807	-2.21244	0.95927
C	-4.45587	-2.44275	1.47336
C	-5.08643	-1.42331	2.19856
C	-4.46678	-0.18978	2.41583
C	-3.19032	0.01235	1.87924
C	0.02560	0.04756	2.70661
C	-0.59427	-0.87567	3.57028
C	-0.61721	-0.68487	4.95280
C	0.03983	0.43308	5.48202
C	0.68559	1.35972	4.66153
C	0.65987	1.16098	3.27788
C	-0.21449	2.00658	-5.66508
C	-1.22314	0.98004	-6.19704
C	4.39066	0.89463	-3.94194
C	4.92525	2.32358	-3.74773
C	-3.08031	-3.53244	-4.42347

C	-3.02606	-3.22539	-5.92588
C	-5.28929	0.79279	-3.00578
C	-6.22443	0.67728	-1.79371
C	-5.14820	-3.77374	1.22943
C	-5.57095	-4.46461	2.53199
C	-5.13408	0.94454	3.18189
C	-5.74962	1.97028	2.21708
C	-1.36659	-1.61007	5.90265
C	-2.60531	-0.89568	6.46839
C	1.37364	2.58323	5.24416
C	0.35999	3.55404	5.86640
C	2.52763	4.99796	0.19205
C	2.66075	5.81534	1.48422
C	5.70348	1.26469	1.53773
C	5.94065	1.67086	2.99979
C	-0.91995	3.28946	-5.20391
C	5.17296	-0.08659	-3.06942
C	-4.28782	-4.41884	-4.08791
C	-4.83593	2.24221	-3.21503
C	-6.34313	-3.61208	0.27892
C	-6.17785	0.48322	4.20182
C	-1.77222	-2.95247	5.29469
C	2.46612	2.20847	6.25384
C	3.40815	5.57979	-0.92188
C	6.84154	1.76920	0.64194
H	-0.47972	-3.44902	0.30055
H	1.46087	-5.63707	-4.76581
H	0.45095	2.27789	-6.49611
H	-1.81275	1.40578	-7.01686
H	-0.71413	0.08702	-6.57323
H	-1.91896	0.66030	-5.41435
H	-1.50919	3.72401	-6.01933
H	-1.60136	3.08725	-4.37066
H	-0.19717	4.03972	-4.86795
H	4.40981	3.03663	-4.39873
H	4.77828	2.64800	-2.71198
H	5.99707	2.37261	-3.97162
H	4.81037	-1.11310	-3.17555
H	6.23277	-0.07170	-3.34488
H	5.10762	0.17563	-2.00848
H	-2.17696	-4.10183	-4.16806
H	-2.15254	-2.61624	-6.17627
H	-2.97575	-4.15224	-6.50786
H	-3.91782	-2.67866	-6.25166
H	-4.31179	-4.66926	-3.02312
H	-5.22929	-3.91543	-4.33413
H	-4.25212	-5.35317	-4.65892
H	-4.90186	-1.49433	-4.39539
H	-5.86346	0.49817	-3.89505
H	-6.60157	-0.34349	-1.68085
H	-5.70080	0.93891	-0.86880

H	-7.08276	1.35027	-1.90035
H	-4.19102	2.33523	-4.09413
H	-5.70194	2.89758	-3.35867
H	-4.28142	2.61973	-2.34913
H	-3.09462	0.89799	-1.33176
H	-2.65605	-2.99552	0.41644
H	-4.41702	-4.42545	0.73338
H	-4.71678	-4.60417	3.20144
H	-6.32569	-3.88099	3.07080
H	-6.00499	-5.44876	2.32311
H	-6.03273	-3.16175	-0.66872
H	-6.80485	-4.58243	0.06325
H	-7.11212	-2.96748	0.71971
H	-6.07857	-1.60217	2.60485
H	-4.33606	1.45689	3.73740
H	-5.00345	2.35744	1.51642
H	-6.55455	1.51268	1.63131
H	-6.17170	2.81961	2.76630
H	-5.77630	-0.27496	4.88131
H	-6.51719	1.33188	4.80482
H	-7.06366	0.06249	3.71264
H	-2.69133	0.96586	2.03813
H	-1.08433	-1.74244	3.14104
H	0.03802	0.57999	6.56092
H	1.12929	1.89795	2.63618
H	0.82522	2.89148	-0.10997
H	1.48355	5.07379	-0.13988
H	2.00343	5.42761	2.26876
H	3.68722	5.79093	1.86651
H	2.39812	6.86431	1.30787
H	3.28403	5.02274	-1.85517
H	3.14997	6.62758	-1.11156
H	4.46886	5.54434	-0.64966
H	4.85489	3.81014	1.02947
H	3.52278	-0.26310	0.97263
H	-0.96562	1.02292	-3.22023
H	2.93075	-0.02610	-1.77204
H	2.48820	1.72847	-5.65545
H	4.56448	0.61999	-4.99263
H	5.70733	0.16808	1.48879
H	6.68938	1.47426	-0.40033
H	7.80085	1.35927	0.97482
H	6.92453	2.86125	0.67228
H	6.90377	1.29180	3.35874
H	5.15487	1.27941	3.65312
H	5.94949	2.76151	3.10746
H	2.04489	1.70550	7.13139
H	2.98994	3.10348	6.60719
H	3.20499	1.53604	5.80748
H	1.86131	3.10254	4.40876
H	-0.40101	3.85197	5.13840

H	0.85958	4.45941	6.22894
H	-0.15525	3.09468	6.71745
H	-2.50513	-2.82442	4.49070
H	-2.23220	-3.58610	6.06019
H	-0.91287	-3.49199	4.88545
H	-0.69169	-1.81533	6.74645
H	-2.34150	0.04578	6.95935
H	-3.11829	-1.52866	7.20115
H	-3.31044	-0.66637	5.66248
H	2.74923	-2.73080	-3.77639
H	1.20769	-1.99437	-3.39687
H	-0.00070	-3.59563	-4.82203
H	1.21689	-2.71461	-5.71552
H	0.46151	-4.18507	-2.34758
H	2.06534	-4.83466	-2.64462
H	-1.23260	-2.75542	-2.56460
H	2.76116	-4.73815	-5.54779
H	1.26230	-5.06806	-6.42335
C	1.66059	-6.58784	2.13543
C	2.73144	-7.11561	1.40799
C	2.88207	-8.50936	1.35330
C	2.00074	-9.36823	2.01174
C	0.94779	-8.80468	2.74142
C	0.76227	-7.42114	2.81351
C	3.74215	-6.28520	0.69393
C	3.93033	-6.30585	-0.73144
C	5.15083	-5.61755	-1.01767
C	5.72934	-5.19776	0.21836
C	4.86401	-5.61077	1.28309
Sc	3.52977	-3.89895	0.00539
O	2.32906	-2.83549	1.32504
C	2.74675	-2.34570	2.61087
C	2.29769	-3.24278	3.75114
C	2.65485	-2.63861	5.10928
C	2.33244	-3.56161	6.28086
C	3.10828	-7.10770	-1.67301
C	3.73521	-7.89671	-2.64605
C	3.00108	-8.74639	-3.48176
C	1.61684	-8.79592	-3.32639
C	0.94947	-8.02061	-2.36861
C	1.70765	-7.18048	-1.55240
C	5.86771	-5.53606	-2.32061
C	5.44826	-4.72996	-3.38591
C	6.16268	-4.68383	-4.58762
C	7.30594	-5.48037	-4.71322
C	7.75457	-6.29776	-3.67376
C	7.02710	-6.30679	-2.47950
C	7.12983	-4.71388	0.35464
C	7.59362	-3.53868	-0.24392
C	8.93907	-3.16365	-0.16036
C	9.82447	-3.98877	0.54059

C	9.39376	-5.17106	1.15422
C	8.04555	-5.51923	1.04856
C	5.20871	-5.48449	2.72146
C	5.90911	-4.35962	3.19544
C	6.40692	-4.30318	4.49980
C	6.15737	-5.38680	5.35158
C	5.43931	-6.50749	4.92803
C	4.97552	-6.54418	3.60988
C	3.69298	-9.62182	-4.51286
C	4.45319	-8.79044	-5.55392
C	-0.56621	-8.12283	-2.27535
C	-1.14762	-7.65415	-0.94143
C	5.73087	-3.77235	-5.72419
C	5.46539	-4.54684	-7.02221
C	9.02121	-7.12133	-3.83709
C	10.17835	-6.51408	-3.03140
C	9.41754	-1.89423	-0.84622
C	10.23210	-0.98637	0.08296
C	10.35264	-6.05002	1.94178
C	11.56688	-6.49150	1.11524
C	7.26901	-3.15319	5.01189
C	7.74850	-2.19458	3.92186
C	5.23028	-7.70415	5.84274
C	6.55573	-8.42953	6.11755
C	2.18227	-10.87410	1.91971
C	2.33294	-11.52704	3.29977
C	-0.37741	-6.82830	3.62520
C	-0.19997	-7.11078	5.12378
C	4.61293	-10.65637	-3.84955
C	-1.23520	-7.38431	-3.44499
C	6.75454	-2.65268	-5.96110
C	8.81847	-8.59894	-3.48121
C	10.20544	-2.21955	-2.12371
C	10.79631	-5.36446	3.24193
C	6.58543	-2.37369	6.14524
C	4.52862	-7.33097	7.15420
C	1.04432	-11.52550	1.12111
C	-1.75105	-7.30559	3.13735
H	4.73333	-2.56675	-0.24885
H	2.90051	-4.49485	6.20943
H	2.90507	-10.17509	-5.04226
H	4.90091	-9.43948	-6.31504
H	3.78507	-8.08539	-6.05813
H	5.25887	-8.21082	-5.09141
H	5.05864	-11.31832	-4.60052
H	5.43088	-10.16934	-3.30746
H	4.06171	-11.27501	-3.13428
H	-0.66940	-8.15468	-0.09450
H	-1.02905	-6.57341	-0.80373
H	-2.22072	-7.87002	-0.90411
H	-0.86887	-7.74247	-4.41205

H	-2.32210	-7.52043	-3.42017
H	-1.02884	-6.30993	-3.38680
H	4.78854	-3.29843	-5.41912
H	4.72886	-5.34156	-6.87223
H	5.08960	-3.87514	-7.80179
H	6.38184	-5.01165	-7.40208
H	6.92766	-2.07471	-5.04889
H	7.71754	-3.06278	-6.28527
H	6.40581	-1.96643	-6.74097
H	7.87098	-5.46094	-5.64338
H	9.29659	-7.07501	-4.89972
H	10.37993	-5.48514	-3.34348
H	9.94149	-6.49107	-1.96263
H	11.09557	-7.09857	-3.16642
H	8.00810	-9.04319	-4.06741
H	9.73264	-9.16919	-3.67917
H	8.57662	-8.72802	-2.42060
H	7.36026	-6.91888	-1.64601
H	6.88060	-2.90544	-0.76459
H	8.51925	-1.33873	-1.14548
H	9.67398	-0.74482	0.99278
H	11.17392	-1.45775	0.38482
H	10.48545	-0.04780	-0.42214
H	9.60664	-2.82406	-2.81145
H	10.50293	-1.30145	-2.64331
H	11.11656	-2.78198	-1.88959
H	10.87216	-3.70510	0.61324
H	9.79766	-6.95562	2.22146
H	11.26131	-7.01583	0.20487
H	12.18212	-5.63577	0.81603
H	12.20434	-7.16563	1.69807
H	9.93334	-5.09803	3.85929
H	11.44586	-6.02415	3.82842
H	11.35541	-4.44569	3.03182
H	7.69336	-6.43447	1.51889
H	6.11313	-3.54790	2.50492
H	6.56253	-5.36242	6.36201
H	4.45935	-7.43147	3.25808
H	3.70733	-8.92551	0.78007
H	3.11488	-11.05010	1.36717
H	3.16191	-11.08436	3.86072
H	1.42375	-11.40915	3.89930
H	2.52445	-12.60106	3.19997
H	0.96662	-11.08981	0.12052
H	1.21168	-12.60312	1.01388
H	0.08042	-11.38606	1.62322
H	0.25402	-9.45972	3.26451
H	1.51349	-5.51186	2.16961
H	4.81604	-7.86585	-2.73352
H	1.21583	-6.58015	-0.79374
H	1.03683	-9.46527	-3.96119

H	-0.81068	-9.18964	-2.38459
H	-0.33906	-5.74066	3.48418
H	-1.89967	-7.06967	2.07995
H	-2.55064	-6.82282	3.70964
H	-1.86569	-8.38846	3.26044
H	-0.99300	-6.62803	5.70544
H	0.76335	-6.73997	5.48639
H	-0.24329	-8.18597	5.33111
H	5.13169	-6.63613	7.74894
H	4.35673	-8.22342	7.76598
H	3.56032	-6.85722	6.96713
H	4.57532	-8.40366	5.30675
H	7.04090	-8.73375	5.18489
H	6.39014	-9.32609	6.72552
H	7.25403	-7.78275	6.66059
H	5.72430	-1.81304	5.76697
H	7.28103	-1.65385	6.59081
H	6.22916	-3.03537	6.94025
H	8.16412	-3.62401	5.44561
H	8.26901	-2.71871	3.11500
H	8.43721	-1.45798	4.34893
H	6.91185	-1.64081	3.48119
H	2.76846	-4.22763	3.64909
H	1.21229	-3.38822	3.67947
H	3.72707	-2.40909	5.12341
H	2.12731	-1.68461	5.23073
H	2.33935	-1.33773	2.74993
H	3.84203	-2.25963	2.61200
H	4.55874	-4.11503	-3.27145
H	1.26767	-3.81814	6.30708
H	2.58364	-3.09173	7.23758

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Complex 1 - 2nd xyl. dimer

C	12.71329	15.46700	1.54137
C	11.96140	14.45722	2.16855
C	11.85923	13.15874	1.63808
C	12.54935	12.85987	0.45847
C	13.22894	13.86417	-0.26975
C	13.32658	15.13507	0.29844
C	10.94715	12.10842	2.25007
H	11.48850	11.15441	2.19818
C	10.57720	12.36367	3.70894
H	10.01747	11.51044	4.10571
H	11.47493	12.51665	4.31481
H	9.93821	13.24657	3.81632
C	9.68058	11.96817	1.38726
H	9.03352	11.17806	1.78313
H	9.10976	12.90349	1.38696
H	9.92035	11.72286	0.34800
C	12.62757	12.98061	-2.54236

H	12.17871	12.07667	-2.12270
H	11.83083	13.72267	-2.66862
H	13.01351	12.72851	-3.53555
C	14.39380	14.73574	-2.37760
H	15.23632	15.15437	-1.82413
H	14.76628	14.42301	-3.35788
H	13.66725	15.54004	-2.53698
C	12.96098	16.78314	2.17829
C	12.79309	17.09798	3.57751
C	13.43404	18.34881	3.82359
C	13.96310	18.82766	2.57747
C	13.63058	17.89050	1.56153
C	11.77744	16.48823	4.48302
C	12.05639	15.67897	5.58752
H	13.08438	15.38268	5.76529
C	11.03537	15.22423	6.43044
C	11.35908	14.37707	7.64961
H	12.39585	14.03676	7.53464
C	10.47727	13.12773	7.76232
H	10.52532	12.52231	6.85266
H	10.80238	12.50689	8.60382
H	9.42743	13.38706	7.93790
C	11.28201	15.21548	8.93418
H	11.94624	16.08327	8.88028
H	10.26337	15.58506	9.09839
H	11.56716	14.61878	9.80796
C	9.71601	15.59028	6.14201
H	8.91102	15.25033	6.79061
C	9.39467	16.37518	5.03114
C	7.94998	16.73982	4.73113
H	7.33541	16.28908	5.52228
C	7.71985	18.25649	4.77671
H	8.01609	18.67400	5.74399
H	8.29849	18.76949	4.00080
H	6.66269	18.49341	4.61355
C	7.48121	16.15356	3.39248
H	7.59722	15.06543	3.37380
H	6.42524	16.38605	3.21534
H	8.05726	16.56559	2.55669
C	10.43851	16.81493	4.21249
H	10.22594	17.43931	3.34778
C	13.45807	19.13848	5.08124
C	14.58906	19.90128	5.41987
H	15.45715	19.87452	4.76758
C	14.62117	20.72209	6.54942
C	15.84330	21.57908	6.83716
H	16.64223	21.23368	6.16685
C	15.56894	23.05198	6.49901
H	15.25720	23.16429	5.45655
H	14.77177	23.45571	7.13362
H	16.46502	23.66275	6.65878

C	16.35273	21.43542	8.27635
H	16.55725	20.39030	8.52735
H	17.27693	22.00714	8.41497
H	15.62407	21.81498	9.00095
C	13.49092	20.77167	7.37024
H	13.49695	21.41271	8.24909
C	12.34773	20.02411	7.07422
C	11.10521	20.11451	7.94544
H	10.39620	19.36534	7.56921
C	11.39246	19.77760	9.41407
H	11.84820	18.78783	9.51287
H	12.07414	20.50592	9.86715
H	10.46673	19.78626	9.99997
C	10.43727	21.49152	7.81950
H	10.19479	21.71979	6.77701
H	9.51057	21.53130	8.40327
H	11.09808	22.28412	8.18813
C	12.34409	19.21914	5.93165
H	11.44564	18.66241	5.69031
C	14.38415	20.23267	2.31924
C	15.69480	20.61479	2.01867
H	16.46115	19.84409	1.97705
C	16.01807	21.95772	1.77112
C	17.44579	22.40688	1.50063
C	18.29047	22.37306	2.78249
C	18.12077	21.61830	0.37389
C	14.99624	22.90862	1.81062
H	15.24528	23.94939	1.60935
C	13.67094	22.55945	2.09703
C	12.56454	23.60055	2.10925
C	12.80143	24.68351	3.16986
C	13.38772	21.21984	2.35678
H	12.36727	20.92328	2.58811
C	13.59982	18.22163	0.11536
C	12.34506	18.19490	-0.51630
H	11.47906	17.86654	0.05411
C	12.17846	18.59856	-1.84128
C	10.80041	18.58897	-2.48214
H	10.11138	18.14170	-1.75296
C	10.30668	20.01437	-2.76857
H	10.30443	20.62193	-1.85839
H	10.94995	20.51496	-3.50082
H	9.28858	20.00044	-3.17388
C	10.75280	17.72659	-3.74993
H	11.07207	16.70015	-3.54442
H	9.73601	17.69154	-4.15654
H	11.40659	18.12883	-4.53171
C	13.30275	19.04842	-2.54115
H	13.18792	19.38521	-3.56946
C	14.56734	19.08855	-1.94682
C	15.76246	19.62979	-2.71339

C	15.62368	21.14196	-2.94466
C	14.70527	18.66266	-0.62011
H	15.68008	18.65933	-0.14213
C	17.07860	14.73613	3.80652
C	16.45222	15.05712	5.04551
C	16.54106	16.32304	5.62591
C	17.22920	17.33319	4.91392
C	17.93325	17.04427	3.74010
C	17.83812	15.75053	3.19651
C	15.98444	16.63004	7.01360
H	15.19806	17.38884	6.89749
C	17.08200	17.23429	7.90707
H	17.50180	18.15532	7.49490
H	16.67276	17.47123	8.89464
H	17.90395	16.52264	8.04418
C	15.38595	15.41475	7.72087
H	14.56625	14.96297	7.15901
H	16.14027	14.63779	7.88681
H	14.99136	15.71294	8.69704
C	18.85219	18.10070	3.14954
H	18.31292	19.05530	3.21199
C	20.11330	18.22492	4.02281
H	20.76509	19.01912	3.64313
H	19.86702	18.45535	5.06396
H	20.68164	17.28816	4.01285
C	19.23098	17.86588	1.68959
H	18.33687	17.72254	1.07604
H	19.79458	18.72370	1.30861
H	19.86909	16.98343	1.57369
C	16.83505	13.42491	3.15810
C	16.17227	12.30928	3.76725
C	15.84196	11.37926	2.74441
C	16.36394	11.87217	1.50008
C	17.00012	13.12372	1.75584
C	16.20833	11.96973	5.21196
C	17.46313	11.99489	5.83909
H	18.32292	12.32346	5.26058
C	17.62947	11.59093	7.16676
C	18.99774	11.60455	7.82812
C	16.50590	11.14574	7.86593
H	16.62883	10.81432	8.89576
C	15.23821	11.10517	7.27369
C	14.04356	10.56996	8.04456
H	13.15908	10.72164	7.41242
C	14.18479	9.06098	8.29419
H	14.33855	8.51797	7.35683
H	15.04218	8.85019	8.94332
H	13.29005	8.66026	8.78435
C	13.80750	11.31805	9.36278
H	13.69224	12.39340	9.19686
H	12.90298	10.94872	9.85881

H	14.64172	11.17721	10.05908
C	15.10103	11.52925	5.94858
H	14.12635	11.53554	5.47045
C	15.42435	9.97079	2.99025
C	16.41599	8.98342	2.92006
H	17.43161	9.28864	2.68215
C	16.12769	7.63769	3.15589
C	17.21537	6.57760	3.11690
C	17.93682	6.53187	1.76390
H	17.23254	6.37374	0.94181
H	18.47179	7.46668	1.56530
H	18.67187	5.71941	1.74652
C	14.80712	7.29149	3.45496
C	13.78807	8.24581	3.53153
C	12.36384	7.79413	3.81511
C	11.69561	8.58218	4.94601
H	12.27870	8.52063	5.86916
H	11.58704	9.64071	4.68956
H	10.69386	8.18774	5.15009
C	11.50904	7.82405	2.53966
C	14.11443	9.58932	3.30465
C	16.32822	11.09944	0.23209
C	15.20330	10.32109	-0.09192
H	14.35008	10.32264	0.58002
C	15.15787	9.51746	-1.23325
C	16.26738	9.50301	-2.08316
H	16.25133	8.87673	-2.97236
C	17.40256	10.26920	-1.80430
C	19.32047	8.85898	-2.63887
C	17.42118	11.05437	-0.64811
H	18.31487	11.62461	-0.42178
C	18.00913	13.74932	0.85332
C	17.72400	14.59121	-0.22486
H	16.69701	14.90424	-0.37840
C	18.73876	15.05926	-1.06815
C	18.40667	15.93788	-2.26248
H	17.37612	16.28847	-2.12302
C	19.30275	17.17795	-2.36319
H	19.27766	17.76467	-1.44053
H	20.34612	16.90934	-2.56182
H	18.97208	17.82023	-3.18618
C	18.45392	15.12646	-3.56580
H	17.78017	14.26566	-3.52048
H	18.16341	15.74523	-4.42228
H	19.46558	14.74863	-3.75286
C	20.05839	14.67512	-0.80539
H	20.85857	15.02500	-1.45464
C	20.38633	13.85920	0.28099
C	21.83186	13.47877	0.55659
H	22.43959	13.93490	-0.23673
C	22.05038	11.96131	0.48943

H	21.73566	11.55708	-0.47764
H	23.10837	11.71525	0.63252
H	21.48132	11.44278	1.26872
C	22.32183	14.04513	1.89629
H	23.37774	13.80169	2.05828
H	22.21529	15.13391	1.92914
H	21.75172	13.62803	2.73367
C	19.34842	13.40543	1.09952
H	19.56597	12.75664	1.94474
Sc	15.24647	16.60775	3.12736
Sc	14.54671	13.59882	2.21673
H	14.40359	14.92822	3.56353
H	15.38531	15.27998	1.78024
H	11.47548	14.67022	3.10781
H	13.89566	15.89938	-0.21021
H	18.33723	15.54442	2.26248
H	12.49374	11.85296	0.05415
H	17.28049	18.33695	5.32601
H	15.87825	14.28716	5.53968
C	13.75938	13.54315	-1.66387
C	12.36082	24.22229	0.72068
C	15.99537	18.89748	-4.04085
C	19.97404	10.64514	7.13349
C	19.58338	13.02039	7.91061
C	18.21509	6.76257	4.26752
H	17.70864	6.75476	5.23759
H	18.96371	5.96228	4.26446
H	18.74456	7.71730	4.17719
C	13.94511	8.64085	-1.50122
C	13.40709	8.77630	-2.93061
C	14.25092	7.17281	-1.16834
H	14.57900	7.06650	-0.13018
H	13.36399	6.54580	-1.31588
H	15.04651	6.78466	-1.81456
C	18.62035	10.22360	-2.71318
C	18.28079	10.58671	-4.16436
H	17.79809	11.56672	-4.22626
H	19.18788	10.61510	-4.77816
H	17.60346	9.85205	-4.61375
H	19.32473	10.97936	-2.34149
H	19.60011	8.61318	-1.60981
H	20.22934	8.85162	-3.25135
H	18.66540	8.06034	-3.00467
H	13.18119	9.81808	-3.17725
H	12.48958	8.19005	-3.05172
H	14.12748	8.40790	-3.66916
H	12.42433	6.74601	4.13889
H	10.50119	7.44005	2.73470
H	11.95859	7.21666	1.74814
H	11.40984	8.84659	2.15930
H	13.35364	10.36378	3.37028

H	14.56401	6.24516	3.63724
H	16.72152	5.60680	3.26127
H	19.74181	13.44239	6.91225
H	20.55039	13.01198	8.42604
H	18.91444	13.69440	8.45490
H	20.93078	10.61098	7.66669
H	20.17844	10.96368	6.10534
H	19.56845	9.62968	7.09261
H	18.85895	11.24437	8.85674
H	14.51869	12.75594	-1.55822
H	16.64752	19.46911	-2.08434
H	16.10502	17.81952	-3.88895
H	16.90177	19.26881	-4.53197
H	15.16245	19.05150	-4.73590
H	16.51906	21.54735	-3.42982
H	15.47010	21.67380	-2.00096
H	14.76676	21.36158	-3.59149
H	13.25303	24.77021	0.39763
H	11.52289	24.92845	0.73047
H	12.15261	23.45379	-0.03001
H	11.63701	23.07610	2.37556
H	12.91076	24.24415	4.16590
H	11.96251	25.38784	3.19716
H	13.70869	25.25948	2.95590
H	18.22244	20.55890	0.62951
H	19.12588	22.00894	0.17909
H	17.54590	21.68406	-0.55409
H	17.39051	23.45549	1.17755
H	17.83609	22.98002	3.57157
H	19.30057	22.75523	2.59576
H	18.38501	21.34978	3.16192
H	13.15261	8.97221	-0.81636
H	16.16846	17.17846	1.66270
H	13.63895	13.02293	3.68820

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Complex 3

La	11.22872	11.61988	1.15480
C	12.25879	11.02726	-1.15971
C	10.92614	10.68793	-1.58344
C	10.19513	9.64892	-0.94833
C	8.85451	9.38940	-1.26544
C	8.15866	10.15606	-2.19467
C	8.86664	11.20830	-2.81052
C	10.18964	11.47490	-2.51336
C	14.59541	14.87967	-0.17913
C	15.36544	13.55755	-0.17247
C	14.59541	12.73206	0.85318
C	12.46540	10.08838	3.19447
C	12.19844	11.30400	3.91543
C	10.79161	11.36627	4.18426

C	10.18594	10.19859	3.63275
C	11.20949	9.39778	3.04492
C	8.89853	12.59452	0.86847
C	9.38993	13.95534	0.72927
C	9.88841	14.68572	1.83901
C	10.35094	15.99838	1.70626
C	10.38328	16.64517	0.46895
C	9.96043	15.90384	-0.64897
C	9.49833	14.60197	-0.53144
C	6.72585	9.87222	-2.55927
C	13.74107	9.62822	2.58312
C	15.00607	9.99598	3.07225
C	16.18815	9.57310	2.45109
C	16.10169	8.74477	1.33310
C	14.86708	8.31841	0.82878
C	13.70813	8.78485	1.44783
C	13.17429	12.25752	4.52291
C	13.30920	13.58480	4.09759
C	14.14844	14.48641	4.75970
C	14.84620	14.04414	5.88787
C	14.72848	12.73263	6.35742
C	13.89741	11.85096	5.65660
C	10.07001	12.33823	5.04444
C	8.77531	12.76802	4.71147
C	8.04229	13.63138	5.52775
C	8.61856	14.06876	6.72293
C	9.89722	13.65187	7.10365
C	10.60789	12.79570	6.25843
C	8.82197	9.71108	3.98519
C	7.72939	9.75790	3.11507
C	6.46354	9.30292	3.51122
C	6.31715	8.77368	4.79407
C	7.39307	8.69643	5.68717
C	8.63302	9.17566	5.26781
C	11.03858	7.94499	2.78221
C	11.87362	7.03757	3.45348
C	11.70022	5.65654	3.34744
C	10.66583	5.17523	2.53821
C	9.81311	6.04499	1.85237
C	10.01092	7.42312	1.98513
C	17.55594	9.94297	3.00330
C	17.71602	11.44292	3.27370
C	14.85867	7.31935	-0.32077
C	15.27903	5.93340	0.19777
C	14.26864	15.92159	4.27501
C	15.72178	16.31464	3.97758
C	15.44760	12.30841	7.62905
C	14.45543	12.02016	8.76461
C	6.64832	14.07361	5.11562
C	5.58204	13.58237	6.10408
C	10.49778	14.08977	8.42954

C	10.61901	15.61499	8.53868
C	5.26389	9.39817	2.58294
C	4.90990	10.85682	2.26138
C	7.22300	8.10813	7.07725
C	6.24007	8.92464	7.92722
C	12.57498	4.72035	4.16610
C	11.83437	4.26158	5.43198
C	8.68010	5.50840	0.99344
C	7.65679	4.72962	1.83142
C	10.82957	18.07703	0.33083
C	17.87775	9.11213	4.25414
C	13.53737	7.21255	-1.08224
C	13.62651	16.90348	5.26509
C	16.38442	11.11529	7.41138
C	6.56552	15.59342	4.92005
C	9.71508	13.51383	9.61814
C	5.45984	8.58602	1.29694
C	6.81153	6.63054	7.02178
C	13.09120	3.51504	3.37307
C	9.19675	4.66147	-0.17718
H	18.29108	9.67018	2.23365
H	18.72953	11.66300	3.62712
H	17.54437	12.02830	2.36446
H	17.01598	11.79864	4.03674
H	18.88321	9.33851	4.62686
H	17.16427	9.32264	5.05693
H	17.82740	8.04054	4.03740
H	16.25225	5.96551	0.69681
H	14.54438	5.56341	0.92082
H	15.34039	5.21283	-0.62538
H	13.21638	8.17436	-1.49259
H	13.64752	6.51582	-1.91973
H	12.73509	6.82504	-0.44460
H	13.70632	15.98833	3.33415
H	16.18402	15.62609	3.26302
H	15.77123	17.32618	3.55966
H	16.33272	16.30559	4.88685
H	12.57613	16.65375	5.44221
H	14.14253	16.88199	6.23137
H	13.67545	17.92964	4.88383
H	15.48953	14.73656	6.42791
H	16.06723	13.15979	7.94197
H	13.81870	12.88712	8.96489
H	13.80375	11.17583	8.51451
H	14.98650	11.76829	9.68929
H	17.13091	11.33054	6.64149
H	16.91468	10.86773	8.33744
H	15.82853	10.22310	7.10288
H	13.76917	10.82990	6.00949
H	8.31828	12.40841	3.79645
H	6.43917	13.60554	4.14503

H	5.61766	12.49418	6.21291
H	5.72704	14.02301	7.09690
H	4.57855	13.86046	5.76248
H	7.30112	15.93710	4.18656
H	5.57023	15.88478	4.56625
H	6.75231	16.12667	5.85909
H	8.05832	14.73727	7.37341
H	11.51360	13.67570	8.47130
H	11.20818	16.02472	7.71282
H	9.63547	16.09742	8.51873
H	11.10570	15.89903	9.47858
H	9.65778	12.42240	9.56205
H	10.19220	13.78323	10.56733
H	8.68964	13.89933	9.63996
H	11.59300	12.46203	6.56487
H	7.86562	10.17271	2.11925
H	5.33612	8.41601	5.10282
H	9.48036	9.13565	5.94811
H	12.66422	7.42652	4.09019
H	13.44904	5.30244	4.48791
H	11.50610	5.11756	6.02949
H	10.94437	3.67758	5.17155
H	12.47894	3.63316	6.05722
H	13.61743	3.82585	2.46567
H	13.78482	2.92603	3.98290
H	12.27578	2.84686	3.07500
H	10.51217	4.10230	2.44930
H	9.33749	8.10438	1.47358
H	15.06906	10.62354	3.95195
H	12.74590	8.46809	1.06172
H	17.01811	8.40682	0.85040
H	15.62799	7.65078	-1.03352
H	8.16058	6.37768	0.56897
H	9.89649	5.22807	-0.79916
H	8.36757	4.33021	-0.81231
H	9.71777	3.76660	0.18071
H	6.81196	4.40772	1.21205
H	7.26956	5.34364	2.65007
H	8.10470	3.83169	2.27155
H	5.82991	6.50997	6.55004
H	6.74890	6.20663	8.03033
H	7.53194	6.04084	6.44664
H	8.20442	8.15954	7.56740
H	6.55192	9.97127	7.99543
H	6.17633	8.51948	8.94341
H	5.23181	8.90334	7.49874
H	6.29120	8.98334	0.70496
H	4.56025	8.62606	0.67248
H	5.67389	7.53614	1.51936
H	4.41049	8.96246	3.12029
H	4.72950	11.42987	3.17607

H	4.00656	10.91020	1.64317
H	5.71889	11.34956	1.71111
H	8.34132	12.42184	1.79009
H	8.36802	12.20768	-0.00379
H	9.15450	14.07025	-1.41507
H	9.98050	16.37039	-1.63293
H	9.81698	14.25318	2.83578
H	10.67377	16.53421	2.59728
H	9.98852	18.73774	0.08598
H	11.57110	18.19845	-0.46747
H	11.27509	18.44763	1.25885
H	10.71850	8.94954	-0.29424
H	10.70220	12.28528	-3.02735
H	8.35553	8.54785	-0.78908
H	8.35894	11.82127	-3.55397
H	6.33750	9.01187	-2.00717
H	6.61880	9.65441	-3.62890
H	6.07407	10.72652	-2.34036
H	15.31693	13.08522	-1.15931
H	16.41884	13.66832	0.09819
H	14.87897	15.49776	0.67964
H	14.74823	15.46581	-1.08928
H	12.89618	10.18720	-0.87470
H	12.78668	11.74987	-1.78287
H	14.56674	11.66546	0.61677
H	14.98230	12.86016	1.86849
H	12.74596	13.93021	3.23470
C	13.16088	14.39756	-0.03845
H	12.75325	14.07542	-1.00439
H	12.47656	15.11751	0.41313
O	13.23888	13.25011	0.83899

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Complex 3 - THF

La	10.44700	11.97112	1.99709
C	8.05038	12.77322	1.36928
C	8.71918	14.04720	1.29601
C	9.31916	14.63298	2.44835
C	10.12489	15.78035	2.36518
C	10.40852	16.38848	1.14739
C	9.84989	15.79731	-0.00441
C	9.05281	14.66895	0.05844
C	11.25937	17.62570	1.04648
C	12.19172	11.90668	0.11156
C	11.11394	11.43353	-0.72806
C	10.39780	10.24750	-0.41008
C	9.26654	9.84542	-1.13728
C	8.76963	10.60227	-2.19105
C	9.45622	11.79466	-2.49934
C	10.57047	12.20481	-1.79195
C	7.56597	10.17401	-2.98693

C	12.22678	9.99993	3.40190
C	11.99913	11.14816	4.21935
C	10.61755	11.15384	4.62575
C	10.00163	9.99256	4.03908
C	10.99245	9.28392	3.30076
C	13.52399	9.52700	2.85788
C	14.69429	9.57292	3.62943
C	15.90661	9.06357	3.15077
C	15.94057	8.51279	1.86895
C	14.79825	8.45067	1.06375
C	13.60175	8.94975	1.57827
C	13.05930	12.15735	4.50387
C	13.54434	12.98719	3.48392
C	14.57282	13.90759	3.70705
C	15.13876	13.96618	4.98427
C	14.70473	13.13741	6.02399
C	13.65894	12.24337	5.76871
C	9.87391	12.20269	5.37044
C	8.48885	12.37015	5.16306
C	7.74060	13.34262	5.83035
C	8.39380	14.18623	6.73127
C	9.76565	14.06202	6.96776
C	10.48528	13.07546	6.28908
C	8.67952	9.41221	4.40645
C	7.59493	9.35707	3.52418
C	6.37090	8.79102	3.90526
C	6.25655	8.26420	5.19302
C	7.32137	8.29684	6.10200
C	8.52124	8.87880	5.69328
C	10.86968	7.87178	2.85524
C	11.73043	6.92095	3.42508
C	11.65546	5.56812	3.09450
C	10.69452	5.16300	2.16171
C	9.81241	6.07635	1.57919
C	9.91024	7.42505	1.93907
C	17.16868	9.09955	3.99641
C	16.98010	8.41370	5.35551
C	14.90592	7.89585	-0.34785
C	15.26657	9.01766	-1.33557
C	15.08240	14.78351	2.57559
C	15.03623	16.27494	2.93108
C	15.35844	13.23163	7.39439
C	15.83276	11.87300	7.92378
C	6.24882	13.47337	5.57140
C	5.88416	14.84797	4.99412
C	10.46671	14.97676	7.95819
C	9.92633	14.79297	9.38292
C	5.17519	8.77716	2.96663
C	5.49208	8.14232	1.60788
C	7.18660	7.70741	7.49531
C	6.93402	6.19419	7.44870

C	12.59859	4.56695	3.74015
C	13.56367	3.95623	2.71479
C	8.77462	5.62083	0.56678
C	9.42957	5.12973	-0.73178
C	17.68901	10.53364	4.16314
C	13.65837	7.14305	-0.81869
C	16.49215	14.36274	2.13666
C	14.43426	13.91721	8.41010
C	5.42878	13.16953	6.83266
C	10.39408	16.44803	7.52748
C	4.58957	10.18564	2.78849
C	6.10775	8.42301	8.31915
C	11.84045	3.47415	4.50537
C	7.83298	4.55580	1.14449
H	17.93434	8.53315	3.44880
H	18.61324	10.54873	4.75249
H	17.89891	10.99056	3.19104
H	16.95099	11.16436	4.66974
H	17.92476	8.38782	5.91010
H	16.24856	8.94409	5.97442
H	16.62879	7.38421	5.23393
H	13.35120	6.37775	-0.09988
H	12.81125	7.82042	-0.97116
H	13.85398	6.65360	-1.77878
H	16.19280	9.52237	-1.04300
H	15.39976	8.61884	-2.34772
H	14.47154	9.77049	-1.36879
H	14.40970	14.62656	1.72214
H	16.51682	13.30825	1.84668
H	16.82637	14.96113	1.28190
H	17.21549	14.50450	2.94728
H	14.02872	16.58183	3.22754
H	15.71515	16.51157	3.75765
H	15.34004	16.88391	2.07287
H	15.95144	14.66347	5.17923
H	16.24634	13.86731	7.27714
H	14.12493	14.90723	8.06099
H	13.53067	13.32131	8.58026
H	14.93874	14.03862	9.37508
H	16.51753	11.38761	7.22259
H	16.35585	11.99618	8.87824
H	14.99159	11.19338	8.09845
H	13.31081	11.57608	6.55377
H	7.97149	11.71778	4.46889
H	5.98679	12.71824	4.81912
H	5.65722	12.17291	7.22211
H	5.63693	13.89558	7.62654
H	4.35568	13.21416	6.61612
H	6.43951	15.05534	4.07440
H	4.81430	14.89723	4.76332
H	6.10519	15.65057	5.70671

H	7.82582	14.94929	7.25884
H	11.52509	14.68916	7.96666
H	10.82045	16.59010	6.52954
H	9.35882	16.80563	7.50170
H	10.94692	17.08460	8.22733
H	10.00198	13.74955	9.70430
H	10.48716	15.41072	10.09310
H	8.87262	15.08574	9.44973
H	11.54508	12.98649	6.48864
H	7.69959	9.78903	2.53044
H	5.30875	7.81943	5.49202
H	9.36160	8.91831	6.38218
H	12.47312	7.25137	4.14633
H	13.20281	5.12246	4.46964
H	11.16672	3.90693	5.25133
H	11.23722	2.85857	3.82879
H	12.53983	2.80733	5.02198
H	14.14004	4.73456	2.20587
H	14.26828	3.27331	3.20257
H	13.02202	3.38586	1.95183
H	10.62802	4.11182	1.88885
H	9.22063	8.13865	1.49680
H	14.64890	9.99391	4.62848
H	12.69973	8.87755	0.98146
H	16.88010	8.11455	1.48705
H	15.74114	7.18125	-0.34227
H	8.16229	6.49797	0.31733
H	10.06762	5.90231	-1.17139
H	8.66941	4.85212	-1.47074
H	10.05340	4.24777	-0.54872
H	7.04639	4.30341	0.42470
H	7.35691	4.90492	2.06584
H	8.37214	3.63156	1.37957
H	5.97633	5.96621	6.96769
H	6.90464	5.77493	8.46060
H	7.71943	5.67911	6.88725
H	8.14757	7.86570	8.00285
H	6.30786	9.49688	8.38462
H	6.06768	8.02073	9.33751
H	5.11527	8.29410	7.87335
H	6.22119	8.73811	1.04798
H	4.58665	8.07528	0.99466
H	5.89903	7.13391	1.72615
H	4.40415	8.15866	3.44598
H	4.31503	10.62459	3.75277
H	3.69244	10.15829	2.15980
H	5.31256	10.85407	2.30811
H	7.44420	12.60744	2.26252
H	7.57348	12.42621	0.45319
H	8.64442	14.24804	-0.85569
H	10.04596	16.24835	-0.97602

H	9.05497	14.25334	3.43559
H	10.52100	16.20700	3.28447
H	10.71660	18.44750	0.56426
H	12.16416	17.44952	0.45211
H	11.57477	17.97394	2.03418
H	10.79850	9.55904	0.33598
H	11.07229	13.12876	-2.06831
H	8.78290	8.90583	-0.87817
H	9.10211	12.40796	-3.32670
H	7.14243	9.24317	-2.59894
H	7.81887	10.00815	-4.04119
H	6.77498	10.93295	-2.96377
H	12.88750	11.14443	0.46883
H	12.70546	12.79931	-0.24934
H	13.15940	12.88349	2.46663

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Complex 3 - THF + H2

La	-1.58271	-0.77513	0.28158
C	-1.74601	-1.90595	2.61291
C	-3.04343	-1.28905	2.58255
C	-3.20687	0.12095	2.68624
C	-4.46085	0.73585	2.54487
C	-5.60218	0.00825	2.22112
C	-5.43510	-1.37568	2.02081
C	-4.20936	-2.00114	2.17650
C	-6.95243	0.65766	2.07885
C	-2.43139	-1.90361	-1.87592
C	-2.69010	-3.11927	-1.12757
C	-1.67222	-3.73945	-0.36061
C	-1.92122	-4.87339	0.42486
C	-3.18932	-5.43705	0.50628
C	-4.21843	-4.81021	-0.22730
C	-3.98690	-3.68657	-0.99780
C	-3.46208	-6.67321	1.32140
C	0.83758	-0.25905	-1.26973
C	0.18504	0.99986	-1.11858
C	0.25568	1.38379	0.26083
C	0.96694	0.35680	0.96568
C	1.29904	-0.66639	0.02477
C	1.19910	-0.90692	-2.55692
C	1.77293	-0.13470	-3.57619
C	2.21317	-0.71218	-4.77216
C	2.05073	-2.08698	-4.94543
C	1.47312	-2.89333	-3.95758
C	1.06812	-2.28963	-2.76672
C	-0.32927	1.84538	-2.22782
C	-1.34381	1.40124	-3.08777
C	-1.80613	2.19203	-4.14199
C	-1.21381	3.44441	-4.34237
C	-0.19226	3.91672	-3.51347

C	0.23066	3.10980	-2.45178
C	-0.21204	2.68745	0.79274
C	0.60095	3.45134	1.64593
C	0.21250	4.71695	2.08839
C	-1.01727	5.23206	1.66082
C	-1.85266	4.50921	0.80586
C	-1.43926	3.23800	0.39175
C	1.51294	0.43603	2.34737
C	0.73525	0.70943	3.47813
C	1.30189	0.81119	4.75508
C	2.68284	0.65603	4.88442
C	3.50000	0.40164	3.77631
C	2.89975	0.28953	2.52285
C	2.13986	-1.85556	0.31683
C	3.34209	-2.05425	-0.37782
C	4.18309	-3.13114	-0.08899
C	3.79386	-4.03467	0.90664
C	2.59911	-3.87391	1.61466
C	1.78742	-2.77602	1.31268
C	2.86202	0.12905	-5.85904
C	4.09019	0.89218	-5.34594
C	1.27377	-4.37559	-4.23469
C	0.01740	-4.59070	-5.09534
C	-2.93122	1.70012	-5.03710
C	-4.17461	2.59330	-4.92336
C	0.42610	5.28317	-3.75918
C	1.94926	5.21365	-3.92716
C	1.15557	5.53573	2.95549
C	0.45586	6.22250	4.13369
C	-3.18646	5.05958	0.32089
C	-3.20933	6.58319	0.16828
C	0.44441	1.07052	5.98342
C	-0.50884	-0.09752	6.27106
C	5.00703	0.27391	3.92162
C	5.40212	-0.88766	4.84250
C	5.49961	-3.29665	-0.83054
C	5.55159	-4.60502	-1.63020
C	2.19043	-4.85550	2.70084
C	2.10674	-6.29598	2.17885
C	1.85189	1.08271	-6.51095
C	1.21878	-5.25024	-2.98028
C	-2.48746	1.55944	-6.49896
C	0.03816	6.27909	-2.65758
C	1.92231	6.56109	2.10583
C	-4.33670	4.59711	1.22743
C	-0.31868	2.39740	5.89022
C	5.64091	1.59102	4.39105
C	6.70035	-3.18367	0.11925
C	3.12064	-4.76635	3.91860
H	3.20892	-0.56642	-6.63564
H	2.32632	1.66638	-7.30814

H	1.01499	0.52904	-6.94760
H	1.43811	1.78325	-5.77791
H	4.58109	1.42888	-6.16545
H	3.81257	1.63167	-4.58724
H	4.82154	0.21241	-4.89754
H	2.07050	-5.06655	-2.31824
H	0.30165	-5.07614	-2.40703
H	1.22570	-6.30891	-3.26003
H	0.06821	-4.01853	-6.02701
H	-0.10373	-5.64944	-5.35133
H	-0.87820	-4.26785	-4.55330
H	-3.20837	0.69912	-4.68062
H	-1.62377	0.89407	-6.58618
H	-3.29831	1.14941	-7.11125
H	-2.20773	2.52882	-6.92600
H	-4.51603	2.66990	-3.88612
H	-3.96721	3.60800	-5.28114
H	-4.99765	2.19132	-5.52465
H	-1.55196	4.07377	-5.16395
H	0.00885	5.65688	-4.70434
H	-1.04914	6.38037	-2.58670
H	0.40535	5.95005	-1.67978
H	0.46052	7.26939	-2.86221
H	2.22987	4.52125	-4.72677
H	2.35472	6.20100	-4.17413
H	2.43890	4.87874	-3.00645
H	1.01556	3.45525	-1.78432
H	1.56625	3.05733	1.94913
H	1.89195	4.83542	3.37187
H	2.46817	6.07309	1.29240
H	1.23456	7.28733	1.65778
H	2.64431	7.11413	2.71726
H	-0.11056	5.50639	4.73626
H	1.19204	6.70815	4.78326
H	-0.23919	6.99975	3.79703
H	-1.31756	6.22365	1.98681
H	-3.35836	4.62768	-0.67465
H	-4.39024	3.50570	1.26830
H	-4.19692	4.96692	2.24965
H	-5.29950	4.97057	0.86048
H	-2.36909	6.94207	-0.43323
H	-4.13732	6.89906	-0.31972
H	-3.16976	7.08907	1.13941
H	-2.07036	2.68621	-0.30280
H	-0.33366	0.85480	3.36145
H	3.12811	0.74156	5.87414
H	3.52029	0.09209	1.65335
H	3.62849	-1.34570	-1.15060
H	5.56750	-2.46939	-1.54926
H	6.68425	-2.23657	0.66745
H	6.70085	-3.99464	0.85595

H	7.64252	-3.24028	-0.43721
H	4.72486	-4.66395	-2.34420
H	6.49059	-4.67941	-2.19001
H	5.48912	-5.47830	-0.97141
H	4.43902	-4.87992	1.13746
H	0.86428	-2.62797	1.87049
H	1.89630	0.93201	-3.41706
H	0.65560	-2.90533	-1.97608
H	2.38893	-2.54788	-5.87312
H	2.13877	-4.70238	-4.82980
H	1.18530	-4.56385	3.03330
H	1.43897	-6.36981	1.31476
H	1.73339	-6.96887	2.95870
H	3.08980	-6.66681	1.86844
H	2.78961	-5.44536	4.71246
H	3.14017	-3.75088	4.32519
H	4.14711	-5.04139	3.65092
H	5.03759	-0.72934	5.86353
H	6.49202	-0.98834	4.89267
H	4.98933	-1.83429	4.48187
H	5.40616	0.05264	2.92292
H	5.38690	2.41503	3.71695
H	6.73266	1.50522	4.42887
H	5.29442	1.86269	5.39442
H	-1.24273	-0.22440	5.46802
H	-1.06238	0.07553	7.20081
H	0.03885	-1.03968	6.37115
H	1.13216	1.14847	6.83658
H	0.36699	3.23514	5.73246
H	-0.88193	2.58447	6.81118
H	-1.03370	2.39242	5.06055
H	-0.99668	-1.42702	3.24388
H	-1.73605	-2.99251	2.66601
H	-4.13075	-3.07354	2.02081
H	-6.29742	-1.97809	1.74037
H	-2.36841	0.73371	3.01423
H	-4.53803	1.80718	2.71452
H	-7.67335	0.24605	2.79527
H	-7.37358	0.50242	1.07812
H	-6.89577	1.73628	2.25073
H	-0.63676	-3.40448	-0.45472
H	-4.80658	-3.23915	-1.55551
H	-1.09641	-5.32545	0.97109
H	-5.22308	-5.22871	-0.19104
H	-2.57610	-6.98302	1.88283
H	-3.76138	-7.51539	0.68546
H	-4.27267	-6.51341	2.04196
H	-1.49118	-1.91295	-2.43556
H	-3.25797	-1.57820	-2.51068
H	-1.77542	0.41524	-2.93247
H	-3.79958	0.16464	-0.88982

H -3.97264 0.51860 -0.24769

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Complex 3 - 1st xyl. hydro black path. TS

La 12.66432 11.29631 3.51495
C 11.42333 11.48641 5.75993
C 10.36657 12.05955 4.94772
C 10.46277 13.38049 4.43627
C 9.50548 13.90311 3.56277
C 8.43207 13.13926 3.10427
C 8.35701 11.81394 3.55792
C 9.29347 11.28370 4.43568
C 7.41707 13.69337 2.14088
C 11.60151 9.38098 1.76312
C 11.75331 8.57647 2.97886
C 13.02220 8.34241 3.56062
C 13.15626 7.61005 4.74983
C 12.04945 7.10655 5.42577
C 10.78330 7.35832 4.86489
C 10.63565 8.07456 3.68982
C 12.18620 6.31759 6.70006
C 15.11698 11.99196 2.46913
C 14.48861 13.28034 2.58408
C 14.45949 13.64923 3.96509
C 15.06654 12.59588 4.71268
C 15.50521 11.59215 3.79991
C 15.10554 11.13566 1.25049
C 14.23617 11.41928 0.17483
C 14.16856 10.60883 -0.96307
C 14.97629 9.47186 -1.02391
C 15.84010 9.13893 0.02259
C 15.89453 9.97192 1.14228
C 14.16344 14.20253 1.46226
C 12.87893 14.71853 1.24071
C 12.62532 15.61565 0.20057
C 13.69345 16.01455 -0.61284
C 14.98980 15.53198 -0.41439
C 15.20573 14.61850 0.62308
C 14.08843 14.96362 4.54136
C 13.43368 15.04941 5.78010
C 13.13274 16.27655 6.37400
C 13.51217 17.44856 5.71289
C 14.17647 17.40693 4.48348
C 14.45334 16.16279 3.91054
C 15.48441 12.67941 6.14022
C 14.83438 11.98214 7.16245
C 15.25374 12.08325 8.49549
C 16.35776 12.88757 8.78444
C 17.03932 13.59346 7.78514
C 16.58461 13.48253 6.47114
C 16.51572 10.57844 4.20961

C	17.82544	10.71507	3.72008
C	18.86420	9.88511	4.14615
C	18.57694	8.89686	5.09386
C	17.29126	8.73780	5.61686
C	16.27305	9.58537	5.16487
C	13.25243	10.95424	-2.12655
C	13.69660	12.24746	-2.82368
C	16.72696	7.90917	-0.08110
C	16.53376	6.94343	1.09466
C	11.22061	16.14535	-0.03426
C	11.13823	17.66003	0.19856
C	16.13756	16.02654	-1.27944
C	16.90467	14.88374	-1.95571
C	12.40885	16.32542	7.70922
C	11.04102	17.01111	7.59007
C	14.64040	18.68080	3.79571
C	15.84035	19.29712	4.53035
C	14.50481	11.38460	9.61918
C	14.27048	9.89365	9.35187
C	18.24495	14.45752	8.11279
C	19.39737	13.62871	8.69675
C	20.27943	10.10627	3.63692
C	20.95488	8.81519	3.15942
C	17.00641	7.68033	6.67005
C	17.22346	6.25970	6.13078
C	11.77726	11.02971	-1.71457
C	18.20233	8.30407	-0.23544
C	10.69296	15.77302	-1.42627
C	17.08860	16.92437	-0.47436
C	13.26562	16.98464	8.79820
C	13.51633	19.71046	3.62850
C	13.17930	12.09875	9.92389
C	17.87861	15.62369	9.04064
C	21.13613	10.80929	4.70094
C	17.82904	7.91535	7.94452
H	13.34792	10.13821	-2.85608
H	11.14738	11.24896	-2.58403
H	11.43777	10.08351	-1.28237
H	11.60732	11.81571	-0.97133
H	13.06591	12.45255	-3.69611
H	13.62567	13.10601	-2.14788
H	14.73424	12.17343	-3.16447
H	18.34926	8.95818	-1.10061
H	18.55575	8.84067	0.65162
H	18.83248	7.41715	-0.36681
H	15.48546	6.64440	1.19343
H	17.13271	6.03731	0.95087
H	16.84573	7.39734	2.04125
H	10.56988	15.66022	0.70485
H	10.71447	14.69021	-1.58162
H	9.65985	16.11554	-1.55262

H	11.29359	16.23579	-2.21719
H	11.47541	17.92298	1.20558
H	11.76363	18.20635	-0.51625
H	10.10880	18.01553	0.07823
H	13.51700	16.72163	-1.42171
H	15.69620	16.64342	-2.07416
H	16.55288	17.76523	-0.02288
H	17.56930	16.36194	0.33381
H	17.87937	17.32872	-1.11630
H	16.23731	14.25614	-2.55303
H	17.68261	15.28174	-2.61654
H	17.39634	14.23901	-1.21933
H	16.20232	14.22440	0.80365
H	13.16664	14.13524	6.30149
H	12.23128	15.28610	8.01513
H	14.22303	16.46744	8.91197
H	13.47705	18.03279	8.55846
H	12.74827	16.96430	9.76402
H	10.41561	16.51855	6.83920
H	10.50878	16.98379	8.54744
H	11.14720	18.06232	7.29946
H	13.29228	18.41174	6.16852
H	14.97776	18.39588	2.79040
H	12.66076	19.28400	3.09631
H	13.15781	20.07735	4.59657
H	13.87149	20.57837	3.06199
H	16.66365	18.58090	4.61365
H	16.20944	20.18327	4.00157
H	15.56261	19.60352	5.54520
H	14.98246	16.12656	2.96362
H	13.97277	11.36984	6.90978
H	16.68981	12.96632	9.81852
H	17.09222	14.02899	5.67989
H	18.03194	11.50195	2.99781
H	20.20642	10.78036	2.77287
H	20.68129	11.75391	5.01420
H	21.24477	10.18034	5.59172
H	22.13960	11.02289	4.31594
H	20.35551	8.30546	2.39928
H	21.93687	9.03528	2.72702
H	21.11377	8.11372	3.98566
H	19.37616	8.24800	5.44445
H	15.27606	9.48209	5.58386
H	13.59601	12.29195	0.22729
H	16.57389	9.71675	1.94477
H	14.93172	8.83189	-1.90397
H	16.43001	7.37807	-0.99577
H	15.94665	7.77641	6.94264
H	16.61589	6.07121	5.23993
H	16.96085	5.51204	6.88758
H	18.27155	6.09750	5.85594

H	17.55383	7.19456	8.72252
H	17.67018	8.92430	8.33645
H	18.90117	7.79899	7.75143
H	19.11801	13.18189	9.65743
H	20.27901	14.25656	8.86774
H	19.68227	12.81555	8.02216
H	18.59516	14.88843	7.16530
H	17.08581	16.23985	8.60578
H	18.74916	16.26440	9.22044
H	17.52707	15.26228	10.01350
H	13.61220	9.73961	8.49005
H	13.79273	9.41972	10.21641
H	15.21178	9.37190	9.15519
H	15.13406	11.46275	10.51645
H	13.34453	13.15501	10.15752
H	12.67376	11.63525	10.77878
H	12.49991	12.04723	9.06580
H	11.90132	12.18619	6.44730
H	11.17604	10.53813	6.24224
H	9.17819	10.26263	4.78976
H	7.53271	11.18555	3.22402
H	11.25306	14.03484	4.80054
H	9.59998	14.93921	3.24283
H	7.61247	13.35765	1.11436
H	7.42898	14.78742	2.13381
H	6.40156	13.37212	2.39644
H	13.92491	8.62156	3.01211
H	9.64312	8.22880	3.27451
H	14.15404	7.41422	5.13296
H	9.89700	6.96767	5.36142
H	13.23557	6.12747	6.94104
H	11.67969	5.34851	6.62684
H	11.74158	6.84857	7.55016
H	12.42889	9.26039	1.05775
H	10.64805	9.20668	1.25967
H	12.05930	14.39911	1.88007
H	11.41634	11.82704	1.76614
H	11.41272	10.80943	1.73456

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Complex 3 - 1st xyl. hydro black path. prod

La	-1.66104	-1.04081	0.09112
C	-2.69259	-0.85724	2.48305
C	-3.93864	-0.40777	1.89682
C	-3.96966	0.71026	1.02535
C	-5.14363	1.10676	0.37242
C	-6.33870	0.41529	0.53459
C	-6.31988	-0.70672	1.38791
C	-5.16637	-1.11306	2.03445
C	-7.60763	0.84246	-0.15432
C	-4.09299	-2.46672	-2.86876

C	-3.31513	-2.96796	-1.68614
C	-1.98060	-3.39379	-1.80120
C	-1.30372	-3.96089	-0.71285
C	-1.93010	-4.12579	0.53260
C	-3.24623	-3.65220	0.66010
C	-3.92222	-3.08868	-0.42401
C	-1.25130	-4.82672	1.67686
C	0.80201	-0.47337	-1.17979
C	0.19948	0.83052	-1.10833
C	0.17988	1.24451	0.26022
C	0.79054	0.21512	1.04199
C	1.19925	-0.83060	0.16219
C	0.88174	-1.33039	-2.39602
C	0.21530	-0.97500	-3.58799
C	0.28776	-1.75865	-4.74454
C	1.01206	-2.95216	-4.70398
C	1.66312	-3.36296	-3.53815
C	1.58977	-2.55048	-2.40432
C	-0.04515	1.76458	-2.24580
C	-1.30999	2.24495	-2.60748
C	-1.46369	3.18689	-3.62800
C	-0.31960	3.66073	-4.28216
C	0.95914	3.20682	-3.94673
C	1.07755	2.25182	-2.93086
C	-0.22267	2.56702	0.80390
C	-0.89499	2.66209	2.03285
C	-1.24050	3.88980	2.59939
C	-0.88944	5.05955	1.91980
C	-0.20943	5.01179	0.69957
C	0.11323	3.76552	0.15509
C	1.25874	0.37484	2.44758
C	0.71429	-0.32941	3.52549
C	1.18015	-0.13964	4.83313
C	2.23124	0.75513	5.04028
C	2.81384	1.46576	3.98359
C	2.30860	1.27056	2.69858
C	2.22817	-1.81952	0.58870
C	3.53337	-1.66593	0.09425
C	4.58797	-2.47465	0.52329
C	4.31887	-3.46545	1.47347
C	3.03704	-3.64311	2.00094
C	2.00464	-2.81207	1.54960
C	-0.37305	-1.32069	-6.04288
C	0.26926	-0.04029	-6.59296
C	2.48187	-4.64401	-3.53890
C	2.09942	-5.60351	-2.40580
C	-2.84833	3.68819	-4.00430
C	-3.02226	5.17439	-3.66370
C	2.18689	3.77099	-4.64406
C	3.03277	2.68401	-5.31878
C	-1.98450	3.93930	3.92339

C	-3.37834	4.56265	3.76816
C	0.22312	6.28503	-0.00976
C	1.39982	6.94952	0.72042
C	0.52575	-0.82945	6.01962
C	0.32118	-2.33409	5.81477
C	3.97004	2.42230	4.22051
C	5.20698	1.69231	4.76208
C	5.99783	-2.21191	0.01749
C	6.78475	-3.48739	-0.30198
C	2.77204	-4.70653	3.05355
C	2.94905	-6.12366	2.49048
C	-1.89116	-1.15823	-5.91132
C	3.98499	-4.33272	-3.50639
C	-3.18153	3.42070	-5.47818
C	3.04114	4.60688	-3.68011
C	-1.17224	4.65882	5.00809
C	-0.92822	7.27920	-0.20439
C	-0.80140	-0.14477	6.38180
C	3.57299	3.58875	5.13503
C	6.76829	-1.33378	1.01622
C	3.64162	-4.50279	4.30183
H	-0.19152	-2.11999	-6.77463
H	-2.33198	-0.85515	-6.86763
H	-2.36253	-2.09892	-5.60956
H	-2.14719	-0.39465	-5.16912
H	-0.16651	0.22443	-7.56307
H	0.11454	0.80341	-5.91255
H	1.34765	-0.17013	-6.72765
H	4.27274	-3.68506	-4.34027
H	4.25199	-3.81915	-2.57666
H	4.57656	-5.25337	-3.56773
H	1.03395	-5.85431	-2.43961
H	2.66650	-6.53770	-2.48406
H	2.31965	-5.17076	-1.42361
H	-3.56612	3.12258	-3.39605
H	-3.08533	2.35807	-5.72066
H	-4.20802	3.73017	-5.70430
H	-2.51492	3.97710	-6.14654
H	-2.83040	5.35891	-2.60261
H	-2.33014	5.79696	-4.24174
H	-4.04059	5.50966	-3.89100
H	-0.41946	4.40364	-5.07187
H	1.82515	4.44508	-5.43259
H	2.45444	5.41113	-3.22540
H	3.44115	3.98641	-2.87057
H	3.89049	5.05925	-4.20438
H	2.44525	2.11783	-6.04680
H	3.88676	3.12936	-5.84139
H	3.42762	1.97240	-4.58561
H	2.05950	1.88444	-2.64248
H	-1.14377	1.75531	2.57499

H	-2.12347	2.90077	4.25119
H	-0.19566	4.18517	5.14703
H	-1.00120	5.70925	4.74713
H	-1.70225	4.63870	5.96707
H	-3.97121	4.02190	3.02428
H	-3.92172	4.53917	4.71943
H	-3.31274	5.60885	3.44863
H	-1.14564	6.02448	2.35206
H	0.57467	5.99022	-1.00724
H	-1.76836	6.81794	-0.73190
H	-1.30223	7.65627	0.75395
H	-0.59402	8.14473	-0.78715
H	2.24222	6.25859	0.82384
H	1.74788	7.83513	0.17653
H	1.10596	7.26815	1.72695
H	0.65344	3.73015	-0.78482
H	-0.10363	-1.01947	3.34007
H	2.60077	0.90165	6.05416
H	2.73673	1.82221	1.86518
H	3.72263	-0.88478	-0.63862
H	5.89959	-1.64131	-0.91588
H	6.23727	-0.39710	1.21071
H	6.88990	-1.85251	1.97382
H	7.76624	-1.09019	0.63455
H	6.24123	-4.13397	-0.99738
H	7.74852	-3.23452	-0.75658
H	6.99797	-4.06898	0.60149
H	5.12766	-4.10198	1.82354
H	1.01148	-2.92388	1.97661
H	-0.36881	-0.06403	-3.61245
H	2.10874	-2.86667	-1.50914
H	1.07746	-3.56959	-5.59901
H	2.27086	-5.15612	-4.48772
H	1.72369	-4.59860	3.36277
H	2.30625	-6.29287	1.62061
H	2.70383	-6.87746	3.24702
H	3.98386	-6.29505	2.17397
H	3.37008	-5.21938	5.08487
H	3.52637	-3.49183	4.70363
H	4.70326	-4.64988	4.07517
H	5.00924	1.25439	5.74688
H	6.05002	2.38402	4.87016
H	5.51319	0.88166	4.09376
H	4.23807	2.84681	3.24376
H	2.71507	4.13327	4.72941
H	4.40410	4.29413	5.24629
H	3.30316	3.23515	6.13643
H	-0.39733	-2.53506	5.01245
H	-0.07405	-2.79451	6.72689
H	1.26013	-2.83426	5.56044
H	1.20525	-0.70438	6.87400

H	-0.65387	0.92108	6.58106
H	-1.24645	-0.60037	7.27394
H	-1.52280	-0.23440	5.56190
H	-2.05747	-0.04781	2.85256
H	-2.78118	-1.65147	3.22624
H	-5.20391	-1.96541	2.71061
H	-7.24353	-1.25900	1.55692
H	-3.09197	1.35457	0.94282
H	-5.11372	1.98432	-0.26941
H	-7.99111	0.06123	-0.82228
H	-7.44843	1.74121	-0.75697
H	-8.40397	1.06400	0.56658
H	-1.45411	-3.27672	-2.74474
H	-4.93376	-2.72135	-0.28046
H	-0.27151	-4.27373	-0.84281
H	-3.75350	-3.72902	1.61688
H	-0.17752	-4.92600	1.50600
H	-1.66292	-5.83539	1.80113
H	-1.40644	-4.29380	2.61985
H	-4.55439	-3.31034	-3.39868
H	-4.88557	-1.78485	-2.55517
H	-2.18058	1.83805	-2.09907
H	-2.67663	-0.17039	-1.51338
H	-3.44739	-1.93412	-3.56682

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Complex 3 - 1st xyl. hydro black path. prod - p-xyl.

La	-1.69582	0.12545	0.60674
C	-2.84122	0.81090	3.13531
C	-3.38189	-0.35481	2.56595
C	-4.37456	-0.27721	1.53014
C	-4.46996	-1.22958	0.52741
C	-3.64753	-2.38017	0.50130
C	-2.81054	-2.56774	1.61627
C	-2.67271	-1.60660	2.61482
C	-3.79989	-3.42660	-0.56968
C	0.60554	0.06848	-1.08216
C	0.24581	1.44673	-1.04269
C	0.45601	1.91912	0.29223
C	0.96661	0.83563	1.07292
C	1.04832	-0.31405	0.22278
C	0.59463	-0.77539	-2.30083
C	-0.53117	-0.80493	-3.13695
C	-0.53658	-1.55542	-4.31660
C	0.61579	-2.27079	-4.65461
C	1.76022	-2.25529	-3.85083
C	1.73091	-1.51036	-2.66877
C	-0.05572	2.29675	-2.22594
C	-1.25549	3.00654	-2.36599
C	-1.48954	3.83232	-3.46616
C	-0.48539	3.95384	-4.43501

C	0.72511	3.26662	-4.32714
C	0.92264	2.43646	-3.21766
C	0.23710	3.31095	0.75904
C	-0.53059	3.58688	1.90010
C	-0.74494	4.89591	2.34003
C	-0.15041	5.94347	1.63022
C	0.63312	5.70667	0.49590
C	0.80781	4.38852	0.06719
C	1.43764	0.91257	2.47695
C	1.09718	-0.05806	3.43144
C	1.59270	-0.00355	4.73807
C	2.45209	1.04532	5.07888
C	2.81616	2.03067	4.15580
C	2.29692	1.95212	2.86271
C	1.61395	-1.63251	0.60149
C	2.90315	-1.70766	1.14788
C	3.47807	-2.92899	1.50602
C	2.72736	-4.09744	1.33116
C	1.43749	-4.06513	0.79209
C	0.90354	-2.82737	0.41998
C	-1.74473	-1.56586	-5.23779
C	-1.90784	-0.21517	-5.94944
C	3.00588	-3.01597	-4.27428
C	3.33075	-4.16438	-3.31067
C	-2.81190	4.56779	-3.60682
C	-2.62381	6.09028	-3.61452
C	1.80262	3.42932	-5.38640
C	2.09673	2.10984	-6.11199
C	-1.63097	5.16413	3.54564
C	-2.94000	5.85066	3.12888
C	1.32730	6.84270	-0.23735
C	2.53747	7.34839	0.56273
C	1.20419	-1.01470	5.80661
C	0.95038	-2.42637	5.27261
C	3.78442	3.14089	4.52848
C	5.19187	2.58863	4.79620
C	4.89432	-2.97800	2.05540
C	5.83511	-3.75190	1.12136
C	0.62236	-5.33829	0.63300
C	1.30529	-6.35877	-0.28602
C	-3.03513	-1.96172	-4.50938
C	4.21368	-2.08522	-4.44892
C	-3.59155	4.10273	-4.84429
C	3.08702	4.03418	-4.80267
C	-0.91405	5.96858	4.63686
C	0.38224	7.99815	-0.58625
C	-0.00334	-0.51370	6.61517
C	3.28590	3.97306	5.71664
C	4.94282	-3.54616	3.47978
C	0.28963	-5.96593	1.99428
H	-1.55452	-2.32589	-6.00830

H	-3.87274	-2.01849	-5.21346
H	-2.93060	-2.93899	-4.02688
H	-3.29840	-1.22857	-3.73922
H	-2.76077	-0.23782	-6.63745
H	-2.07373	0.59139	-5.22794
H	-1.01216	0.03606	-6.52563
H	3.99476	-1.28117	-5.15829
H	4.50143	-1.62289	-3.49845
H	5.08070	-2.64210	-4.82164
H	2.49664	-4.87005	-3.24860
H	4.21700	-4.71529	-3.64542
H	3.52751	-3.79169	-2.29996
H	-3.41300	4.31343	-2.72388
H	-3.76188	3.02217	-4.81974
H	-4.56609	4.60092	-4.89961
H	-3.04721	4.33441	-5.76664
H	-2.10103	6.42631	-2.71404
H	-2.03847	6.41552	-4.48177
H	-3.59206	6.60157	-3.65783
H	-0.64617	4.59653	-5.29938
H	1.41421	4.13731	-6.13130
H	2.88625	4.99057	-4.30947
H	3.53846	3.36490	-4.06203
H	3.82946	4.20609	-5.59012
H	1.19099	1.70097	-6.56941
H	2.84216	2.25812	-6.90163
H	2.48641	1.35564	-5.42028
H	1.85466	1.88767	-3.10937
H	-0.96928	2.76330	2.46265
H	-1.89121	4.18755	3.97482
H	0.00455	5.46882	4.95820
H	-0.64447	6.97065	4.28570
H	-1.56004	6.09032	5.51327
H	-3.47554	5.26064	2.37849
H	-3.60074	5.98762	3.99226
H	-2.74537	6.83851	2.69663
H	-0.30109	6.96651	1.96756
H	1.70394	6.42851	-1.18182
H	-0.48211	7.64662	-1.15715
H	0.00862	8.50069	0.31279
H	0.90336	8.75132	-1.18715
H	3.24099	6.53647	0.77179
H	3.07227	8.13041	0.01178
H	2.22175	7.77051	1.52359
H	1.40562	4.19082	-0.81824
H	0.45439	-0.88266	3.13492
H	2.85142	1.08376	6.09137
H	2.57731	2.70241	2.12859
H	3.46768	-0.78972	1.28825
H	5.25439	-1.94184	2.10244
H	4.31931	-2.95906	4.16062

H	4.58876	-4.58267	3.50820
H	5.96830	-3.53637	3.86533
H	5.82523	-3.33156	0.11103
H	6.86468	-3.71903	1.49451
H	5.54287	-4.80520	1.04688
H	3.15978	-5.05439	1.61601
H	-0.08494	-2.79946	-0.03792
H	-1.40415	-0.21928	-2.85340
H	2.60620	-1.47564	-2.02580
H	0.62696	-2.84932	-5.57778
H	2.79046	-3.45995	-5.25584
H	-0.32652	-5.05374	0.15741
H	1.50927	-5.92931	-1.27053
H	0.67113	-7.24179	-0.42155
H	2.25835	-6.69791	0.13431
H	-0.35369	-6.84415	1.87084
H	-0.22379	-5.25455	2.64895
H	1.19929	-6.29038	2.51122
H	5.19260	1.91149	5.65772
H	5.89493	3.40136	5.01030
H	5.56881	2.02998	3.93385
H	3.85042	3.81112	3.66139
H	2.29648	4.39464	5.51633
H	3.97339	4.80042	5.92388
H	3.21362	3.36842	6.62743
H	0.03790	-2.47334	4.66798
H	0.81866	-3.12735	6.10354
H	1.77734	-2.78162	4.65123
H	2.05507	-1.07619	6.49960
H	0.18875	0.47321	7.04706
H	-0.24129	-1.20446	7.43197
H	-0.89036	-0.42924	5.97724
H	-3.42449	1.72930	3.11079
H	-2.11519	0.72947	3.94059
H	-1.96543	-1.77032	3.42401
H	-2.21555	-3.47659	1.68158
H	-4.97883	0.62431	1.46000
H	-5.18124	-1.07117	-0.27869
H	-3.95592	-2.97274	-1.55230
H	-4.65951	-4.07956	-0.36991
H	-2.91480	-4.06634	-0.63388
H	-2.03390	2.88020	-1.61864
H	-2.82787	0.66660	-1.08347

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Complex 3 - 2nd xyl. hydro black path.

La	-1.95771	-0.62688	0.43470
C	-3.23448	-0.25876	3.05069
C	-4.09483	-0.26595	1.94390
C	-4.22514	0.88222	1.08206
C	-4.54327	0.74964	-0.26741

C	-4.74762	-0.50375	-0.87555
C	-4.80314	-1.61542	-0.00151
C	-4.53404	-1.50256	1.35351
C	-5.07747	-0.63592	-2.33806
C	0.46830	-0.63912	-1.11947
C	0.00018	0.71193	-1.09140
C	0.14981	1.19996	0.24917
C	0.69775	0.14705	1.04392
C	0.89154	-0.98877	0.19644
C	0.69238	-1.47947	-2.32782
C	-0.35088	-2.03327	-3.07642
C	-0.09716	-2.82020	-4.20444
C	1.23176	-3.02945	-4.58518
C	2.30132	-2.48771	-3.86508
C	2.01281	-1.71785	-2.73497
C	-0.49834	1.49292	-2.24971
C	-1.63522	2.31416	-2.14231
C	-2.09841	3.07664	-3.21526
C	-1.39364	3.01845	-4.42326
C	-0.25540	2.22347	-4.56902
C	0.17537	1.46050	-3.47785
C	-0.11756	2.57925	0.72453
C	-0.87989	2.82337	1.87783
C	-1.11928	4.12012	2.33784
C	-0.55979	5.19264	1.63390
C	0.21352	4.98977	0.48710
C	0.41627	3.67970	0.04149
C	1.14283	0.25651	2.45549
C	0.74655	-0.67048	3.42897
C	1.21844	-0.59607	4.74242
C	2.11596	0.42581	5.06841
C	2.53604	1.36869	4.12476
C	2.03339	1.27461	2.82526
C	1.55685	-2.26238	0.56470
C	2.79287	-2.24785	1.22712
C	3.46213	-3.43087	1.54879
C	2.87006	-4.64947	1.19938
C	1.63988	-4.70138	0.53617
C	0.99793	-3.50102	0.22205
C	-1.23084	-3.47454	-4.97560
C	-2.24098	-2.45218	-5.51061
C	3.73478	-2.73969	-4.30198
C	4.51832	-3.53616	-3.24991
C	-3.31747	3.97122	-3.06259
C	-2.94057	5.45506	-3.17267
C	0.50292	2.20521	-5.88600
C	0.41794	0.83500	-6.57122
C	-1.96306	4.35272	3.58072
C	-3.18928	5.22858	3.29108
C	0.88766	6.13783	-0.24793
C	2.28042	6.40761	0.34436

C	0.76170	-1.55723	5.82926
C	0.40871	-2.95665	5.31922
C	3.55088	2.44312	4.48006
C	4.93300	1.83214	4.75330
C	4.80498	-3.38404	2.26001
C	5.92026	-4.02695	1.42452
C	1.00700	-6.02867	0.15172
C	1.84544	-6.77099	-0.89808
C	-1.92843	-4.54753	-4.12671
C	4.46234	-1.43637	-4.65883
C	-4.43079	3.61368	-4.05600
C	1.96189	2.64849	-5.71380
C	-1.13012	4.93603	4.72998
C	0.05937	7.42553	-0.28437
C	-0.41190	-0.95596	6.61942
C	3.09551	3.31580	5.65602
C	4.73110	-4.01487	3.65700
C	0.74094	-6.91658	1.37459
H	-0.78152	-3.97832	-5.84246
H	-2.71699	-5.04710	-4.70116
H	-1.21679	-5.30845	-3.79149
H	-2.38554	-4.10735	-3.23364
H	-3.01610	-2.94854	-6.10527
H	-2.73923	-1.92008	-4.69331
H	-1.75197	-1.70494	-6.14252
H	3.92574	-0.88183	-5.43505
H	4.55630	-0.78318	-3.78436
H	5.47339	-1.64437	-5.02653
H	4.02923	-4.48951	-3.02943
H	5.53519	-3.74594	-3.60046
H	4.59549	-2.98140	-2.30882
H	-3.71062	3.80984	-2.04911
H	-4.72836	2.56436	-3.96473
H	-5.31696	4.23475	-3.88476
H	-4.10877	3.77648	-5.09019
H	-2.16987	5.71816	-2.44253
H	-2.55146	5.69072	-4.16934
H	-3.81358	6.09327	-2.99619
H	-1.72885	3.61366	-5.27082
H	0.01400	2.93555	-6.54531
H	2.02386	3.63778	-5.24957
H	2.51996	1.94794	-5.08362
H	2.46728	2.69464	-6.68473
H	-0.62329	0.55360	-6.75671
H	0.94250	0.84996	-7.53338
H	0.86864	0.05158	-5.95312
H	1.06026	0.83923	-3.57157
H	-1.27876	1.98204	2.44231
H	-2.32914	3.37025	3.90822
H	-0.28738	4.28266	4.97378
H	-0.72707	5.92035	4.46696

H	-1.74123	5.05597	5.63144
H	-3.80370	4.80470	2.49039
H	-3.81517	5.32462	4.18500
H	-2.89543	6.23819	2.98382
H	-0.73128	6.20523	1.98994
H	1.02962	5.80726	-1.28584
H	-0.95010	7.24652	-0.66720
H	-0.03347	7.87778	0.70919
H	0.54083	8.16726	-0.93026
H	2.90237	5.50749	0.32269
H	2.79826	7.19451	-0.21566
H	2.19997	6.73209	1.38808
H	1.01137	3.50689	-0.85176
H	0.06980	-1.47107	3.14454
H	2.50028	0.47641	6.08622
H	2.35379	1.99199	2.07419
H	3.24223	-1.29390	1.49046
H	5.05985	-2.32396	2.39120
H	3.97015	-3.52348	4.27064
H	4.47866	-5.07947	3.59851
H	5.69349	-3.92952	4.17423
H	5.99506	-3.56097	0.43718
H	6.88927	-3.92339	1.92558
H	5.73868	-5.09693	1.27385
H	3.38030	-5.57819	1.44743
H	0.04092	-3.52194	-0.29627
H	-1.37356	-1.88187	-2.74177
H	2.82053	-1.29118	-2.14584
H	1.44058	-3.64021	-5.46281
H	3.68843	-3.35107	-5.21364
H	0.03638	-5.79722	-0.30611
H	1.99693	-6.15206	-1.78756
H	1.35040	-7.69878	-1.20669
H	2.83223	-7.03656	-0.50220
H	0.23127	-7.84062	1.07943
H	0.11437	-6.40157	2.10953
H	1.67450	-7.19951	1.87356
H	4.90463	1.16859	5.62480
H	5.67313	2.61505	4.95348
H	5.28135	1.24343	3.89899
H	3.64506	3.09598	3.60218
H	2.12937	3.78590	5.45021
H	3.82463	4.10968	5.85214
H	2.99328	2.72861	6.57520
H	-0.50563	-2.94774	4.71547
H	0.22930	-3.63203	6.16234
H	1.20998	-3.37959	4.70617
H	1.60444	-1.66420	6.52695
H	-0.14995	0.01931	7.04128
H	-0.70916	-1.61579	7.44248
H	-1.28133	-0.81364	5.96814

H	-2.95668	0.68690	3.50881
H	-3.19433	-1.12931	3.69994
H	-4.53231	-2.39710	1.97043
H	-5.04068	-2.59377	-0.41018
H	-3.98895	1.86439	1.48422
H	-4.58215	1.64401	-0.88571
H	-4.79520	-1.62201	-2.71750
H	-4.55321	0.11546	-2.93597
H	-6.15272	-0.51004	-2.52119
H	-2.15111	2.38880	-1.18676
H	-2.11036	-2.51559	-0.50084
H	-1.87930	-2.64119	2.02532
H	-1.94977	-2.92869	1.31426

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Complex 3 - 2nd xyl. hydro black path. TS

La	-1.48890	-0.11271	0.65215
C	-3.02221	-0.25280	3.00580
C	-3.93881	0.28805	2.00301
C	-3.78518	1.59417	1.47585
C	-4.59851	2.06212	0.43235
C	-5.56892	1.25415	-0.15517
C	-5.69366	-0.05893	0.33396
C	-4.90430	-0.53392	1.36900
C	-6.44633	1.74606	-1.27392
C	0.87184	-0.13470	-1.03093
C	0.39328	1.20760	-1.00252
C	0.55273	1.71190	0.32977
C	1.13413	0.66839	1.12292
C	1.31806	-0.47167	0.28339
C	1.10224	-0.95182	-2.25285
C	0.06288	-1.37343	-3.08842
C	0.32141	-2.11351	-4.24602
C	1.64870	-2.41460	-4.56471
C	2.71320	-2.00633	-3.75482
C	2.42194	-1.27761	-2.59821
C	-0.08717	1.95268	-2.19381
C	-1.38034	2.48997	-2.27356
C	-1.81837	3.17784	-3.40663
C	-0.92182	3.34645	-4.46824
C	0.37630	2.83478	-4.42308
C	0.77514	2.13052	-3.28207
C	0.18367	3.06453	0.80714
C	-0.41787	3.25749	2.06363
C	-0.78295	4.52696	2.52053
C	-0.52070	5.62945	1.70150
C	0.09287	5.48236	0.45310
C	0.43200	4.19856	0.01926
C	1.58733	0.78168	2.53205
C	1.19225	-0.14206	3.50998
C	1.66234	-0.05547	4.82445

C	2.55835	0.96929	5.14370
C	2.97921	1.90607	4.19338
C	2.47563	1.80470	2.89497
C	1.94583	-1.76025	0.65901
C	3.17578	-1.79280	1.33011
C	3.78896	-3.00194	1.66775
C	3.14260	-4.19606	1.33046
C	1.91622	-4.20166	0.65751
C	1.33599	-2.97645	0.32223
C	-0.81642	-2.61294	-5.12032
C	-1.67423	-1.46434	-5.66592
C	4.14489	-2.35595	-4.12629
C	4.79095	-3.28263	-3.08765
C	-3.23696	3.71386	-3.49055
C	-3.27110	5.23826	-3.66087
C	1.32465	3.03402	-5.59332
C	1.63793	1.70551	-6.29483
C	-1.44330	4.69905	3.87902
C	-2.86708	5.25976	3.75549
C	0.44045	6.68818	-0.40430
C	1.66958	7.41869	0.15740
C	1.20323	-1.01049	5.91558
C	0.87976	-2.42069	5.41544
C	4.00196	2.97687	4.53690
C	5.40090	2.36479	4.70358
C	5.13380	-3.00900	2.37687
C	6.22242	-3.67871	1.52711
C	1.21716	-5.50340	0.30291
C	2.06265	-6.37427	-0.63545
C	-1.68149	-3.63751	-4.37220
C	5.00268	-1.10416	-4.35434
C	-4.03445	3.01886	-4.60308
C	2.61229	3.75640	-5.17520
C	-0.59634	5.56559	4.82047
C	-0.73528	7.65566	-0.58433
C	0.00751	-0.41746	6.67864
C	3.61387	3.79688	5.77285
C	5.04727	-3.65444	3.76617
C	0.80524	-6.28343	1.55926
H	-0.36203	-3.12503	-5.97996
H	-2.47254	-4.02788	-5.02293
H	-1.07885	-4.48239	-4.02403
H	-2.15743	-3.18450	-3.49574
H	-2.45808	-1.84790	-6.32887
H	-2.16214	-0.91567	-4.85370
H	-1.06750	-0.75061	-6.23138
H	4.56664	-0.45893	-5.12342
H	5.09563	-0.51386	-3.43610
H	6.01399	-1.37941	-4.67427
H	4.21184	-4.20260	-2.96431
H	5.80806	-3.55695	-3.39010

H	4.85066	-2.79788	-2.10756
H	-3.72622	3.47584	-2.53647
H	-4.03975	1.93313	-4.46722
H	-5.07241	3.36990	-4.61545
H	-3.60207	3.22769	-5.58772
H	-2.72827	5.73951	-2.85397
H	-2.81396	5.54281	-4.60863
H	-4.30325	5.60601	-3.65954
H	-1.24042	3.88624	-5.35841
H	0.80760	3.67802	-6.31794
H	2.39253	4.71534	-4.69517
H	3.19625	3.15545	-4.46995
H	3.24633	3.94949	-6.04746
H	0.72341	1.22755	-6.65824
H	2.30249	1.86665	-7.15128
H	2.12721	1.00192	-5.61338
H	1.77434	1.70841	-3.22575
H	-0.57347	2.40258	2.71965
H	-1.51697	3.70007	4.32977
H	0.41102	5.15520	4.93469
H	-0.49926	6.58851	4.44034
H	-1.05691	5.62326	5.81274
H	-3.49599	4.62529	3.12302
H	-3.34161	5.33139	4.74026
H	-2.86017	6.26347	3.31652
H	-0.79009	6.62438	2.04807
H	0.70748	6.30576	-1.39818
H	-1.61966	7.14160	-0.97286
H	-1.01529	8.13423	0.36069
H	-0.47013	8.45363	-1.28609
H	2.52639	6.74329	0.24277
H	1.95709	8.25534	-0.48928
H	1.46212	7.82091	1.15542
H	0.91250	4.07457	-0.94663
H	0.52842	-0.95409	3.22479
H	2.94292	1.02661	6.16081
H	2.79383	2.51819	2.13887
H	3.66515	-0.85690	1.58697
H	5.42485	-1.95976	2.51958
H	4.30786	-3.14574	4.39182
H	4.75962	-4.70943	3.69782
H	6.01557	-3.60737	4.27715
H	6.31474	-3.19647	0.54918
H	7.19527	-3.62355	2.02843
H	5.99732	-4.73715	1.35541
H	3.60780	-5.14385	1.59424
H	0.39072	-2.96565	-0.21739
H	-0.95844	-1.15013	-2.79170
H	3.22679	-0.95269	-1.94345
H	1.85992	-2.99017	-5.46544
H	4.10349	-2.90371	-5.07784

H	0.29830	-5.23570	-0.23507
H	2.32970	-5.82819	-1.54506
H	1.51257	-7.27589	-0.92738
H	2.99211	-6.69591	-0.15238
H	0.24594	-7.18650	1.29010
H	0.17502	-5.67358	2.21388
H	1.68229	-6.59629	2.13716
H	5.42216	1.66061	5.54287
H	6.14715	3.14296	4.89945
H	5.70393	1.81942	3.80448
H	4.04121	3.66585	3.68269
H	2.62424	4.24855	5.65654
H	4.33713	4.60200	5.94208
H	3.59473	3.17922	6.67740
H	-0.01566	-2.43254	4.78458
H	0.68707	-3.08676	6.26309
H	1.70242	-2.84145	4.83011
H	2.03509	-1.09478	6.62918
H	0.24528	0.56914	7.08862
H	-0.29037	-1.06946	7.50757
H	-0.85566	-0.30339	6.01322
H	-2.55005	0.50330	3.63942
H	-3.46645	-1.03808	3.62140
H	-5.04122	-1.55233	1.72420
H	-6.43449	-0.72076	-0.10945
H	-3.08729	2.28467	1.94854
H	-4.47378	3.08755	0.09127
H	-6.19553	1.25623	-2.22218
H	-6.34138	2.82460	-1.41980
H	-7.50271	1.53712	-1.07291
H	-2.06738	2.37665	-1.43534
H	-2.15256	-1.28009	-0.96940
H	-1.97077	-1.20253	2.56863
H	-1.27783	-1.77529	2.15870

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Complex 3 - 2nd xyl. hydro black path. prod

La	-1.90978	-0.69937	0.33714
C	-4.41337	0.42481	3.33361
C	-4.52304	0.01992	1.89151
C	-4.47624	0.95582	0.85169
C	-4.61086	0.55925	-0.49060
C	-4.79028	-0.78467	-0.83719
C	-4.79324	-1.73029	0.20680
C	-4.66369	-1.33703	1.53956
C	-4.97350	-1.21793	-2.26377
C	0.52487	-0.64541	-1.14920
C	0.04275	0.70048	-1.10434
C	0.16953	1.16562	0.24590
C	0.73577	0.11134	1.02867
C	0.93706	-1.00975	0.16938

C	0.80516	-1.45113	-2.37138
C	-0.19549	-1.99069	-3.18581
C	0.11921	-2.74655	-4.31953
C	1.46614	-2.93687	-4.64188
C	2.49457	-2.40676	-3.85629
C	2.14580	-1.66835	-2.72199
C	-0.45585	1.48393	-2.25988
C	-1.62989	2.25371	-2.17509
C	-2.09836	3.00725	-3.25224
C	-1.35669	2.99930	-4.43918
C	-0.17671	2.26292	-4.55999
C	0.25453	1.50204	-3.46778
C	-0.14821	2.51350	0.77097
C	-0.81883	2.66536	1.99605
C	-1.08591	3.92613	2.53564
C	-0.66644	5.05711	1.82787
C	0.00385	4.94706	0.60493
C	0.25027	3.67205	0.08892
C	1.26131	0.26582	2.41335
C	0.79420	-0.47899	3.49924
C	1.33361	-0.30659	4.78053
C	2.37035	0.61176	4.95500
C	2.87406	1.36389	3.88562
C	2.30263	1.18462	2.62605
C	1.52976	-2.31693	0.53526
C	2.71997	-2.39231	1.27182
C	3.30585	-3.62177	1.58293
C	2.67379	-4.79298	1.15188
C	1.48055	-4.75542	0.42375
C	0.92398	-3.51135	0.11898
C	-0.97207	-3.39836	-5.15193
C	-1.97978	-2.38098	-5.70030
C	3.94910	-2.64634	-4.22461
C	4.67447	-3.47476	-3.15553
C	-3.37499	3.82316	-3.13465
C	-3.11705	5.32330	-3.32802
C	0.62393	2.30620	-5.85092
C	0.63168	0.94678	-6.56209
C	-1.78921	4.05520	3.87663
C	-3.07041	4.89475	3.78396
C	0.52126	6.17321	-0.13054
C	1.83384	6.66714	0.49740
C	0.79637	-1.09744	5.96169
C	1.09118	-2.59690	5.82162
C	4.02188	2.34052	4.07956
C	5.30263	1.62515	4.53162
C	4.61840	-3.67231	2.34807
C	5.77008	-4.15303	1.45368
C	0.79856	-6.03256	-0.03776
C	1.66494	-6.80755	-1.04016
C	-1.68321	-4.50264	-4.35575

C	4.69569	-1.33563	-4.50621
C	-4.45968	3.32921	-4.10232
C	2.05210	2.81913	-5.62161
C	-0.84579	4.60971	4.95307
C	-0.50315	7.31041	-0.21218
C	-0.70339	-0.85205	6.17629
C	3.65754	3.47665	5.04451
C	4.52263	-4.52467	3.61996
C	0.38942	-6.92341	1.14281
H	-0.48148	-3.87332	-6.01277
H	-2.44303	-4.99906	-4.97045
H	-0.97225	-5.26122	-4.01390
H	-2.17736	-4.09044	-3.46883
H	-2.72711	-2.87711	-6.32991
H	-2.51228	-1.87286	-4.88930
H	-1.48191	-1.61453	-6.30138
H	4.20117	-0.75884	-5.29418
H	4.74492	-0.70598	-3.61102
H	5.72443	-1.53610	-4.82603
H	4.16891	-4.42969	-2.98428
H	5.70675	-3.68259	-3.45928
H	4.70669	-2.94442	-2.19794
H	-3.75236	3.68672	-2.11116
H	-4.67305	2.26512	-3.95758
H	-5.39195	3.88736	-3.96120
H	-4.14827	3.46143	-5.14407
H	-2.36404	5.68786	-2.62365
H	-2.75703	5.53594	-4.34050
H	-4.03699	5.89864	-3.17582
H	-1.69594	3.58837	-5.28954
H	0.12056	3.02346	-6.51377
H	2.04867	3.80013	-5.13598
H	2.62496	2.13433	-4.98742
H	2.58566	2.91232	-6.57392
H	-0.38716	0.61683	-6.78736
H	1.18594	1.00660	-7.50564
H	1.10100	0.17514	-5.94321
H	1.16864	0.92177	-3.54264
H	-1.10052	1.77837	2.56187
H	-2.07667	3.04148	4.18645
H	0.04472	3.98269	5.05303
H	-0.51692	5.62487	4.70404
H	-1.34691	4.65086	5.92676
H	-3.75846	4.49557	3.03127
H	-3.59218	4.91346	4.74717
H	-2.84952	5.93212	3.50985
H	-0.85596	6.04370	2.24435
H	0.74522	5.85657	-1.15804
H	-1.45145	6.96778	-0.63740
H	-0.71500	7.73733	0.77431
H	-0.12217	8.12276	-0.84033

H	2.58776	5.87424	0.51308
H	2.24114	7.51584	-0.06366
H	1.67176	6.99269	1.53111
H	0.77962	3.57194	-0.85475
H	-0.02511	-1.17405	3.33168
H	2.79318	0.74214	5.95014
H	2.67349	1.76330	1.78308
H	3.20131	-1.47466	1.59832
H	4.84659	-2.64390	2.65826
H	3.71145	-4.17971	4.26759
H	4.33520	-5.57808	3.38389
H	5.45864	-4.47705	4.18770
H	5.87493	-3.51917	0.56775
H	6.72074	-4.13833	1.99895
H	5.59818	-5.17890	1.10923
H	3.12211	-5.75611	1.38807
H	0.00089	-3.46483	-0.45702
H	-1.23190	-1.86225	-2.88694
H	2.92130	-1.25310	-2.08339
H	1.72258	-3.52623	-5.52158
H	3.95108	-3.23153	-5.15454
H	-0.12006	-5.73276	-0.55869
H	1.91812	-6.18528	-1.90396
H	1.13894	-7.69841	-1.40194
H	2.60266	-7.13964	-0.58035
H	-0.15619	-7.80645	0.79121
H	-0.25333	-6.38077	1.84293
H	1.26511	-7.27604	1.69922
H	5.16961	1.15821	5.51383
H	6.13672	2.33166	4.60980
H	5.58680	0.83849	3.82579
H	4.22477	2.79376	3.09989
H	2.77374	4.02051	4.69768
H	4.48417	4.19063	5.13318
H	3.44290	3.09266	6.04803
H	0.60368	-3.01302	4.93382
H	0.72723	-3.14843	6.69606
H	2.16620	-2.77846	5.72782
H	1.32287	-0.73780	6.85669
H	-0.91365	0.21415	6.30986
H	-1.05959	-1.38401	7.06586
H	-1.28555	-1.20589	5.31837
H	-4.27024	1.50270	3.43931
H	-5.32033	0.14824	3.88269
H	-4.66728	-2.08809	2.32314
H	-4.89380	-2.78371	-0.03441
H	-4.34555	2.00928	1.08611
H	-4.58792	1.31251	-1.27330
H	-4.37114	-2.10716	-2.46854
H	-4.67614	-0.43176	-2.96214
H	-6.02400	-1.46284	-2.46061

H -2.17099 2.29797 -1.23115
H -2.23884 -2.37585 -0.93353
H -3.56685 -0.08923 3.80011
H -1.91013 -1.37857 2.35788

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Complex 3 - 2nd xyl. hydro black path. prod - p-xyl.

C 13.43140 11.45061 2.40744
C 13.30630 10.56728 1.32388
C 13.92538 9.31118 1.40266
C 14.66573 8.93571 2.52525
C 14.76115 9.83640 3.59381
C 14.14787 11.09280 3.55397
C 12.53632 10.94548 0.11864
C 11.53345 10.15239 -0.53783
C 11.07098 10.89737 -1.68020
C 11.74692 12.14719 -1.68712
C 12.66231 12.17300 -0.58494
La 10.08696 12.00371 0.67721
C 10.77520 9.05281 0.09777
C 10.14885 8.03372 -0.64047
C 9.32633 7.08786 -0.02601
C 9.08864 7.18605 1.35149
C 9.68197 8.17897 2.12848
C 10.53082 9.09669 1.49243
C 10.18555 10.40659 -2.77438
C 8.82495 10.72480 -2.86481
C 8.04218 10.26503 -3.92785
C 8.64929 9.47575 -4.91138
C 10.00619 9.14542 -4.85747
C 10.76142 9.61623 -3.77765
C 11.66944 13.17478 -2.75510
C 10.48523 13.86733 -3.03175
C 10.43201 14.83489 -4.04032
C 11.59002 15.09656 -4.77848
C 12.78709 14.41549 -4.53302
C 12.81077 13.46060 -3.51516
C 13.70282 13.20593 -0.35472
C 13.37905 14.54267 -0.11126
C 14.37488 15.50709 0.07817
C 15.71145 15.10949 0.00201
C 16.07264 13.77947 -0.24671
C 15.05592 12.83962 -0.41674
C 8.69293 5.96338 -0.82716
C 7.70287 6.49590 -1.87130
C 9.44392 8.23419 3.62762
C 10.67290 7.73949 4.40440
C 6.57469 10.65018 -4.02044
C 5.65088 9.42726 -4.08238
C 10.64566 8.32659 -5.96663
C 11.65324 9.16350 -6.76774

C	9.14337	15.59649	-4.30341
C	9.27267	17.07273	-3.90223
C	14.03833	14.70042	-5.34663
C	13.83110	14.40694	-6.83849
C	14.01291	16.94757	0.39802
C	13.13420	17.58238	-0.68726
C	17.53101	13.36240	-0.33764
C	18.25342	14.06413	-1.49594
C	15.37522	7.59215	2.56424
C	16.90049	7.76724	2.55714
C	14.25894	12.06302	4.71854
C	15.70325	12.54251	4.91853
C	9.75414	5.06310	-1.47374
C	9.01543	9.62719	4.10730
C	6.31944	11.58921	-5.20794
C	11.29306	7.03876	-5.44214
C	8.67674	15.46244	-5.75876
C	14.54393	16.13312	-5.12927
C	13.34945	17.05548	1.77884
C	18.27346	13.58142	0.98740
C	14.92605	6.72776	3.74920
C	13.69005	11.47263	6.01561
H	8.44098	12.73135	-0.46617
H	10.90311	13.56755	1.85856
H	8.12566	5.34586	-0.11763
H	7.22128	5.66694	-2.40133
H	6.91952	7.09735	-1.39956
H	8.20328	7.12491	-2.61460
H	9.28008	4.22143	-1.99020
H	10.34714	5.61388	-2.21147
H	10.44307	4.65903	-0.72539
H	10.94463	6.72342	4.10260
H	11.53985	8.38465	4.22605
H	10.47346	7.73274	5.48154
H	8.13634	9.98511	3.55937
H	8.75756	9.60751	5.17120
H	9.82408	10.35967	3.99285
H	6.33258	11.20366	-3.10392
H	5.80410	8.76900	-3.22217
H	4.60046	9.73845	-4.09073
H	5.82650	8.83838	-4.98946
H	6.94446	12.48455	-5.14379
H	6.54245	11.09333	-6.15938
H	5.27081	11.90603	-5.23447
H	8.05882	9.11557	-5.75244
H	9.83952	8.03421	-6.65320
H	11.18453	10.06606	-7.17132
H	12.49272	9.47935	-6.13878
H	12.06087	8.58497	-7.60429
H	10.56685	6.41946	-4.90611
H	11.70024	6.44529	-6.26812

H	12.11881	7.25847	-4.75639
H	11.82199	9.38462	-3.71278
H	9.59589	13.65620	-2.43998
H	8.37128	15.14741	-3.66503
H	9.56174	17.17324	-2.85168
H	10.03264	17.58050	-4.50681
H	8.32324	17.60078	-4.04655
H	8.57414	14.41205	-6.04803
H	7.70760	15.95328	-5.90130
H	9.38612	15.92926	-6.45113
H	11.55994	15.84965	-5.56371
H	14.81800	14.01866	-4.98126
H	13.49577	13.37726	-6.99671
H	13.07776	15.07258	-7.27418
H	14.76314	14.55280	-7.39602
H	14.73711	16.32481	-4.06950
H	15.47361	16.30589	-5.68318
H	13.80999	16.86972	-5.47480
H	13.73402	12.92668	-3.30477
H	12.33230	14.82244	-0.03739
H	16.48794	15.85904	0.14612
H	15.31319	11.80036	-0.60809
H	13.83742	8.62639	0.56246
H	15.09967	7.05864	1.64464
H	17.22807	8.35105	1.69151
H	17.24223	8.28835	3.45832
H	17.40338	6.79435	2.52379
H	13.84255	6.57638	3.74154
H	15.40788	5.74452	3.71355
H	15.19252	7.18982	4.70613
H	15.33385	9.55386	4.47479
H	12.95693	12.43007	2.35146
H	10.32327	7.98291	-1.70951
H	11.10268	9.78785	2.11317
H	8.43265	6.45971	1.82847
H	8.61553	7.54588	3.84135
H	13.65273	12.94066	4.46017
H	12.65018	11.15638	5.88602
H	13.72171	12.21260	6.82274
H	14.26574	10.60038	6.34469
H	15.75841	13.27811	5.72865
H	16.09220	13.00881	4.00865
H	16.36617	11.70988	5.17949
H	18.30210	14.64316	1.25626
H	19.30886	13.22965	0.91562
H	17.78677	13.04247	1.80584
H	17.54255	12.28414	-0.54668
H	17.74698	13.88003	-2.44851
H	19.28577	13.70711	-1.58323
H	18.28958	15.14840	-1.34281
H	12.41490	16.48529	1.81256

H	13.11866	18.09959	2.01905
H	14.00470	16.66177	2.56229
H	14.95340	17.51455	0.43546
H	13.61440	17.53147	-1.66910
H	12.93792	18.63542	-0.45667
H	12.16728	17.07461	-0.76558
H	8.37901	11.36123	-2.10016

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Complex 3 - 1st xyl. hydro red path. TS

La	12.84934	11.91880	4.27246
C	10.67268	12.62793	5.63640
C	9.25199	13.05942	5.67783
C	8.90614	14.41626	5.55809
C	7.57570	14.82329	5.54796
C	6.52919	13.89965	5.64980
C	6.87147	12.54742	5.75478
C	8.20073	12.13500	5.76968
C	5.09116	14.34724	5.67274
C	11.89750	10.19981	2.57636
C	11.76269	9.39945	3.75755
C	12.89961	9.04638	4.54282
C	12.77441	8.41420	5.79311
C	11.53323	8.13680	6.35077
C	10.39803	8.51244	5.59813
C	10.50023	9.12882	4.36629
C	11.38549	7.45480	7.68387
C	15.31348	11.97560	2.52373
C	14.75822	13.28339	2.65492
C	14.88004	13.68616	4.03111
C	15.53379	12.61419	4.73476
C	15.80698	11.56994	3.80535
C	15.50184	11.19956	1.27234
C	15.97184	11.81071	0.10113
C	16.22059	11.06970	-1.05912
C	15.97618	9.69521	-1.03962
C	15.50334	9.04695	0.10596
C	15.28222	9.81231	1.25157
C	14.27250	14.10125	1.50656
C	13.07731	13.82550	0.83291
C	12.66072	14.59119	-0.25926
C	13.48176	15.63985	-0.68917
C	14.69475	15.93253	-0.05923
C	15.07460	15.15276	1.03920
C	14.20270	14.82746	4.69645
C	13.76312	14.70664	6.03189
C	13.09709	15.73869	6.70344
C	12.84274	16.92324	6.01266
C	13.24337	17.08299	4.68065
C	13.91534	16.04078	4.04254
C	16.08998	12.69516	6.11209

C	15.64333	11.89370	7.16966
C	16.17166	12.02229	8.46127
C	17.18870	12.95527	8.66960
C	17.67717	13.76115	7.63294
C	17.10735	13.62623	6.36741
C	16.77002	10.45789	4.01788
C	17.92119	10.41985	3.21570
C	18.89470	9.43329	3.36931
C	18.70365	8.45711	4.35325
C	17.57694	8.46361	5.17861
C	16.62236	9.47127	4.99985
C	16.75558	11.73266	-2.31768
C	18.10949	12.41354	-2.07755
C	15.20339	7.55740	0.06203
C	13.71255	7.31383	-0.22199
C	11.33390	14.29924	-0.93892
C	10.33468	15.44534	-0.72624
C	15.56125	17.08091	-0.55181
C	16.98207	16.63104	-0.91489
C	12.73054	15.57411	8.16964
C	11.30473	16.03036	8.49864
C	12.96245	18.37701	3.93571
C	13.68003	19.57127	4.57974
C	15.63781	11.20069	9.62333
C	15.72898	9.69124	9.37207
C	18.80746	14.74821	7.86858
C	20.09931	14.03475	8.29097
C	20.13490	9.43580	2.49154
C	20.22378	8.17412	1.62287
C	17.38097	7.39415	6.24011
C	17.14645	6.01200	5.61445
C	15.73887	12.71296	-2.91710
C	15.64859	6.80455	1.31992
C	11.50144	13.98113	-2.43013
C	15.59480	18.23583	0.45864
C	13.75684	16.29113	9.06048
C	11.45665	18.64278	3.80338
C	14.20320	11.60989	9.98679
C	18.42137	15.83622	8.87971
C	21.41453	9.63200	3.31605
C	18.54443	7.35354	7.23964
H	16.91766	10.93360	-3.05401
H	16.12591	13.15875	-3.84060
H	14.79763	12.20685	-3.15309
H	15.51087	13.52460	-2.21846
H	18.50766	12.82430	-3.01216
H	18.01905	13.23988	-1.36459
H	18.84239	11.70625	-1.67667
H	16.69829	7.00043	1.55717
H	15.05096	7.08784	2.19296
H	15.52289	5.72545	1.18002

H	13.40234	7.79971	-1.15238
H	13.50213	6.24177	-0.30957
H	13.09157	7.71575	0.58615
H	10.91747	13.40620	-0.45522
H	12.19361	13.14767	-2.58214
H	10.53800	13.71049	-2.87584
H	11.88931	14.84382	-2.98319
H	10.18188	15.64293	0.33900
H	10.68923	16.37152	-1.19264
H	9.36373	15.19941	-1.17024
H	13.17513	16.24786	-1.53849
H	15.09301	17.46137	-1.46972
H	14.58592	18.59959	0.67681
H	16.05030	17.92089	1.40417
H	16.18147	19.07592	0.07045
H	16.96808	15.83479	-1.66504
H	17.55914	17.46917	-1.32078
H	17.52062	16.25660	-0.03742
H	16.01403	15.35340	1.55011
H	13.99261	13.80607	6.59572
H	12.79380	14.50129	8.39714
H	14.76896	15.92150	8.87095
H	13.75109	17.37027	8.86998
H	13.52750	16.13610	10.12084
H	10.56169	15.51612	7.88197
H	11.07398	15.82283	9.54895
H	11.17994	17.10832	8.34774
H	12.33168	17.73897	6.51781
H	13.36561	18.25512	2.92252
H	10.94845	17.80628	3.31436
H	10.99042	18.79135	4.78372
H	11.27474	19.54619	3.21079
H	14.75878	19.39860	4.64486
H	13.51509	20.48281	3.99479
H	13.31062	19.75818	5.59422
H	14.22733	16.18016	3.01533
H	14.85378	11.16459	6.99097
H	17.61047	13.05217	9.66845
H	17.46168	14.24682	5.54815
H	18.05600	11.18399	2.45507
H	20.04396	10.29507	1.81397
H	21.36471	10.54821	3.91254
H	21.57693	8.79518	4.00446
H	22.29105	9.69714	2.66182
H	19.33186	8.06219	0.99916
H	21.09778	8.21827	0.96340
H	20.31911	7.27251	2.23828
H	19.45213	7.67778	4.48170
H	15.74663	9.48204	5.64243
H	16.16269	12.87879	0.10562
H	14.94712	9.32293	2.15979

H	16.16343	9.11055	-1.93962
H	15.77055	7.14736	-0.78532
H	16.47523	7.66092	6.80157
H	16.29384	6.02567	4.92886
H	16.95091	5.26145	6.38858
H	18.02390	5.68360	5.04639
H	18.33987	6.63875	8.04447
H	18.71755	8.33646	7.68835
H	19.47581	7.04269	6.75389
H	19.97702	13.53164	9.25654
H	20.92181	14.75135	8.39223
H	20.39296	13.27879	7.55636
H	19.00254	15.24455	6.90869
H	17.52679	16.37780	8.55747
H	19.23444	16.56126	8.99591
H	18.21669	15.40850	9.86747
H	15.08474	9.38599	8.54001
H	15.40557	9.13325	10.25756
H	16.75236	9.38905	9.13249
H	16.27346	11.42823	10.48959
H	14.13988	12.67993	10.20663
H	13.85251	11.05956	10.86681
H	13.51117	11.39439	9.16470
H	11.30509	13.29751	6.23942
H	10.77151	11.59580	6.01551
H	8.43352	11.07635	5.85755
H	6.08197	11.80186	5.82996
H	9.69527	15.15913	5.46311
H	7.34456	15.88284	5.45526
H	4.75467	14.56537	6.69455
H	4.42509	13.57739	5.27069
H	4.94532	15.25823	5.08367
H	13.89739	9.14385	4.11170
H	9.59767	9.39705	3.82267
H	13.67792	8.11697	6.32255
H	9.40821	8.30075	5.99940
H	12.36000	7.22153	8.12234
H	10.82978	6.51383	7.59376
H	10.83948	8.07996	8.40075
H	12.76457	10.01297	1.94166
H	10.98676	10.41298	2.02060
H	12.44944	13.00461	1.17245
H	11.24758	13.14496	3.29988
H	10.91236	12.96253	4.19480

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Complex 3 - 1st xyl. hydro red path. prod

La	-0.95659	-0.18263	0.97254
C	-6.23660	0.87699	-1.13891
C	-6.61054	-0.58148	-1.18848
C	-5.63697	-1.56430	-1.41105

C	-5.98465	-2.91050	-1.48993
C	-7.31366	-3.32787	-1.34820
C	-8.28173	-2.34625	-1.11828
C	-7.93696	-0.99792	-1.03966
C	-7.68304	-4.78459	-1.45300
C	-1.13569	-2.52298	2.12332
C	-2.28673	-1.83753	2.65331
C	-2.16028	-0.90932	3.72429
C	-3.19799	-0.04321	4.07976
C	-4.40167	-0.00289	3.37020
C	-4.52298	-0.87803	2.27895
C	-3.50522	-1.75597	1.92354
C	-5.52526	0.92004	3.75881
C	1.02335	-0.25113	-1.20397
C	0.69351	1.11212	-0.97436
C	1.10174	1.44156	0.36312
C	1.74955	0.28348	0.92301
C	1.69346	-0.76230	-0.04301
C	0.81853	-1.01661	-2.45618
C	1.19997	-0.48812	-3.69665
C	1.04071	-1.21864	-4.87766
C	0.47354	-2.49305	-4.80016
C	0.07976	-3.05330	-3.58159
C	0.26738	-2.30501	-2.41759
C	0.16903	2.05433	-2.00394
C	-1.14876	2.03335	-2.47485
C	-1.57829	2.92532	-3.46182
C	-0.65865	3.84043	-3.98679
C	0.66902	3.88092	-3.55190
C	1.06664	2.98050	-2.55730
C	0.58327	2.57027	1.16773
C	0.23219	2.35901	2.52079
C	-0.34054	3.36512	3.31279
C	-0.58653	4.60690	2.73105
C	-0.26632	4.85626	1.38926
C	0.30801	3.84097	0.62703
C	2.54249	0.28558	2.17631
C	2.35070	-0.64631	3.20642
C	3.11875	-0.60518	4.37598
C	4.10531	0.37860	4.48974
C	4.33065	1.32043	3.48009
C	3.53332	1.26538	2.33667
C	2.51471	-2.00472	-0.04742
C	3.59297	-2.06836	-0.94208
C	4.43052	-3.18231	-1.00511
C	4.17511	-4.25594	-0.14544
C	3.11266	-4.22976	0.76122
C	2.28868	-3.09849	0.79424
C	1.46601	-0.64954	-6.22096
C	2.95243	-0.27031	-6.24334
C	-0.51473	-4.45073	-3.53806

C	-1.89085	-4.47825	-2.86118
C	-3.02008	2.89936	-3.94164
C	-3.74616	4.21399	-3.62454
C	1.64481	4.88559	-4.14304
C	2.85659	4.20523	-4.79346
C	-0.61274	3.10376	4.78476
C	-1.96601	3.64726	5.25548
C	-0.53346	6.21653	0.76764
C	0.27644	7.32442	1.45490
C	2.88940	-1.55416	5.54333
C	2.34548	-2.92587	5.14102
C	5.43133	2.36031	3.60207
C	6.82036	1.70708	3.62962
C	5.59067	-3.21710	-1.98587
C	5.43145	-4.34260	-3.01679
C	2.83903	-5.40689	1.68409
C	2.29004	-6.61591	0.91347
C	0.58504	0.53717	-6.63365
C	0.44818	-5.44481	-2.87478
C	-3.12197	2.56049	-5.43456
C	2.09148	5.92263	-3.10335
C	0.53163	3.65517	5.64934
C	-2.03130	6.55067	0.75655
C	1.98243	-0.90076	6.59870
C	5.22972	3.27882	4.81444
C	6.94311	-3.31275	-1.26666
C	4.07246	-5.80315	2.50627
H	1.31980	-1.44466	-6.96494
H	0.88351	0.92102	-7.61600
H	-0.46776	0.24363	-6.68881
H	0.66132	1.35663	-5.91116
H	3.24942	0.06975	-7.24180
H	3.16754	0.54179	-5.54059
H	3.58318	-1.12251	-5.97153
H	1.40730	-5.47669	-3.40054
H	0.65273	-5.15954	-1.83757
H	0.02536	-6.45597	-2.87185
H	-2.58319	-3.78087	-3.34256
H	-2.32450	-5.48337	-2.91071
H	-1.81950	-4.20162	-1.80371
H	-3.52503	2.09910	-3.38604
H	-2.63985	1.60373	-5.65519
H	-4.17049	2.49368	-5.74540
H	-2.64133	3.32787	-6.05174
H	-3.71046	4.43832	-2.55392
H	-3.29288	5.05735	-4.15755
H	-4.79802	4.15845	-3.92639
H	-0.97676	4.54180	-4.75672
H	1.10655	5.42451	-4.93461
H	1.23201	6.44378	-2.66999
H	2.64509	5.44952	-2.28450

H	2.74850	6.67244	-3.55824
H	2.54593	3.49053	-5.56160
H	3.51028	4.94752	-5.26469
H	3.45457	3.66238	-4.05313
H	2.09421	2.98520	-2.19930
H	0.49826	1.42024	3.00653
H	-0.62894	2.01364	4.91822
H	1.49241	3.22340	5.35423
H	0.60563	4.74353	5.54636
H	0.36449	3.42676	6.70786
H	-2.78431	3.28210	4.62731
H	-2.16143	3.33955	6.28832
H	-1.99220	4.74208	5.23628
H	-1.02717	5.40059	3.32887
H	-0.20057	6.16097	-0.27652
H	-2.60491	5.77773	0.23612
H	-2.42940	6.63538	1.77391
H	-2.20970	7.50594	0.25090
H	1.34804	7.10335	1.43489
H	0.11720	8.28582	0.95448
H	-0.02023	7.44407	2.50283
H	0.55590	4.04010	-0.40836
H	1.58647	-1.40824	3.08641
H	4.71544	0.40171	5.39143
H	3.69144	1.98369	1.53606
H	3.77708	-1.22519	-1.60321
H	5.57430	-2.26506	-2.53300
H	7.07109	-2.49319	-0.55280
H	7.03280	-4.25377	-0.71251
H	7.76880	-3.27241	-1.98594
H	4.48170	-4.25438	-3.55278
H	6.24382	-4.31339	-3.75160
H	5.45456	-5.32741	-2.53690
H	4.81915	-5.13204	-0.18524
H	1.44229	-3.07800	1.47403
H	1.63386	0.50640	-3.73150
H	-0.01449	-2.72609	-1.45531
H	0.33658	-3.06836	-5.71504
H	-0.65505	-4.77007	-4.57985
H	2.06079	-5.08577	2.38935
H	1.37243	-6.36085	0.37526
H	2.06546	-7.44322	1.59622
H	3.01773	-6.97698	0.17814
H	3.81832	-6.58731	3.22784
H	4.47821	-4.94918	3.05723
H	4.87174	-6.19385	1.86685
H	6.94396	1.07643	4.51702
H	7.60697	2.46952	3.65157
H	6.97905	1.07699	2.74921
H	5.37924	2.98713	2.70183
H	4.25655	3.77783	4.77653

H	6.00664	4.05056	4.84756
H	5.28239	2.71766	5.75405
H	1.31498	-2.86202	4.77378
H	2.33577	-3.59837	6.00498
H	2.95473	-3.38514	4.35770
H	3.87042	-1.71473	6.01240
H	2.38788	0.05775	6.93685
H	1.86778	-1.55152	7.47276
H	0.98436	-0.71327	6.18630
H	-6.34145	1.34454	-2.12610
H	-6.87933	1.43505	-0.45014
H	-8.71365	-0.25766	-0.85756
H	-9.32194	-2.64067	-0.99489
H	-4.59464	-1.26665	-1.51034
H	-5.20736	-3.65223	-1.66291
H	-7.62790	-5.13551	-2.49079
H	-8.70187	-4.96608	-1.09878
H	-7.00603	-5.41347	-0.86502
H	-1.25005	-0.92149	4.32258
H	-3.65488	-2.41172	1.06938
H	-3.06221	0.61619	4.93456
H	-5.43431	-0.87499	1.68496
H	-5.21672	1.61755	4.54295
H	-6.38908	0.36046	4.13772
H	-5.87635	1.50980	2.90483
H	-0.35869	-2.77276	2.84742
H	-1.34235	-3.34077	1.43013
H	-1.84033	1.30617	-2.05134
H	-2.34463	-0.07346	-0.62300
H	-5.19663	1.00760	-0.82548

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Complex 3 - 1st xyl. hydro red path. prod - p-xyl.

La	-0.92844	-0.19563	0.98183
C	-1.13033	-2.53859	2.18098
C	-2.30054	-1.83314	2.62596
C	-2.22234	-0.86209	3.66537
C	-3.25128	0.05187	3.90572
C	-4.40237	0.09615	3.11279
C	-4.48020	-0.83334	2.06332
C	-3.47216	-1.75919	1.82033
C	-5.51568	1.07422	3.37561
C	1.04908	-0.25173	-1.19207
C	0.71463	1.10968	-0.96092
C	1.12186	1.43911	0.37711
C	1.77495	0.28259	0.93517
C	1.72072	-0.76241	-0.03196
C	0.83674	-1.01681	-2.44304
C	1.21714	-0.49123	-3.68493
C	1.04335	-1.21889	-4.86564
C	0.46217	-2.48700	-4.78618

C	0.06843	-3.04377	-3.56599
C	0.27240	-2.29915	-2.40254
C	0.17713	2.04853	-1.98695
C	-1.14334	2.01498	-2.44951
C	-1.58979	2.90608	-3.42940
C	-0.68390	3.83338	-3.95702
C	0.64650	3.88583	-3.53138
C	1.06105	2.98605	-2.54291
C	0.59076	2.55898	1.18602
C	0.25410	2.34225	2.54160
C	-0.33128	3.33771	3.33870
C	-0.60900	4.57283	2.75843
C	-0.30552	4.82680	1.41294
C	0.28450	3.82405	0.64691
C	2.57216	0.28816	2.18590
C	2.38472	-0.64069	3.21944
C	3.15436	-0.59338	4.38772
C	4.13761	0.39421	4.49736
C	4.35928	1.33282	3.48372
C	3.56092	1.27093	2.34131
C	2.53633	-2.00813	-0.03491
C	3.60832	-2.08291	-0.93616
C	4.43875	-3.20213	-0.99886
C	4.18217	-4.26997	-0.13240
C	3.12563	-4.23294	0.78080
C	2.30889	-3.09640	0.81386
C	1.46454	-0.65182	-6.21111
C	2.95101	-0.27357	-6.24046
C	-0.54960	-4.43088	-3.51915
C	-1.93086	-4.42902	-2.85198
C	-3.03620	2.86640	-3.89454
C	-3.77944	4.16161	-3.53919
C	1.60778	4.90274	-4.12534
C	2.82011	4.23701	-4.78985
C	-0.57643	3.06526	4.81377
C	-1.86903	3.69033	5.34711
C	-0.61128	6.17924	0.79185
C	0.17481	7.30846	1.47190
C	2.92921	-1.53980	5.55790
C	2.40372	-2.91941	5.15799
C	5.45772	2.37584	3.59984
C	6.84825	1.72566	3.62605
C	5.59281	-3.24841	-1.98625
C	5.42242	-4.37909	-3.00972
C	2.84925	-5.40511	1.70915
C	2.28021	-6.60966	0.94606
C	0.58261	0.53536	-6.62087
C	0.39051	-5.43819	-2.84335
C	-3.15113	2.55929	-5.39324
C	2.05403	5.93816	-3.08386
C	0.63400	3.51426	5.64788

C	-2.11732	6.47455	0.79194
C	2.00875	-0.89260	6.60531
C	5.25753	3.29824	4.80950
C	6.94895	-3.34622	-1.27432
C	4.08616	-5.81288	2.52033
H	1.31443	-1.44743	-6.95382
H	0.87710	0.91865	-7.60466
H	-0.47063	0.24244	-6.67124
H	0.66245	1.35490	-5.89884
H	3.24398	0.06437	-7.24082
H	3.16968	0.53989	-5.54039
H	3.58240	-1.12562	-5.96962
H	1.35339	-5.48939	-3.36071
H	0.59125	-5.15171	-1.80571
H	-0.05002	-6.44174	-2.83888
H	-2.60695	-3.72061	-3.34015
H	-2.38392	-5.42563	-2.89926
H	-1.86224	-4.14777	-1.79561
H	-3.52151	2.04599	-3.35064
H	-2.65458	1.61676	-5.64151
H	-4.20232	2.48043	-5.69215
H	-2.69304	3.34884	-5.99947
H	-3.73418	4.36167	-2.46412
H	-3.34576	5.02406	-4.05792
H	-4.83400	4.09566	-3.82952
H	-1.01480	4.53473	-4.72154
H	1.05800	5.44105	-4.90940
H	1.19369	6.44944	-2.64057
H	2.61836	5.46558	-2.27207
H	2.70074	6.69608	-3.54013
H	2.50944	3.52365	-5.55922
H	3.46304	4.98782	-5.26242
H	3.42917	3.69556	-4.05758
H	2.09085	3.00114	-2.19162
H	0.54012	1.40843	3.02486
H	-0.66462	1.97590	4.92595
H	1.54994	3.01823	5.31369
H	0.78452	4.59594	5.55848
H	0.48482	3.27976	6.70779
H	-2.73250	3.41368	4.73404
H	-2.05585	3.35804	6.37374
H	-1.81203	4.78393	5.37036
H	-1.06329	5.35751	3.35748
H	-0.28513	6.13082	-0.25480
H	-2.67468	5.68598	0.27734
H	-2.50938	6.55061	1.81234
H	-2.32445	7.42398	0.28624
H	1.25156	7.11495	1.44447
H	-0.01268	8.26483	0.97159
H	-0.11731	7.42184	2.52183
H	0.51915	4.02767	-0.39067

H	1.62123	-1.40402	3.10372
H	4.74851	0.42256	5.39837
H	3.71565	1.98677	1.53784
H	3.79326	-1.24407	-1.60252
H	5.57776	-2.29956	-2.53894
H	7.08506	-2.52289	-0.56631
H	7.03726	-4.28423	-0.71485
H	7.77062	-3.31434	-1.99862
H	4.46997	-4.28963	-3.54069
H	6.23063	-4.35758	-3.74937
H	5.44402	-5.36130	-2.52448
H	4.82043	-5.15027	-0.17221
H	1.46662	-3.06780	1.49918
H	1.66035	0.49921	-3.72114
H	-0.01023	-2.71760	-1.43935
H	0.31290	-3.05948	-5.70095
H	-0.68784	-4.75360	-4.56023
H	2.08136	-5.07440	2.42128
H	1.36062	-6.34562	0.41562
H	2.05299	-7.43326	1.63243
H	2.99723	-6.97983	0.20478
H	3.83044	-6.59278	3.24596
H	4.50624	-4.96222	3.06563
H	4.87519	-6.21354	1.87439
H	6.97540	1.09829	4.51528
H	7.63327	2.48987	3.64343
H	7.00608	1.09293	2.74738
H	5.40205	2.99944	2.69758
H	4.28382	3.79618	4.77211
H	6.03380	4.07082	4.83817
H	5.31293	2.74047	5.75097
H	1.37473	-2.86901	4.78458
H	2.39704	-3.58868	6.02452
H	3.02270	-3.37433	4.37979
H	3.90929	-1.68717	6.03322
H	2.40215	0.07129	6.94234
H	1.89579	-1.54137	7.48111
H	1.01130	-0.71729	6.18607
H	-1.35160	-0.86557	4.31971
H	-3.57895	-2.44882	0.98646
H	-3.14975	0.75000	4.73406
H	-5.35116	-0.82792	1.41127
H	-5.21631	1.83344	4.10383
H	-6.40544	0.57122	3.77417
H	-5.82286	1.59134	2.45997
H	-0.38189	-2.75858	2.94341
H	-1.29754	-3.37231	1.49689
H	-1.82282	1.27745	-2.02407
H	-2.26502	-0.11228	-0.63694

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Complex 3 - 2nd xyl. hydro red path.

C	1.40649	-3.39512	-0.67979
C	1.93159	-2.11619	-0.45582
C	3.31499	-1.99020	-0.26502
C	4.16011	-3.10247	-0.27830
C	3.59567	-4.36650	-0.48062
C	2.22156	-4.52967	-0.68656
C	1.07478	-0.90552	-0.45066
C	0.24225	-0.47586	-1.53115
C	-0.24579	0.82590	-1.23420
C	0.25144	1.19757	0.05887
C	1.08380	0.12764	0.53391
La	-1.52688	-0.68449	0.79404
C	-1.34150	-3.10477	1.64719
C	-2.34887	-2.64930	2.57190
C	-2.01803	-1.81285	3.67458
C	-2.99811	-1.24613	4.49531
C	-4.36013	-1.42541	4.24578
C	-4.70148	-2.17539	3.10797
C	-3.73917	-2.75159	2.28760
C	-5.41837	-0.85389	5.15115
C	0.06355	-1.18141	-2.82543
C	1.17995	-1.45449	-3.62700
C	1.04340	-2.08088	-4.86839
C	-0.23839	-2.45474	-5.28431
C	-1.37139	-2.20757	-4.50502
C	-1.20661	-1.55727	-3.27772
C	-0.95220	1.71784	-2.19915
C	-2.34528	1.79587	-2.30968
C	-2.95297	2.67665	-3.20931
C	-2.13656	3.48177	-4.01114
C	-0.74271	3.41414	-3.94398
C	-0.16534	2.52671	-3.02951
C	-0.28297	2.29516	0.89284
C	-0.57965	2.06257	2.25353
C	-1.16154	3.04349	3.06686
C	-1.45190	4.28495	2.50025
C	-1.17461	4.55695	1.15416
C	-0.60250	3.55806	0.36582
C	1.90145	0.14129	1.76921
C	1.97318	-0.97051	2.62444
C	2.78582	-0.96244	3.76260
C	3.54160	0.18381	4.03101
C	3.49795	1.30938	3.20238
C	2.66743	1.27459	2.08067
C	2.24877	-2.35592	-5.75189
C	3.01470	-1.07206	-6.09797
C	-2.74755	-2.63222	-4.98807
C	-3.42849	-3.59487	-4.00570
C	-4.46843	2.76578	-3.28485
C	-5.00240	2.61078	-4.71425

C	0.11650	4.28130	-4.84925
C	1.00342	5.24566	-4.05028
C	-1.43237	2.76450	4.53598
C	-0.53479	3.62016	5.44051
C	-1.45300	5.92752	0.55979
C	-2.90479	6.37585	0.76776
C	2.86928	-2.13871	4.72538
C	2.02053	-1.87527	5.97987
C	4.37168	2.52313	3.47257
C	4.16690	3.09798	4.87955
C	5.65760	-2.92958	-0.08173
C	6.15220	-3.62731	1.19231
C	1.61389	-5.90808	-0.88843
C	1.73305	-6.76502	0.37991
C	3.18286	-3.40221	-5.12928
C	-3.64160	-1.41819	-5.27472
C	-4.97815	4.06792	-2.64993
C	0.95518	3.43482	-5.81643
C	-2.91193	2.94704	4.89739
C	-0.47027	6.97367	1.10630
C	2.50693	-3.48928	4.10437
C	5.85270	2.20354	3.22123
C	6.45249	-3.39636	-1.30884
C	2.20859	-6.63425	-2.10157
H	1.86601	-2.77341	-6.69334
H	3.83505	-1.28626	-6.79228
H	2.35751	-0.33106	-6.56337
H	3.45118	-0.61559	-5.20278
H	4.02773	-3.61473	-5.79429
H	3.58610	-3.05376	-4.17267
H	2.65307	-4.34103	-4.94164
H	-2.80372	-4.47314	-3.81423
H	-3.62533	-3.10573	-3.04556
H	-4.38859	-3.94023	-4.40562
H	-3.17920	-0.75353	-6.01121
H	-4.61663	-1.73520	-5.66201
H	-3.81314	-0.83729	-4.36246
H	-4.86507	1.93145	-2.69162
H	-4.64813	1.68294	-5.17236
H	-6.09788	2.59521	-4.71472
H	-4.68756	3.44212	-5.35477
H	-4.64537	4.15675	-1.61116
H	-4.60624	4.94269	-3.19547
H	-6.07334	4.10623	-2.66226
H	-2.59102	4.17559	-4.71619
H	-0.57029	4.88969	-5.45343
H	0.40472	5.87983	-3.38861
H	1.72409	4.70169	-3.42977
H	1.57195	5.89780	-4.72258
H	0.32113	2.77297	-6.41406
H	1.52331	4.07548	-6.50019

H	1.67141	2.80745	-5.27496
H	0.91672	2.45185	-2.95231
H	-0.27060	1.12772	2.72422
H	-1.17509	1.71210	4.71575
H	0.52268	3.45919	5.21154
H	-0.74670	4.68730	5.31197
H	-0.69803	3.37224	6.49505
H	-3.55323	2.30529	4.28619
H	-3.08353	2.69809	5.95041
H	-3.23529	3.98282	4.74843
H	-1.89276	5.06233	3.11984
H	-1.28523	5.84536	-0.52171
H	-3.60965	5.63843	0.37256
H	-3.13410	6.52421	1.82879
H	-3.08787	7.32786	0.25806
H	0.56710	6.67770	0.92241
H	-0.63680	7.94739	0.63253
H	-0.59376	7.10263	2.18751
H	-0.38633	3.76402	-0.67703
H	1.40962	-1.86257	2.36844
H	4.19279	0.18587	4.90375
H	2.62953	2.13320	1.41492
H	3.73855	-1.00168	-0.10677
H	5.84079	-1.85374	0.04084
H	5.62038	-3.25920	2.07479
H	6.00003	-4.71093	1.13691
H	7.22327	-3.45026	1.34152
H	6.12791	-2.87367	-2.21385
H	7.52342	-3.20892	-1.17211
H	6.32349	-4.47059	-1.48126
H	4.24076	-5.24269	-0.48256
H	0.33811	-3.50883	-0.84293
H	2.16410	-1.16244	-3.27028
H	-2.06700	-1.33971	-2.64736
H	-0.35704	-2.95259	-6.24618
H	-2.60391	-3.17083	-5.93491
H	0.54404	-5.75944	-1.08610
H	2.09808	-6.03756	-3.01165
H	1.70779	-7.59580	-2.26023
H	3.27618	-6.83784	-1.96279
H	1.24251	-7.73504	0.24144
H	1.26999	-6.26800	1.23780
H	2.78260	-6.95555	0.63078
H	6.21215	1.43482	3.91447
H	6.47281	3.09608	3.36081
H	6.01052	1.83347	2.20354
H	4.07383	3.29761	2.75329
H	3.11826	3.35582	5.05592
H	4.76683	4.00437	5.01529
H	4.47083	2.38478	5.65366
H	1.43857	-3.55357	3.86924

H	2.72763	-4.29852	4.80806
H	3.06485	-3.67763	3.18239
H	3.91774	-2.19727	5.05124
H	2.29977	-0.93379	6.46291
H	2.14269	-2.68306	6.70996
H	0.95699	-1.81580	5.72239
H	-0.96830	-1.68353	3.93755
H	-4.05475	-3.33581	1.42627
H	-2.68703	-0.65784	5.35642
H	-5.75218	-2.31654	2.86114
H	-6.23815	-0.40335	4.58111
H	-5.00717	-0.08456	5.81099
H	-5.86058	-1.62931	5.78929
H	-0.35762	-3.32089	2.06426
H	-1.66457	-3.85538	0.92350
H	-2.95708	1.13569	-1.69592
H	-3.05900	-0.70877	-0.66552
H	-3.97747	0.32893	1.98843
H	-3.75587	0.96651	1.66665

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Complex 3 - 2nd xyl. hydro red path. TS

C	1.66543	-3.01137	-0.25374
C	2.35012	-1.81675	0.01692
C	3.70608	-1.89491	0.36541
C	4.37108	-3.12147	0.44303
C	3.65098	-4.29119	0.17871
C	2.29646	-4.25450	-0.16824
C	1.67707	-0.50278	-0.10574
C	0.90431	-0.08116	-1.23430
C	0.56089	1.28352	-1.06374
C	1.09022	1.71805	0.19874
C	1.80000	0.61173	0.77942
La	-0.83854	0.12733	1.16634
C	-1.32881	-2.26996	2.08210
C	-1.75926	-3.25843	3.10110
C	-0.83201	-4.03429	3.81367
C	-1.24163	-4.92347	4.80394
C	-2.59262	-5.07950	5.12886
C	-3.51992	-4.30920	4.41695
C	-3.11595	-3.41745	3.42936
C	-3.03390	-6.02262	6.21708
C	0.65174	-0.87868	-2.46163
C	1.72763	-1.24225	-3.28133
C	1.52795	-1.97397	-4.45446
C	0.22345	-2.35949	-4.77949
C	-0.87170	-2.02079	-3.98024
C	-0.64335	-1.26450	-2.82554
C	-0.06142	2.14483	-2.10916
C	-1.44442	2.26397	-2.29028
C	-1.97477	3.09834	-3.27875

C	-1.09132	3.81559	-4.09306
C	0.29417	3.70786	-3.95137
C	0.79409	2.86575	-2.95205
C	0.59310	2.89500	0.94426
C	0.23245	2.76098	2.30572
C	-0.37929	3.79864	3.02406
C	-0.62195	5.00237	2.36392
C	-0.26601	5.18369	1.02021
C	0.32276	4.12779	0.32458
C	2.55900	0.66566	2.05046
C	2.40333	-0.29263	3.06177
C	3.09641	-0.18945	4.27592
C	3.97232	0.88289	4.45141
C	4.16963	1.84914	3.45559
C	3.44999	1.72997	2.26830
C	2.68731	-2.32918	-5.37033
C	3.34043	-1.07318	-5.96401
C	-2.27213	-2.46843	-4.36257
C	-2.90079	-3.36094	-3.28376
C	-3.47977	3.22819	-3.44747
C	-3.93823	2.88745	-4.87145
C	1.22722	4.48093	-4.86845
C	2.12375	5.45414	-4.09134
C	-0.75302	3.60423	4.48366
C	-0.01414	4.59048	5.39790
C	-0.49189	6.51723	0.32839
C	-1.95417	6.97426	0.40152
C	2.90511	-1.20882	5.38621
C	1.45519	-1.24815	5.88714
C	5.14586	2.99594	3.65461
C	4.73746	3.89795	4.82668
C	5.85663	-3.16462	0.76274
C	6.18898	-4.11906	1.91598
C	1.51970	-5.53066	-0.44823
C	1.45971	-6.44444	0.78326
C	3.73037	-3.21192	-4.67299
C	-3.18059	-1.27447	-4.68444
C	-3.97275	4.62211	-3.03446
C	2.06513	3.54064	-5.74547
C	-2.27134	3.68726	4.69355
C	0.45101	7.59390	0.88543
C	3.38838	-2.60372	4.96836
C	6.58587	2.49147	3.82137
C	6.67801	-3.51167	-0.48784
C	2.07524	-6.28106	-1.66601
H	2.26919	-2.90850	-6.20484
H	4.12844	-1.34475	-6.67545
H	2.60553	-0.45354	-6.48678
H	3.79720	-0.45854	-5.18059
H	4.53531	-3.48051	-5.36631
H	4.18367	-2.69594	-3.81995

H	3.28190	-4.13671	-4.29824
H	-2.26840	-4.22775	-3.06734
H	-3.04559	-2.80812	-2.34934
H	-3.88143	-3.72727	-3.60748
H	-2.75395	-0.66035	-5.48360
H	-4.17134	-1.61534	-5.00527
H	-3.31413	-0.63530	-3.80534
H	-3.94053	2.49961	-2.76785
H	-3.60440	1.88892	-5.16740
H	-5.03123	2.91634	-4.94089
H	-3.54399	3.60265	-5.60203
H	-3.69298	4.85042	-2.00149
H	-3.54302	5.39912	-3.67673
H	-5.06354	4.68873	-3.11437
H	-1.48684	4.47304	-4.86546
H	0.59405	5.07934	-5.53765
H	1.52851	6.14684	-3.48783
H	2.80066	4.91887	-3.41631
H	2.74077	6.04524	-4.77710
H	1.42606	2.87513	-6.33359
H	2.69422	4.11209	-6.43721
H	2.72434	2.91326	-5.13577
H	1.86785	2.75815	-2.81761
H	0.52418	1.86882	2.86322
H	-0.43792	2.59073	4.76490
H	1.07009	4.50885	5.27655
H	-0.29868	5.62589	5.18087
H	-0.25460	4.39426	6.44828
H	-2.79818	2.95065	4.07914
H	-2.52543	3.49569	5.74152
H	-2.65638	4.67945	4.43369
H	-1.08858	5.82160	2.90592
H	-0.24455	6.37298	-0.73108
H	-2.62880	6.21361	-0.00213
H	-2.26150	7.18206	1.43233
H	-2.09619	7.89497	-0.17431
H	1.49834	7.28951	0.79581
H	0.32240	8.53815	0.34508
H	0.24858	7.78569	1.94512
H	0.58803	4.26318	-0.71822
H	1.73917	-1.13933	2.89737
H	4.51595	0.96186	5.39122
H	3.57991	2.47026	1.48288
H	4.25532	-0.97823	0.56321
H	6.14464	-2.15303	1.07854
H	5.61041	-3.87729	2.81230
H	5.97496	-5.16042	1.65145
H	7.25310	-4.05918	2.16943
H	6.48297	-2.80362	-1.29914
H	7.75142	-3.49274	-0.26804
H	6.42781	-4.51373	-0.85375

H	4.15750	-5.25203	0.23820
H	0.62100	-2.97275	-0.55370
H	2.73037	-0.93887	-2.99143
H	-1.47455	-0.96922	-2.18717
H	0.05577	-2.94011	-5.68603
H	-2.17778	-3.07022	-5.27687
H	0.49050	-5.23268	-0.68762
H	2.07409	-5.64350	-2.55502
H	1.47082	-7.16903	-1.88211
H	3.10448	-6.61501	-1.49342
H	0.85937	-7.33639	0.57304
H	1.01090	-5.93024	1.63836
H	2.46009	-6.78011	1.07877
H	6.69224	1.88519	4.72768
H	7.28348	3.33238	3.90101
H	6.89101	1.87479	2.97038
H	5.11300	3.60582	2.74194
H	3.72716	4.29418	4.68660
H	5.42530	4.74543	4.92058
H	4.75450	3.35066	5.77555
H	2.81983	-2.98354	4.11294
H	3.27065	-3.31665	5.79164
H	4.44445	-2.58445	4.68229
H	3.53308	-0.88178	6.22602
H	1.11676	-0.25499	6.19878
H	1.36325	-1.92235	6.74551
H	0.76827	-1.60980	5.11513
H	0.22680	-3.94864	3.57864
H	-3.86501	-2.83959	2.89197
H	-0.49439	-5.51474	5.32966
H	-4.58066	-4.41262	4.63745
H	-3.99053	-6.49649	5.97450
H	-3.16663	-5.49826	7.17211
H	-2.29867	-6.81612	6.38210
H	-0.33654	-2.53325	1.67848
H	-2.04468	-2.24375	1.23609
H	-2.10923	1.68581	-1.64938
H	-2.44724	0.13281	-0.21506
H	-1.54101	-1.01952	2.93311
H	-1.69300	-0.13259	3.28034

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Complex 3 - 2nd xyl. hydro red path. prod

C	1.28283	-2.98760	-0.31662
C	1.95046	-1.76458	-0.15412
C	3.32343	-1.79156	0.13041
C	4.02132	-2.99505	0.25148
C	3.31825	-4.19491	0.09513
C	1.94881	-4.20950	-0.18733
C	1.24085	-0.47432	-0.31232
C	0.39792	-0.12615	-1.41456

C	0.02011	1.22959	-1.27974
C	0.61145	1.74079	-0.07183
C	1.39181	0.68483	0.50868
La	-1.14741	0.16461	1.16778
C	-2.06661	-2.68566	1.90033
C	-2.95658	-3.81198	2.36101
C	-2.43881	-4.89099	3.08275
C	-3.26903	-5.91549	3.53113
C	-4.64379	-5.89749	3.27561
C	-5.15699	-4.81794	2.54814
C	-4.33021	-3.79230	2.09878
C	-5.54697	-6.99028	3.78410
C	0.10012	-0.99651	-2.58063
C	1.13617	-1.35282	-3.45318
C	0.90103	-2.17148	-4.56057
C	-0.39892	-2.64326	-4.76932
C	-1.45576	-2.30868	-3.91822
C	-1.19272	-1.47197	-2.82779
C	-0.74473	2.00368	-2.29708
C	-2.14415	2.03745	-2.32683
C	-2.83033	2.78544	-3.28781
C	-2.08592	3.50019	-4.23283
C	-0.68931	3.47216	-4.24597
C	-0.03177	2.71806	-3.26763
C	0.14844	2.95723	0.63299
C	-0.13588	2.90557	2.01670
C	-0.71603	3.98417	2.70044
C	-0.99129	5.14729	1.98298
C	-0.70426	5.24868	0.61433
C	-0.15527	4.15044	-0.04617
C	2.16867	0.76666	1.76569
C	2.01192	-0.19042	2.77977
C	2.70363	-0.09442	3.99191
C	3.59318	0.96955	4.15964
C	3.79121	1.93511	3.16414
C	3.06214	1.82690	1.97964
C	2.01353	-2.52272	-5.53440
C	2.46049	-1.29046	-6.33417
C	-2.85220	-2.84759	-4.17736
C	-3.36996	-3.68795	-3.00248
C	-4.34966	2.82432	-3.28926
C	-4.94271	2.39568	-4.63755
C	0.08662	4.22884	-5.31085
C	1.04763	5.26117	-4.70707
C	-1.02923	3.86960	4.18234
C	-0.29544	4.93384	5.00848
C	-0.96266	6.54028	-0.14281
C	-2.42309	6.99712	-0.03845
C	2.46628	-1.06825	5.13441
C	1.30348	-0.57743	6.01326
C	4.78811	3.06581	3.35380

C	4.44344	3.94247	4.56455
C	5.51697	-2.98909	0.52170
C	5.87260	-3.70744	1.82979
C	1.19506	-5.51552	-0.37808
C	1.35732	-6.46618	0.81483
C	3.20972	-3.19197	-4.84624
C	-3.83721	-1.72252	-4.52247
C	-4.87507	4.20629	-2.87551
C	0.82859	3.26982	-6.25239
C	-2.54214	3.91492	4.43721
C	-0.00344	7.64920	0.31390
C	2.23081	-2.51211	4.68152
C	6.22617	2.53644	3.44700
C	6.30478	-3.57374	-0.65909
C	1.59665	-6.20486	-1.68989
H	1.59628	-3.24542	-6.24907
H	3.21770	-1.56266	-7.07817
H	1.61659	-0.82975	-6.85664
H	2.89727	-0.53239	-5.67455
H	3.96509	-3.48265	-5.58485
H	3.68976	-2.51502	-4.13158
H	2.90482	-4.08842	-4.29853
H	-2.68171	-4.50523	-2.76486
H	-3.49016	-3.07644	-2.10176
H	-4.34709	-4.12367	-3.23896
H	-3.49006	-1.14581	-5.38548
H	-4.82643	-2.13085	-4.75832
H	-3.95159	-1.03079	-3.68124
H	-4.68738	2.10259	-2.53408
H	-4.58556	1.40446	-4.93110
H	-6.03646	2.36267	-4.58385
H	-4.67423	3.09760	-5.43480
H	-4.49484	4.49448	-1.89070
H	-4.56727	4.97645	-3.59188
H	-5.96995	4.20939	-2.83195
H	-2.60223	4.08913	-4.98913
H	-0.65002	4.77808	-5.91299
H	0.51596	5.97047	-4.06476
H	1.82362	4.77883	-4.10244
H	1.55126	5.82958	-5.49686
H	0.13936	2.55441	-6.71111
H	1.33213	3.82273	-7.05333
H	1.58995	2.69640	-5.71242
H	1.05484	2.67529	-3.25207
H	0.16741	2.04670	2.61843
H	-0.67556	2.88403	4.50975
H	0.78570	4.89010	4.84500
H	-0.63181	5.94454	4.75176
H	-0.48365	4.78565	6.07723
H	-3.05312	3.10843	3.90317
H	-2.75445	3.79844	5.50542

H	-2.97398	4.86831	4.11238
H	-1.43238	5.99753	2.49804
H	-0.75649	6.33628	-1.20138
H	-3.10843	6.21562	-0.37930
H	-2.69259	7.25406	0.99183
H	-2.59044	7.88808	-0.65317
H	1.04085	7.34231	0.20003
H	-0.15735	8.56105	-0.27358
H	-0.16414	7.90040	1.36827
H	0.05248	4.21989	-1.10825
H	1.35642	-1.04328	2.61343
H	4.14654	1.04191	5.09445
H	3.19281	2.56837	1.19547
H	3.85684	-0.85185	0.24520
H	5.81753	-1.93860	0.63122
H	5.34942	-3.26158	2.68107
H	5.60318	-4.76860	1.78920
H	6.94931	-3.64739	2.02348
H	6.07931	-3.04143	-1.58823
H	7.38323	-3.50451	-0.47833
H	6.06105	-4.63059	-0.81406
H	3.85107	-5.13878	0.18759
H	0.22690	-2.98748	-0.57794
H	2.13692	-0.97741	-3.25559
H	-1.99155	-1.18558	-2.14561
H	-0.59411	-3.29039	-5.62382
H	-2.78340	-3.50825	-5.05255
H	0.12926	-5.26226	-0.45397
H	1.42391	-5.54743	-2.54704
H	1.01666	-7.12230	-1.84035
H	2.65807	-6.47734	-1.68259
H	0.73792	-7.35946	0.68064
H	1.06069	-5.98504	1.75200
H	2.39498	-6.79972	0.92574
H	6.35813	1.90217	4.33057
H	6.93969	3.36435	3.52219
H	6.48706	1.94021	2.56717
H	4.72656	3.69968	2.45916
H	3.43100	4.34918	4.48311
H	5.14219	4.78238	4.64471
H	4.50160	3.37415	5.49930
H	1.27017	-2.62218	4.16659
H	2.20582	-3.17956	5.54909
H	3.01675	-2.85977	4.00453
H	3.37605	-1.05987	5.75086
H	1.49949	0.42592	6.40432
H	1.14939	-1.25059	6.86403
H	0.37241	-0.53449	5.43699
H	-1.37299	-4.93382	3.29583
H	-4.75530	-2.96706	1.53206
H	-2.83917	-6.74647	4.08622

H	-6.22117	-4.78089	2.32529
H	-6.36321	-7.19370	3.08406
H	-6.00351	-6.71241	4.74225
H	-4.99806	-7.92309	3.94326
H	-1.05179	-3.04510	1.68896
H	-2.48693	-2.23514	0.98545
H	-2.70176	1.45448	-1.59398
H	-2.84878	-0.16266	-0.07475
H	-2.01211	-1.91134	2.69238
H	-1.68050	0.18022	3.25952

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Complex 3 - 2nd xyl. + THF

C	2.58158	1.47223	1.86793
C	1.65497	1.98570	0.94756
C	1.78345	3.32095	0.53912
C	2.79718	4.14115	1.03845
C	3.71176	3.59390	1.94720
C	3.62097	2.26325	2.36843
C	0.54878	1.14887	0.43119
C	0.16882	0.97418	-0.94156
C	-0.98905	0.12334	-0.96556
C	-1.28969	-0.24329	0.37581
C	-0.34808	0.39738	1.23969
La	1.30885	-1.38088	-0.34244
O	3.33715	-2.81216	-1.14240
C	3.20837	-3.74215	-2.25431
C	4.00031	-4.99123	-1.85478
C	4.10875	-4.86667	-0.33086
C	4.23320	-3.36466	-0.14777
C	1.02486	1.28541	-2.10694
C	0.49825	1.61282	-3.36636
C	1.32782	1.82034	-4.47143
C	2.70958	1.66907	-4.31730
C	3.28219	1.34301	-3.08592
C	2.42921	1.15715	-1.99257
C	-1.86727	-0.16395	-2.13679
C	-1.75021	-1.31426	-2.92637
C	-2.61410	-1.54951	-3.99946
C	-3.61100	-0.60622	-4.27421
C	-3.76315	0.54882	-3.50273
C	-2.87858	0.75723	-2.43844
C	-2.47628	-1.01817	0.81416
C	-2.70994	-2.32056	0.35639
C	-3.83950	-3.03880	0.75936
C	-4.74472	-2.42895	1.63280
C	-4.54447	-1.12730	2.10439
C	-3.40393	-0.43734	1.68919
C	-0.42622	0.44742	2.72169
C	-0.31312	-0.69800	3.51303
C	-0.41171	-0.62963	4.90725

C	-0.64352	0.61268	5.50106
C	-0.76834	1.78097	4.73866
C	-0.65198	1.68084	3.35196
C	0.75036	2.21230	-5.82111
C	-0.13721	1.10504	-6.40411
C	4.79602	1.27122	-2.96263
C	5.37952	2.67070	-2.70910
C	-2.48590	-2.82124	-4.82226
C	-2.22875	-2.53055	-6.30662
C	-4.87909	1.53587	-3.80235
C	-5.88091	1.62269	-2.64247
C	-4.06070	-4.45784	0.26244
C	-3.94929	-5.48010	1.40199
C	-5.54375	-0.46667	3.03973
C	-6.91875	-0.30078	2.37802
C	-0.22986	-1.87437	5.75951
C	-1.24814	-2.96881	5.41565
C	-1.03163	3.12600	5.39462
C	-2.37428	3.14308	6.13830
C	2.86670	5.60515	0.63512
C	2.55777	6.52365	1.82625
C	4.60775	1.68251	3.36811
C	4.45690	2.33492	4.74949
C	-0.00365	3.54708	-5.74788
C	5.29439	0.28588	-1.90230
C	-3.71024	-3.73038	-4.64634
C	-4.33878	2.92444	-4.16891
C	-5.39428	-4.60621	-0.48193
C	-5.66154	-1.21448	4.37431
C	1.20725	-2.40637	5.65837
C	0.11630	3.54736	6.32171
C	4.20802	5.97633	-0.00927
C	6.05679	1.77301	2.87217
H	0.22146	-3.02378	-1.19817
H	1.98800	-1.90609	1.62518
H	1.59963	2.35076	-6.50395
H	-0.50664	1.38915	-7.39573
H	0.41907	0.16769	-6.50503
H	-1.00446	0.91021	-5.76508
H	-0.35760	3.84422	-6.74118
H	-0.87737	3.47362	-5.09194
H	0.63775	4.34541	-5.36158
H	5.07204	3.37706	-3.48618
H	5.03510	3.05949	-1.74485
H	6.47461	2.63822	-2.69027
H	4.86125	-0.71051	-2.03614
H	6.38428	0.19399	-1.95671
H	5.05368	0.62831	-0.88939
H	-1.61413	-3.36413	-4.43418
H	-1.33670	-1.91160	-6.44128
H	-2.08502	-3.46274	-6.86445

H	-3.07309	-2.00119	-6.76221
H	-3.87095	-3.97597	-3.59262
H	-4.61978	-3.24586	-5.01871
H	-3.58182	-4.66739	-5.20002
H	-4.29869	-0.77704	-5.10101
H	-5.41961	1.15121	-4.67795
H	-6.29027	0.63752	-2.39929
H	-5.40490	2.01577	-1.73757
H	-6.71394	2.28763	-2.89704
H	-3.65580	2.87105	-5.02267
H	-5.15746	3.60386	-4.43099
H	-3.79340	3.37215	-3.33076
H	-2.97781	1.64241	-1.81463
H	-1.98585	-2.78232	-0.31289
H	-3.25610	-4.67301	-0.45298
H	-2.98165	-5.40345	1.90737
H	-4.73047	-5.32163	2.15408
H	-4.05637	-6.50216	1.02090
H	-5.46899	-3.89083	-1.30670
H	-5.49933	-5.61659	-0.89325
H	-6.24573	-4.43282	0.18564
H	-5.62666	-2.97974	1.95451
H	-5.15939	0.53839	3.25925
H	-6.84260	0.26023	1.44144
H	-7.36728	-1.27348	2.14697
H	-7.60830	0.23291	3.04195
H	-4.68781	-1.29600	4.86631
H	-6.34533	-0.69264	5.05344
H	-6.04923	-2.22894	4.22895
H	-3.23114	0.57344	2.04956
H	-0.10519	-1.64746	3.02860
H	-0.72336	0.66738	6.58573
H	-0.74139	2.57616	2.74090
H	1.06182	3.72683	-0.16599
H	2.08375	5.76612	-0.11802
H	1.58610	6.28458	2.26906
H	3.31546	6.41965	2.61078
H	2.54277	7.57395	1.51424
H	4.40987	5.35991	-0.89026
H	4.20766	7.02616	-0.32279
H	5.03974	5.84261	0.69116
H	4.50580	4.22294	2.34509
H	2.47851	0.44058	2.20537
H	-0.57626	1.71640	-3.47156
H	2.87004	0.99767	-1.00931
H	3.35825	1.82292	-5.17874
H	5.17231	0.92842	-3.93685
H	4.36057	0.61867	3.47806
H	6.17613	1.28676	1.89871
H	6.73849	1.28843	3.57992
H	6.37925	2.81473	2.76561

H	5.13547	1.87154	5.47445
H	3.43441	2.22900	5.12349
H	4.69166	3.40466	4.70997
H	0.22789	2.84867	7.15831
H	-0.06897	4.54193	6.74318
H	1.06777	3.57762	5.78225
H	-1.09203	3.86867	4.58759
H	-3.19995	2.87885	5.47027
H	-2.57611	4.13631	6.55518
H	-2.37707	2.42788	6.96839
H	1.44987	-2.68996	4.62845
H	1.34175	-3.28825	6.29537
H	1.93078	-1.64649	5.97056
H	-0.40253	-1.57826	6.80360
H	-2.27419	-2.60147	5.51277
H	-1.12886	-3.83019	6.08257
H	-1.12035	-3.32423	4.38784
H	4.99708	-4.97798	-2.30838
H	3.49900	-5.90850	-2.17338
H	3.19662	-5.22675	0.15624
H	4.96065	-5.41176	0.08401
H	3.59890	-3.25929	-3.15582
H	2.13822	-3.93720	-2.37681
H	-0.99175	-2.05329	-2.66886
H	5.25247	-3.01019	-0.35209
H	3.89651	-2.99314	0.82503

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Complex 3 - 2nd xyl. + THF RO TS

C	12.69632	15.80383	5.47762
C	11.74341	16.32511	4.58902
C	11.87013	17.66228	4.18556
C	12.90574	18.47219	4.65571
C	13.84572	17.91464	5.53116
C	13.75834	16.58254	5.94795
C	10.61748	15.49986	4.09548
C	10.21192	15.33162	2.72949
C	9.04410	14.49663	2.72430
C	8.75302	14.13880	4.06764
C	9.72044	14.75714	4.91665
La	11.37935	12.95069	3.33821
O	13.39750	11.95007	2.82061
C	13.98792	11.11023	1.87595
C	15.06600	10.29098	2.58978
C	14.43087	9.89475	3.90536
C	13.92558	11.05520	4.69163
C	11.02607	15.67732	1.54242
C	10.44676	16.03560	0.31656
C	11.22923	16.27960	-0.81625
C	12.61569	16.14194	-0.71950
C	13.24184	15.79587	0.48246

C	12.43512	15.56835	1.60045
C	8.16363	14.17971	1.56304
C	8.31394	13.02190	0.78982
C	7.45646	12.74326	-0.27758
C	6.42858	13.64992	-0.56160
C	6.24035	14.80913	0.19557
C	7.12099	15.06193	1.25378
C	7.53996	13.41370	4.51991
C	7.26304	12.10592	4.10398
C	6.09873	11.44792	4.51254
C	5.20452	12.12318	5.34881
C	5.45015	13.43086	5.78095
C	6.62383	14.05962	5.36100
C	9.68685	14.74524	6.39831
C	9.64446	13.54520	7.11598
C	9.58205	13.53163	8.51338
C	9.54187	14.75218	9.19036
C	9.57270	15.97410	8.50625
C	9.65414	15.95253	7.11358
C	10.59182	16.69851	-2.13049
C	9.67388	15.60620	-2.69411
C	14.76189	15.71471	0.52775
C	15.38352	17.11162	0.36620
C	7.62657	11.46698	-1.08550
C	7.90290	11.75332	-2.56733
C	5.08724	15.75080	-0.10996
C	4.07718	15.79408	1.04541
C	5.82024	10.02701	4.05064
C	5.78043	9.04093	5.22620
C	4.46466	14.16305	6.67691
C	3.09922	14.33935	5.99865
C	9.58225	12.22085	9.28250
C	8.40309	11.31923	8.89649
C	9.47920	17.29627	9.25024
C	8.08835	17.48426	9.87349
C	12.97526	19.93630	4.25335
C	12.69546	20.85445	5.45199
C	14.77710	15.98721	6.90614
C	14.69107	16.63593	8.29452
C	9.84746	18.03402	-1.99542
C	15.32388	15.03225	1.77601
C	6.42117	10.53067	-0.92316
C	5.56961	17.16163	-0.47192
C	4.53349	9.94135	3.21844
C	4.31680	13.48096	8.04336
C	10.91838	11.48200	9.11926
C	10.57867	17.45668	10.30732
C	14.30521	20.30068	3.58233
C	16.20583	16.06094	6.35199
H	10.20228	11.28880	2.66631
H	12.36466	12.33366	5.19170

H	11.40925	16.84835	-2.84899
H	9.25583	15.91353	-3.65924
H	10.22283	14.67135	-2.84457
H	8.83943	15.39605	-2.01732
H	9.44649	18.35206	-2.96417
H	9.00680	17.95004	-1.29881
H	10.51018	18.82256	-1.62517
H	15.03380	17.60861	-0.54332
H	15.11800	17.74675	1.21795
H	16.47627	17.04698	0.31966
H	14.88534	14.04360	1.94413
H	16.40801	14.91171	1.67896
H	15.14476	15.63540	2.67351
H	8.50394	10.94781	-0.67838
H	8.78540	12.38817	-2.69054
H	8.07398	10.82076	-3.11676
H	7.05652	12.26439	-3.03973
H	6.24884	10.28843	0.12956
H	5.50639	10.98965	-1.31457
H	6.58177	9.59311	-1.46733
H	5.74453	13.44576	-1.38388
H	4.56758	15.34478	-0.98853
H	3.70575	14.79278	1.28339
H	4.53408	16.20171	1.95374
H	3.21996	16.42702	0.78930
H	6.25552	17.13992	-1.32462
H	4.72294	17.80623	-0.73308
H	6.09408	17.63007	0.36826
H	6.99404	15.95146	1.86627
H	7.97953	11.59575	3.46226
H	6.65539	9.73386	3.40123
H	6.71157	9.07213	5.80041
H	4.95839	9.27454	5.91201
H	5.63363	8.01508	4.86943
H	4.56827	10.62664	2.36610
H	4.38373	8.92506	2.83652
H	3.65424	10.20174	3.81845
H	4.29416	11.62042	5.67015
H	4.87741	15.16548	6.85290
H	3.19838	14.85170	5.03676
H	2.62111	13.37137	5.81148
H	2.42323	14.92587	6.63118
H	5.28430	13.39780	8.54748
H	3.64149	14.05038	8.69212
H	3.90479	12.47082	7.94051
H	6.83279	15.07517	5.68858
H	9.66394	12.60570	6.56965
H	9.48193	14.74516	10.27746
H	9.67864	16.89073	6.56478
H	11.13101	18.07623	3.50390
H	12.17829	20.10285	3.51644

H	11.73102	20.62061	5.91320
H	13.46768	20.74438	6.22148
H	12.68064	21.90544	5.14232
H	14.48770	19.67989	2.70013
H	14.30201	21.34909	3.26441
H	15.15021	20.16704	4.26664
H	14.65835	18.53506	5.90399
H	12.60135	14.77257	5.81775
H	9.36806	16.12998	0.25652
H	12.91372	15.36541	2.55613
H	13.22583	16.31798	-1.60447
H	15.06720	15.11832	-0.34491
H	14.52148	14.92576	7.02360
H	16.27942	15.57410	5.37439
H	16.91049	15.56930	7.03200
H	16.53472	17.09909	6.23228
H	15.39522	16.16437	8.98920
H	13.68412	16.53760	8.71028
H	14.93264	17.70367	8.24847
H	10.49090	16.70011	11.09466
H	10.51293	18.43966	10.78691
H	11.57354	17.36223	9.86216
H	9.61863	18.09199	8.50621
H	7.30257	17.41334	9.11513
H	8.00717	18.46297	10.35993
H	7.88978	16.71720	10.63035
H	11.09294	11.21721	8.07052
H	10.92751	10.55696	9.70701
H	11.75660	12.10484	9.44732
H	9.47226	12.47273	10.34632
H	7.44780	11.83176	9.04190
H	8.39804	10.40753	9.50459
H	8.45637	11.01787	7.84523
H	15.95126	10.91217	2.77121
H	15.37535	9.42359	1.99867
H	13.63160	9.15865	3.75902
H	15.16581	9.42027	4.57951
H	14.43703	11.71064	1.07102
H	13.24745	10.43356	1.42112
H	9.08740	12.30260	1.05895
H	14.60264	11.87754	4.89444
H	13.31041	10.77745	5.53495

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Complex 3 - 2nd xyl. + THF RO prod

C	2.33775	1.37200	2.00242
C	1.64576	1.93786	0.90874
C	2.25225	3.01555	0.24332
C	3.48495	3.52737	0.65017
C	4.14516	2.92809	1.73137
C	3.58773	1.84927	2.41859

C	0.38933	1.32161	0.43386
C	0.14159	0.93298	-0.92590
C	-0.96150	0.03303	-0.92950
C	-1.42233	-0.11464	0.41901
C	-0.59253	0.67917	1.25550
La	1.27746	-1.23621	0.41038
O	2.51157	-2.20872	-1.02011
C	3.36560	-3.06220	-1.72581
C	4.69031	-3.30277	-1.00071
C	4.62846	-4.16207	0.26775
C	3.83722	-3.58088	1.44221
C	0.79476	1.49651	-2.14211
C	0.18522	2.59307	-2.76599
C	0.74524	3.19369	-3.89694
C	1.94281	2.67284	-4.39501
C	2.57520	1.57329	-3.80769
C	1.98476	0.99136	-2.68009
C	-1.61106	-0.51680	-2.14346
C	-0.87203	-1.20972	-3.11410
C	-1.47166	-1.70082	-4.27447
C	-2.84194	-1.48242	-4.45774
C	-3.61012	-0.79919	-3.51289
C	-2.98104	-0.32544	-2.35690
C	-2.65696	-0.81738	0.84370
C	-2.87972	-2.16676	0.55989
C	-4.05962	-2.81176	0.94735
C	-5.03372	-2.07062	1.62121
C	-4.84889	-0.71247	1.91322
C	-3.65680	-0.10297	1.52161
C	-0.68858	0.76074	2.72957
C	-0.76871	-0.40473	3.50425
C	-0.82973	-0.34206	4.90285
C	-0.83544	0.91331	5.51307
C	-0.77422	2.09940	4.76710
C	-0.68840	2.00596	3.37885
C	0.07327	4.37390	-4.57722
C	-1.28777	3.98185	-5.16896
C	3.84702	1.01450	-4.42415
C	4.94378	0.73214	-3.39179
C	-0.65113	-2.45168	-5.30910
C	-0.61405	-1.70815	-6.65143
C	-5.09892	-0.59135	-3.73638
C	-5.93125	-1.43846	-2.76328
C	-4.20291	-4.30018	0.66792
C	-3.43205	-5.11446	1.71994
C	-5.92067	0.08900	2.63361
C	-7.22332	0.15897	1.82494
C	-0.90269	-1.60956	5.73691
C	-2.23823	-2.33788	5.53193
C	-0.83471	3.45796	5.44549
C	-2.20967	3.69730	6.08599

C	4.07460	4.73866	-0.05277
C	4.00876	5.98094	0.84832
C	4.30100	1.21259	3.59966
C	4.46695	2.19951	4.76294
C	-0.05886	5.58107	-3.63933
C	3.54477	-0.23721	-5.26141
C	-1.14142	-3.89456	-5.49064
C	-5.49796	0.88799	-3.66097
C	-5.65047	-4.78398	0.56017
C	-6.18100	-0.44480	4.04864
C	0.28113	-2.54746	5.46292
C	0.28891	3.65112	6.47157
C	5.50518	4.49669	-0.54932
C	5.65362	0.61206	3.19278
H	0.25480	-2.84555	1.40112
H	2.75513	-3.61872	1.26652
H	0.72217	4.67441	-5.41129
H	-1.73422	4.82540	-5.70720
H	-1.18939	3.14433	-5.86616
H	-1.98834	3.67783	-4.38377
H	-0.48884	6.43800	-4.16945
H	-0.71330	5.35594	-2.79004
H	0.91490	5.88236	-3.24014
H	5.16749	1.62198	-2.79556
H	4.65268	-0.06759	-2.70272
H	5.86626	0.41502	-3.89005
H	2.80639	-0.02380	-6.04026
H	4.45345	-0.61330	-5.74490
H	3.14154	-1.03772	-4.63151
H	0.37804	-2.49819	-4.92902
H	-0.22985	-0.69102	-6.52825
H	0.02669	-2.23292	-7.36900
H	-1.61467	-1.63514	-7.09180
H	-1.14074	-4.43551	-4.53929
H	-2.16225	-3.92000	-5.88765
H	-0.49920	-4.43728	-6.19331
H	-3.32938	-1.85354	-5.35785
H	-5.32141	-0.94060	-4.75404
H	-5.69311	-2.50181	-2.86539
H	-5.73405	-1.15464	-1.72421
H	-7.00291	-1.30858	-2.95290
H	-4.91897	1.49209	-4.36653
H	-6.56077	1.01324	-3.89587
H	-5.33259	1.29502	-2.65769
H	-3.55734	0.20761	-1.60644
H	-2.10548	-2.73471	0.05059
H	-3.72187	-4.48293	-0.30317
H	-2.38197	-4.80996	1.76451
H	-3.86751	-4.96575	2.71478
H	-3.47026	-6.18561	1.49042
H	-6.22245	-4.19204	-0.16144

H	-5.67596	-5.82999	0.23717
H	-6.16806	-4.73375	1.52500
H	-5.95802	-2.55474	1.92542
H	-5.53913	1.11400	2.73418
H	-7.05004	0.57954	0.82949
H	-7.66302	-0.83593	1.69376
H	-7.96449	0.78442	2.33523
H	-5.26090	-0.45676	4.64033
H	-6.91572	0.17903	4.57018
H	-6.57396	-1.46724	4.02129
H	-3.49690	0.95051	1.73866
H	-0.78316	-1.37028	2.99893
H	-0.89606	0.96586	6.59885
H	-0.63534	2.91237	2.78025
H	1.73971	3.46718	-0.59999
H	3.44866	4.93266	-0.93328
H	2.98274	6.18349	1.17043
H	4.62051	5.84696	1.74745
H	4.38155	6.86458	0.31867
H	5.55841	3.61804	-1.19891
H	5.86395	5.36169	-1.11736
H	6.20050	4.34126	0.28279
H	5.10870	3.31981	2.04901
H	1.85209	0.60964	2.61526
H	-0.74459	2.97234	-2.34944
H	2.45081	0.12142	-2.22086
H	2.39423	3.13422	-5.27274
H	4.23033	1.78280	-5.10979
H	3.66538	0.39019	3.95534
H	5.54315	-0.11332	2.38036
H	6.12106	0.10245	4.04216
H	6.34617	1.38857	2.85027
H	4.92841	1.70631	5.62522
H	3.50095	2.60387	5.07855
H	5.10699	3.04241	4.48012
H	0.20688	2.93286	7.29456
H	0.24714	4.65615	6.90563
H	1.27309	3.52129	6.01133
H	-0.69928	4.21413	4.66062
H	-3.01208	3.59771	5.34865
H	-2.26731	4.70133	6.52106
H	-2.40203	2.97467	6.88672
H	0.27186	-2.90977	4.42901
H	0.23881	-3.42222	6.12125
H	1.23616	-2.04010	5.63642
H	-0.84780	-1.30388	6.79095
H	-3.08379	-1.68992	5.78215
H	-2.29345	-3.23033	6.16542
H	-2.35824	-2.65495	4.49112
H	5.13327	-2.32458	-0.76489
H	5.37559	-3.78750	-1.70974

H	4.21714	-5.14850	0.01465
H	5.65885	-4.34423	0.59963
H	3.58451	-2.63415	-2.71755
H	2.86780	-4.02942	-1.90562
H	0.19292	-1.37094	-2.96049
H	4.13868	-2.54325	1.64384
H	4.02092	-4.14956	2.35991

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Complex 3 THF ROP dimer

C	2.72645	1.22296	1.05798
C	1.55211	1.66229	0.43539
C	1.50140	2.98685	-0.02317
C	2.58136	3.85786	0.12914
C	3.73888	3.38053	0.75432
C	3.82913	2.06803	1.22703
C	0.35193	0.80271	0.24680
C	-0.21975	0.48971	-1.03029
C	-1.47016	-0.16481	-0.80046
C	-1.67484	-0.25296	0.60595
C	-0.54652	0.33730	1.26029
La	0.62734	-1.98309	0.09599
O	2.13077	-3.34947	-1.19587
C	1.57543	-3.76193	-2.44031
C	2.10436	-2.92798	-3.60122
C	1.55981	-3.34461	-4.97161
C	1.99067	-4.73581	-5.43479
C	0.31693	0.95011	-2.33483
C	-0.53567	1.56522	-3.26084
C	-0.04568	2.12062	-4.44767
C	1.32284	2.03860	-4.70366
C	2.20948	1.41958	-3.81313
C	1.69056	0.87979	-2.63481
C	-2.46467	-0.55948	-1.83092
C	-2.16811	-1.48611	-2.84047
C	-3.10971	-1.84667	-3.80623
C	-4.36414	-1.22752	-3.77099
C	-4.69509	-0.29012	-2.79031
C	-3.73913	0.02229	-1.81776
C	-2.96438	-0.62023	1.25384
C	-3.50374	-1.91061	1.21269
C	-4.74398	-2.19598	1.79405
C	-5.45275	-1.15957	2.41137
C	-4.94490	0.14389	2.46701
C	-3.69775	0.39313	1.88898
C	-0.39656	0.45528	2.72885
C	-0.88160	-0.56053	3.57375
C	-0.80120	-0.45759	4.96505
C	-0.19697	0.67878	5.51345
C	0.30411	1.70612	4.70771
C	0.19223	1.58364	3.32111

C	-0.97028	2.82742	-5.42497
C	-1.97245	1.85666	-6.06246
C	3.68959	1.37756	-4.16853
C	4.61549	1.08568	-2.98766
C	-2.78834	-2.89392	-4.85811
C	-2.78389	-2.30522	-6.27473
C	-6.07647	0.34337	-2.77620
C	-6.94318	-0.24972	-1.65665
C	-5.29962	-3.61058	1.74762
C	-5.53936	-4.18216	3.15134
C	-5.73109	1.27404	3.11351
C	-7.02387	1.57672	2.34336
C	-1.39926	-1.49972	5.89903
C	-2.78991	-1.04943	6.37481
C	0.92496	2.95177	5.31760
C	-0.13662	3.82260	6.00529
C	2.49112	5.28843	-0.37513
C	2.66528	6.30769	0.75883
C	5.09537	1.56192	1.89795
C	5.50516	2.43143	3.09348
C	-1.69050	4.01689	-4.77579
C	3.94911	0.39001	-5.31724
C	-3.73458	-4.09871	-4.76478
C	-6.02603	1.87336	-2.68492
C	-6.57494	-3.69312	0.89790
C	-6.02931	1.00687	4.59424
C	-1.47535	-2.90818	5.30767
C	2.07171	2.62107	6.28127
C	3.48638	5.55144	-1.51349
C	6.24875	1.42575	0.89413
H	-0.86145	-3.46082	0.44979
H	1.60864	-5.53022	-4.78681
H	-0.33808	3.22663	-6.22993
H	-2.60974	2.37665	-6.78668
H	-1.45555	1.04683	-6.58657
H	-2.62223	1.40254	-5.30706
H	-2.29271	4.55439	-5.51662
H	-2.36488	3.68756	-3.97785
H	-0.97694	4.72295	-4.33961
H	4.43939	1.77269	-2.15452
H	4.49054	0.06281	-2.61476
H	5.66092	1.18882	-3.29619
H	3.32365	0.61037	-6.18782
H	4.99751	0.42919	-5.63276
H	3.73083	-0.63526	-4.99984
H	-1.77402	-3.25816	-4.64788
H	-2.07637	-1.47508	-6.35549
H	-2.50415	-3.06705	-7.01089
H	-3.77468	-1.92654	-6.54901
H	-3.72335	-4.53438	-3.76121
H	-4.76698	-3.81128	-4.99232

H	-3.44249	-4.87603	-5.47939
H	-5.10905	-1.48299	-4.52263
H	-6.55309	0.08874	-3.73281
H	-7.04749	-1.33276	-1.77278
H	-6.49735	-0.06510	-0.67391
H	-7.94639	0.19158	-1.66477
H	-5.41809	2.30064	-3.48864
H	-7.03406	2.29551	-2.76022
H	-5.60256	2.20642	-1.73140
H	-3.97675	0.73484	-1.03383
H	-2.92645	-2.70308	0.74054
H	-4.53839	-4.23485	1.26216
H	-4.62450	-4.15893	3.75115
H	-6.30527	-3.61243	3.68931
H	-5.88152	-5.22150	3.09282
H	-6.39622	-3.32473	-0.11647
H	-6.92940	-4.72776	0.82862
H	-7.38213	-3.09385	1.33415
H	-6.42173	-1.37148	2.85976
H	-5.09916	2.17096	3.06250
H	-6.81610	1.81302	1.29536
H	-7.70612	0.71954	2.36231
H	-7.54954	2.42978	2.78702
H	-5.10806	0.84814	5.16177
H	-6.56181	1.85452	5.03994
H	-6.65841	0.11881	4.72100
H	-3.28399	1.39860	1.92414
H	-1.35513	-1.42978	3.12760
H	-0.12775	0.76248	6.59700
H	0.55589	2.38722	2.68875
H	0.59496	3.33815	-0.50958
H	1.48069	5.41903	-0.78461
H	1.93633	6.14107	1.55805
H	3.66555	6.24450	1.20131
H	2.53338	7.32901	0.38485
H	3.32896	4.85488	-2.34229
H	3.37505	6.57143	-1.89795
H	4.52081	5.43663	-1.17086
H	4.58948	4.04747	0.87719
H	2.79483	0.20147	1.42504
H	-1.59341	1.63786	-3.02821
H	2.36826	0.43760	-1.91017
H	1.71638	2.48490	-5.61647
H	3.94247	2.38044	-4.54311
H	4.87597	0.55684	2.28158
H	5.99043	0.73415	0.08734
H	7.14865	1.04519	1.38961
H	6.49764	2.39482	0.44685
H	6.36955	1.99519	3.60561
H	4.69014	2.52518	3.81757
H	5.78827	3.44139	2.77715

H	1.71249	2.07389	7.15989
H	2.55109	3.53840	6.64015
H	2.83473	2.00529	5.79516
H	1.34743	3.53618	4.48971
H	-0.93733	4.09252	5.30989
H	0.30731	4.74716	6.39130
H	-0.59333	3.29350	6.84932
H	-2.18898	-2.96004	4.47868
H	-1.81072	-3.61883	6.07034
H	-0.50319	-3.24479	4.93586
H	-0.74675	-1.54441	6.78279
H	-2.75114	-0.06127	6.84366
H	-3.20088	-1.75692	7.10396
H	-3.48102	-0.99422	5.52717
H	3.20052	-2.99350	-3.59990
H	1.86267	-1.87249	-3.41948
H	0.46342	-3.28361	-4.95951
H	1.88661	-2.60110	-5.70846
H	0.47037	-3.67850	-2.40205
H	1.78135	-4.82842	-2.59340
H	-1.17853	-1.93833	-2.88021
H	3.08200	-4.82536	-5.44900
H	1.62767	-4.93731	-6.44797
C	2.29165	-6.96846	2.30557
C	3.18125	-7.53745	1.38558
C	3.07245	-8.91118	1.12291
C	2.10643	-9.70343	1.74499
C	1.22651	-9.09509	2.64775
C	1.30588	-7.73099	2.94258
C	4.24491	-6.76450	0.69152
C	4.41055	-6.68930	-0.73214
C	5.65255	-6.03006	-0.98951
C	6.25266	-5.69960	0.25855
C	5.37984	-6.14205	1.30133
La	3.85944	-4.04158	0.24828
O	2.37498	-2.67517	1.56187
C	2.60402	-2.13379	2.86236
C	2.52403	-3.18387	3.96271
C	2.67856	-2.57665	5.35854
C	2.61161	-3.61537	6.47492
C	3.50302	-7.31306	-1.72613
C	4.02187	-8.02856	-2.81270
C	3.18524	-8.70546	-3.70764
C	1.80711	-8.65457	-3.50012
C	1.24336	-7.94331	-2.43185
C	2.10429	-7.27501	-1.56021
C	6.34536	-5.87932	-2.29794
C	5.93090	-4.97211	-3.28080
C	6.62325	-4.83561	-4.48679
C	7.74006	-5.64975	-4.70781
C	8.17874	-6.57284	-3.75641

C	7.47474	-6.66802	-2.55131
C	7.65412	-5.23564	0.43288
C	8.13262	-4.04810	-0.13191
C	9.47315	-3.67232	-0.00366
C	10.34261	-4.51221	0.70013
C	9.89839	-5.70623	1.27949
C	8.55191	-6.05068	1.13892
C	5.63689	-5.95077	2.74557
C	6.19298	-4.74319	3.20675
C	6.48864	-4.54350	4.55872
C	6.21026	-5.57754	5.45832
C	5.65934	-6.79357	5.03735
C	5.37471	-6.96324	3.68117
C	3.76069	-9.50661	-4.86374
C	4.49242	-8.60785	-5.86935
C	-0.27095	-7.94766	-2.26615
C	-0.75887	-7.49761	-0.88874
C	6.20583	-3.79352	-5.51078
C	5.98837	-4.38897	-6.90731
C	9.40343	-7.43164	-4.02421
C	10.56967	-7.04497	-3.10473
C	9.96392	-2.37560	-0.62649
C	10.56502	-1.42344	0.41554
C	10.85624	-6.62855	2.01808
C	11.87222	-7.26522	1.05931
C	7.16839	-3.28077	5.06607
C	8.69068	-3.48633	5.12794
C	5.42556	-7.93537	6.01300
C	6.75686	-8.57122	6.44058
C	2.02681	-11.19137	1.44754
C	2.27683	-12.03758	2.70321
C	0.33686	-7.08190	3.91636
C	0.32720	-7.77975	5.28226
C	4.66806	-10.64358	-4.37500
C	-0.95101	-7.12439	-3.37121
C	7.21594	-2.63760	-5.55856
C	9.09398	-8.93084	-3.92268
C	10.95498	-2.63817	-1.76913
C	11.57099	-5.92379	3.17787
C	6.83659	-2.02086	4.26379
C	4.60256	-7.51613	7.23686
C	0.69707	-11.56997	0.78155
C	-1.07883	-7.00209	3.32708
H	5.32995	-2.58446	-0.22887
H	3.40560	-4.36154	6.36592
H	2.91119	-9.96634	-5.38726
H	4.86791	-9.19678	-6.71383
H	3.82513	-7.83530	-6.26395
H	5.34634	-8.10350	-5.40497
H	5.02040	-11.24697	-5.21903
H	5.54955	-10.25309	-3.85545

H	4.13734	-11.30377	-3.68179
H	-0.27518	-8.05741	-0.08276
H	-0.57570	-6.43045	-0.71879
H	-1.83974	-7.65201	-0.80652
H	-0.64857	-7.45609	-4.36922
H	-2.04107	-7.20778	-3.30163
H	-0.69037	-6.06472	-3.27680
H	5.24667	-3.37716	-5.17505
H	5.26634	-5.21057	-6.88401
H	5.61416	-3.62469	-7.59718
H	6.92234	-4.77865	-7.32671
H	7.33798	-2.17850	-4.57298
H	8.19994	-2.99112	-5.88621
H	6.88776	-1.86274	-6.26025
H	8.29234	-5.55932	-5.64133
H	9.71530	-7.22986	-5.05814
H	10.83577	-5.99080	-3.22529
H	10.31000	-7.19795	-2.05222
H	11.45671	-7.64918	-3.32619
H	8.28186	-9.21563	-4.59881
H	9.97656	-9.52604	-4.18179
H	8.79667	-9.20877	-2.90569
H	7.80324	-7.36308	-1.78342
H	7.43281	-3.39981	-0.65315
H	9.08572	-1.87900	-1.05903
H	9.85133	-1.21403	1.21835
H	11.46628	-1.84701	0.87273
H	10.84669	-0.47095	-0.04716
H	10.50795	-3.27620	-2.53738
H	11.26263	-1.69836	-2.24172
H	11.85909	-3.13781	-1.40278
H	11.38946	-4.23145	0.79921
H	10.25257	-7.43963	2.44682
H	11.37046	-7.82088	0.26129
H	12.50112	-6.50165	0.58802
H	12.53185	-7.95849	1.59358
H	10.85439	-5.50563	3.89047
H	12.21736	-6.62567	3.71653
H	12.20289	-5.10390	2.81847
H	8.18975	-6.97725	1.57874
H	6.43894	-3.96821	2.48424
H	6.44718	-5.43018	6.51070
H	4.96253	-7.90762	3.33824
H	3.76135	-9.36402	0.41451
H	2.82869	-11.41677	0.73213
H	3.23979	-11.79233	3.16197
H	1.49759	-11.87331	3.45568
H	2.27877	-13.10505	2.45662
H	0.53947	-10.99726	-0.13718
H	0.68160	-12.63549	0.52667
H	-0.15123	-11.37634	1.44746

H	0.46554	-9.69933	3.13680
H	2.36341	-5.90955	2.54932
H	5.09801	-8.07896	-2.94175
H	1.69071	-6.74582	-0.70684
H	1.15078	-9.19794	-4.17931
H	-0.58808	-8.99229	-2.40282
H	0.68541	-6.05322	4.07610
H	-1.08690	-6.44197	2.38753
H	-1.76087	-6.50413	4.02502
H	-1.47765	-8.00291	3.12684
H	-0.31368	-7.23735	5.98580
H	1.33321	-7.83493	5.70906
H	-0.06080	-8.80167	5.20873
H	5.13795	-6.78404	7.85139
H	4.39150	-8.38285	7.87259
H	3.64772	-7.07023	6.94249
H	4.85068	-8.70063	5.47502
H	7.32998	-8.91154	5.57265
H	6.58498	-9.43250	7.09592
H	7.37677	-7.85217	6.98789
H	7.24810	-2.06451	3.24988
H	7.26781	-1.14003	4.75064
H	5.75614	-1.86584	4.18378
H	6.81440	-3.12274	6.09460
H	8.94967	-4.35366	5.74321
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H	3.63678	-2.04354	5.41790
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H	3.59190	-1.64812	2.88719
H	5.06340	-4.34262	-3.09502
H	1.65257	-4.14533	6.46788
H	2.72355	-3.14816	7.45880

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Complex 3 - 2nd xyl. dimer

C	5.03708	-1.28092	-1.37643
C	3.70612	-1.55282	-1.72685
C	3.29923	-1.29624	-3.04238
C	4.18493	-0.79120	-3.99733
C	5.50711	-0.54113	-3.61191
C	5.95106	-0.77873	-2.30815
C	2.83247	-2.22581	-0.72940
C	2.50514	-1.81345	0.61482
C	1.95015	-2.96717	1.28423
C	1.87302	-4.03132	0.34343
C	2.42006	-3.57785	-0.89084
C	2.47194	-0.42295	1.11567

C	1.92115	-0.10631	2.38033
C	1.82049	1.20799	2.85215
C	2.26545	2.25461	2.02668
C	2.80913	1.99597	0.75880
C	2.87831	0.66860	0.31411
C	1.29893	1.52433	4.24723
C	0.40963	0.43247	4.84501
C	3.37425	3.14810	-0.05985
C	3.52331	2.84351	-1.55115
La	-0.01186	-1.96836	-0.53200
La	-0.29423	1.24199	0.51078
C	-1.98366	3.00553	-1.10632
C	-2.88040	2.07444	-0.49792
C	-2.86490	2.30832	0.91329
C	-1.95807	3.39599	1.18357
C	-1.45659	3.85081	-0.08689
C	-3.83583	1.22813	-1.26069
C	-5.20651	1.29988	-0.98559
C	-6.14095	0.57374	-1.73437
C	-5.67624	-0.23095	-2.77276
C	-4.31516	-0.31565	-3.09096
C	-3.41034	0.42110	-2.32834
C	-7.62826	0.64826	-1.43239
C	-8.16031	2.08575	-1.49541
C	-3.89369	-1.16244	-4.28201
C	-2.47043	-1.71617	-4.19172
C	-3.77910	1.60070	1.85501
C	-3.65356	0.23372	2.12588
C	-4.56985	-0.43606	2.94390
C	-5.63440	0.29029	3.48502
C	-5.80062	1.65630	3.23111
C	-4.86283	2.29628	2.41535
C	-1.49826	3.93405	2.49207
C	-0.30283	4.67795	2.56744
C	0.15385	5.25855	3.75425
C	-0.59180	5.06942	4.91961
C	-1.76545	4.30818	4.90395
C	-2.19937	3.74879	3.69983
C	-0.93426	5.21349	-0.37800
C	0.18098	5.48593	-1.17887
C	0.52794	6.80373	-1.51407
C	-0.26636	7.84899	-1.03951
C	-1.39132	7.61577	-0.23946
C	-1.70147	6.29697	0.08579
C	-1.91217	3.29628	-2.56626
C	-2.86619	4.16089	-3.11611
C	-2.86389	4.48584	-4.47364
C	-1.87552	3.92503	-5.28907
C	-0.90414	3.05975	-4.77685
C	-0.93589	2.75486	-3.41032
C	-4.42244	-1.92992	3.17916

C	-4.61768	-2.33017	4.64541
C	-6.96128	2.41046	3.86201
C	-7.72903	3.28556	2.86514
C	1.40740	6.12081	3.72362
C	2.21046	6.10766	5.02707
C	-2.58521	4.12137	6.17051
C	-3.18514	5.45222	6.64668
C	1.74632	7.13062	-2.36241
C	1.85398	6.26395	-3.62014
C	-2.30403	8.74904	0.19939
C	-3.14139	9.25949	-0.98306
C	-3.91191	5.42786	-5.04115
C	-4.80079	4.73128	-6.08025
C	0.15507	2.45303	-5.68424
C	-0.45787	1.47837	-6.69939
C	1.79279	-3.20583	2.74260
C	2.91558	-3.05993	3.57070
C	2.87328	-3.39577	4.92776
C	1.67284	-3.88052	5.45310
C	0.53010	-4.03583	4.65969
C	0.60769	-3.69493	3.30777
C	1.49959	-5.43917	0.65384
C	2.43278	-6.27499	1.27969
C	2.12540	-7.60445	1.58263
C	0.85186	-8.08162	1.25633
C	-0.10284	-7.27530	0.63168
C	0.23939	-5.95281	0.32916
C	2.69491	-4.43738	-2.07036
C	1.66221	-4.97832	-2.84511
C	1.93625	-5.79587	-3.94664
C	3.27028	-6.07703	-4.25694
C	4.32502	-5.56583	-3.49291
C	4.02002	-4.74267	-2.40724
C	4.10540	-3.27196	5.80987
C	4.56355	-1.81563	5.95884
C	-0.75415	-4.60593	5.23649
C	-1.22226	-3.85630	6.48964
C	3.14696	-8.52514	2.22885
C	3.62524	-7.99948	3.58808
C	-1.48099	-7.82155	0.29867
C	-1.78270	-7.74422	-1.20350
C	0.79989	-6.35201	-4.78861
C	0.82948	-7.88419	-4.86215
C	5.77003	-5.91326	-3.81072
C	6.17946	-5.47026	-5.22104
C	3.72360	-0.57507	-5.42864
C	4.21588	-1.71182	-6.33693
C	7.40445	-0.53614	-1.93402
C	7.55200	0.50223	-0.81473
C	-7.96507	-0.01165	-0.08859
C	-5.36970	-2.72059	2.26383

C	-6.49005	3.24184	5.06400
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C	-1.78607	3.44925	7.29387
C	3.03517	7.06767	-1.53028
C	-1.55215	9.90254	0.87371
C	-3.27996	6.70245	-5.61681
C	0.98596	3.52432	-6.40298
C	2.48039	1.82982	5.18317
C	4.71999	3.59392	0.53749
C	5.25449	-4.16039	5.31465
C	-0.61070	-6.10988	5.51400
C	4.33402	-8.79056	1.29210
C	-2.57669	-7.11644	1.11085
C	4.13343	0.79081	-5.99040
C	8.11758	-1.84495	-1.56675
C	-4.09324	-0.37291	-5.58607
C	0.78795	-5.73508	-6.19439
C	6.04684	-7.40869	-3.60025
H	-8.14082	0.07603	-2.21790
H	-9.04389	0.02074	0.10378
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H	-7.45604	0.49455	0.73829
H	-9.24517	2.10483	-1.34142
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H	-5.13069	-0.04051	-5.69278
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H	-3.84025	-0.98565	-6.45916
H	-2.32069	-2.30708	-3.28027
H	-2.26509	-2.37012	-5.04616
H	-1.72454	-0.91314	-4.21395
H	-2.83622	-0.32864	1.67511
H	-3.39386	-2.19304	2.89846
H	-5.20080	-2.47341	1.21163
H	-5.22402	-3.79924	2.39089
H	-6.41575	-2.49189	2.49736
H	-3.95616	-1.76341	5.30771
H	-5.64839	-2.16358	4.97699
H	-4.40443	-3.39576	4.78069
H	-6.36419	-0.21380	4.11550
H	-7.66105	1.65299	4.24057
H	-5.98789	2.61432	5.80705
H	-5.78494	4.01855	4.74746
H	-7.33660	3.73709	5.55284
H	-8.08887	2.70098	2.01360
H	-8.59628	3.74607	3.35064
H	-7.10541	4.09802	2.47655
H	-4.97044	3.35463	2.18993
H	0.28159	4.83569	1.66636
H	2.05461	5.71598	2.93197
H	0.53793	7.58380	2.35600

H	0.39482	8.01803	4.06738
H	1.95608	8.17778	3.24192
H	2.43967	5.08899	5.35473
H	3.15616	6.64320	4.89401
H	1.67112	6.60797	5.83891
H	-0.25726	5.51547	5.85218
H	-3.41908	3.45494	5.91645
H	-1.39258	2.47970	6.97428
H	-0.93863	4.06729	7.61067
H	-2.41964	3.28452	8.17237
H	-3.78406	5.92141	5.86004
H	-3.82848	5.29794	7.52002
H	-2.39993	6.16092	6.93311
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H	-0.00521	8.86844	-1.31742
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H	-3.62648	4.58659	-2.46566
H	-4.55663	5.72866	-4.20451
H	-2.66933	7.21418	-4.86658
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H	-5.58823	5.40670	-6.43314
H	-4.21885	4.41615	-6.95356
H	-1.86361	4.16733	-6.34995
H	-0.20034	2.06383	-2.99936
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H	2.11702	2.12119	6.17426
H	3.11926	0.94843	5.30095
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H	0.97306	-0.48146	5.06119
H	-0.01721	0.78214	5.78978
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H	5.11853	4.45359	-0.01155
H	4.62000	3.88007	1.58886
H	5.45411	2.78351	0.47941
H	2.58806	2.48575	-1.99422
H	3.82975	3.74678	-2.08738
H	4.28835	2.08220	-1.73566
H	3.84022	-2.69722	3.12815
H	1.63591	-4.15467	6.50577
H	-1.53025	-4.48486	4.46921
H	-0.31310	-6.65055	4.61070
H	0.14942	-6.29600	6.28139
H	-1.55671	-6.53165	5.87198
H	-1.33417	-2.78549	6.29450
H	-2.18840	-4.24321	6.83121
H	-0.51350	-3.97356	7.31684
H	-0.26781	-3.82760	2.67723

H	3.41278	-5.87306	1.52396
H	3.99830	-9.20393	0.33610
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H	-2.38304	-7.18849	2.18583
H	-2.63404	-6.05452	0.84793
H	-3.55737	-7.56235	0.90983
H	0.62885	-4.75359	-2.58201
H	3.49410	-6.71609	-5.10901
H	4.82663	-4.33318	-1.80430
H	2.27309	-1.50772	-3.33435
H	2.62610	-0.61347	-5.41900
H	3.78685	1.60806	-5.35073
H	5.22112	0.87872	-6.08645
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H	6.21760	-0.16001	-4.34281
H	7.90046	-0.13076	-2.82635
H	8.04591	-2.57556	-2.37821
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H	8.60897	0.68197	-0.58940
H	7.09980	1.45735	-1.09945
H	7.06955	0.16339	0.10875
H	5.35724	-1.49447	-0.35928
H	-1.07458	-3.62214	-1.42088
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H	-5.54837	1.93815	-0.17719
H	-2.34876	0.36860	-2.53996
H	3.26306	0.47133	-0.67551
H	-6.39261	-0.80778	-3.35742
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H	7.23882	-5.68446	-5.40213
H	5.60137	-5.99677	-5.98847
H	6.39523	-5.35903	-3.09779
H	5.78761	-7.71952	-2.58357
H	7.10534	-7.63706	-3.76908
H	5.45971	-8.02047	-4.29417
H	0.71904	-4.64374	-6.14702
H	-0.06412	-6.10553	-6.77547
H	1.70170	-5.98754	-6.74437

H	-1.48515	-8.88200	0.58663
H	-2.75856	-8.19103	-1.42492
H	-1.02454	-8.27566	-1.78664
H	-1.80543	-6.70481	-1.54799
H	-0.47186	-5.30582	-0.18453
H	0.60006	-9.11545	1.49073
H	2.64436	-9.48612	2.40485
H	4.85132	-1.38957	4.99125
H	5.43185	-1.74707	6.62363
H	3.76712	-1.19254	6.37727
H	6.10845	-4.10593	5.99898
H	5.60281	-3.84520	4.32495
H	4.94227	-5.20629	5.24120
H	3.81989	-3.63054	6.80813
H	-4.57592	-2.02405	-4.31353
H	0.83673	1.87877	-5.04272
H	-1.00516	0.67333	-6.20117
H	0.32133	1.02574	-7.32297
H	-1.15875	1.99410	-7.36530
H	1.77793	3.06144	-7.00148
H	1.45385	4.21148	-5.69263
H	0.36588	4.11912	-7.08265
H	-2.50005	9.69483	-1.75760
H	-3.84615	10.03285	-0.65725
H	-3.71279	8.44735	-1.44275
H	-2.99879	8.33014	0.93975
H	-0.97160	9.55396	1.73277
H	-2.25661	10.66356	1.22660
H	-0.86226	10.39478	0.17954
H	2.03799	5.21370	-3.37129
H	2.68488	6.60252	-4.24890
H	0.93458	6.30727	-4.21088
H	1.62554	8.17120	-2.69316
H	2.97764	7.72951	-0.66047
H	3.90335	7.36498	-2.12939
H	3.21216	6.05090	-1.16350
H	-0.13542	-6.06309	-4.29234
H	-0.53437	-0.87176	1.44262
H	-1.46030	-0.27553	-0.43878

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Complex 3 - 2nd xyl. H2 lost TS

C	19.87299	13.85468	1.46640
C	18.54960	13.63916	1.05082
C	18.19895	14.00144	-0.25541
C	19.13274	14.54640	-1.14171
C	20.44541	14.73184	-0.69448
C	20.83326	14.39617	0.60640
C	17.63055	12.92168	1.97687
C	17.23035	13.30288	3.31757
C	16.68168	12.11978	3.95404

C	16.69850	11.06456	2.98893
C	17.29258	11.54527	1.79185
C	17.17376	14.67221	3.85456
C	16.68596	14.96746	5.15928
C	16.58162	16.26760	5.65253
C	17.03483	17.34837	4.86194
C	17.59259	17.10622	3.59784
C	17.60780	15.79807	3.09423
C	16.05790	16.52286	7.05910
C	14.73650	15.80438	7.35181
C	18.20702	18.26511	2.82594
C	18.38919	18.00329	1.33036
La	14.86730	12.99079	2.05448
La	14.64105	16.25302	3.22877
C	13.00324	18.04533	1.46492
C	12.09087	17.11780	2.05396
C	12.02321	17.39401	3.45471
C	12.89335	18.50502	3.73779
C	13.46305	18.92798	2.48686
C	11.24135	16.18306	1.27634
C	9.85626	16.13056	1.47759
C	9.03656	15.28398	0.72146
C	9.63053	14.46853	-0.24242
C	11.00918	14.49960	-0.47830
C	11.79550	15.37022	0.27506
C	7.53310	15.23830	0.93850
C	6.88224	16.61863	0.78347
C	11.61104	13.61557	-1.55757
C	12.87900	12.88604	-1.09244
C	11.09293	16.68626	4.38175
C	11.26779	15.33922	4.72380
C	10.35744	14.66873	5.54656
C	9.23892	15.36734	6.01161
C	9.01361	16.70534	5.67329
C	9.95344	17.35061	4.86195
C	13.26601	19.10358	5.04607
C	14.49132	19.79058	5.17386
C	14.88664	20.41637	6.35730
C	14.04372	20.33769	7.46932
C	12.83255	19.64355	7.40182
C	12.46011	19.03837	6.19787
C	13.95949	20.30355	2.20953
C	15.13899	20.61556	1.52388
C	15.48177	21.94667	1.23705
C	14.61506	22.96491	1.63560
C	13.41993	22.69169	2.31143
C	13.11680	21.36264	2.59415
C	13.10804	18.30761	0.00221
C	12.02921	18.93554	-0.63381
C	12.04799	19.22597	-1.99870
C	13.18129	18.87067	-2.73743

C	14.27885	18.24353	-2.14094
C	14.22613	17.96904	-0.76833
C	10.57079	13.20410	5.88881
C	10.59519	12.96155	7.40323
C	7.77788	17.42664	6.18943
C	6.94623	18.05433	5.06439
C	16.18597	21.20548	6.40208
C	17.05445	20.87511	7.62158
C	11.90900	19.57457	8.60727
C	11.34543	20.95843	8.96048
C	16.77528	22.31541	0.52859
C	16.98229	21.53996	-0.77584
C	12.44961	23.80046	2.68317
C	11.85677	24.46371	1.43170
C	10.86594	19.92012	-2.65337
C	10.23430	19.06214	-3.75767
C	15.49170	17.84447	-2.96721
C	15.16644	16.68247	-3.91613
C	16.69445	11.84128	5.42334
C	17.95460	11.82654	6.03882
C	18.11161	11.51532	7.39314
C	16.97059	11.20745	8.13612
C	15.69629	11.20201	7.55707
C	15.57432	11.52580	6.20230
C	16.22318	9.67928	3.21663
C	17.10054	8.59411	3.10581
C	16.65786	7.28105	3.28499
C	15.30129	7.06882	3.55216
C	14.39259	8.12495	3.66418
C	14.87620	9.42866	3.51263
C	17.49750	10.74254	0.56145
C	16.43236	10.03564	-0.02181
C	16.59866	9.27112	-1.17677
C	17.87319	9.20058	-1.75235
C	18.96116	9.87966	-1.19779
C	18.75470	10.65050	-0.04790
C	19.48842	11.47136	8.03555
C	20.22829	12.81052	7.92705
C	14.47175	10.83888	8.38021
C	14.24545	11.81455	9.54269
C	17.62091	6.10748	3.22140
C	18.59762	6.12809	4.40621
C	12.92076	7.84698	3.91977
C	12.05102	8.27566	2.72927
C	15.42028	8.52893	-1.78503
C	15.60062	7.00762	-1.69366
C	20.36770	9.76429	-1.76606
C	20.41585	9.57774	-3.28494
C	18.72597	14.86650	-2.57042
C	19.08284	13.70126	-3.50627
C	22.27389	14.58644	1.05280

C	22.39275	15.57948	2.21588
C	7.17848	14.60562	2.29092
C	9.52377	12.31378	5.20481
C	8.13856	18.47460	7.25097
C	15.90906	22.71398	6.32206
C	12.58502	18.93167	9.82506
C	17.98621	22.17282	1.46100
C	13.07890	24.84669	3.61172
C	11.24771	21.30969	-3.18205
C	16.08673	19.02275	-3.74885
C	17.12577	16.14619	8.09759
C	19.54804	18.65724	3.46957
C	20.33565	10.32767	7.45949
C	14.54532	9.39213	8.88879
C	18.37507	6.03827	1.88798
C	12.42291	8.48704	5.22127
C	19.31208	16.18242	-3.09232
C	22.94030	13.24853	1.40190
C	11.87795	14.41516	-2.84011
C	15.14789	8.96584	-3.23067
C	21.13950	8.63782	-1.05964
H	7.11764	14.59174	0.15313
H	6.09177	14.55514	2.42671
H	7.57736	13.58920	2.36559
H	7.59921	15.18450	3.11970
H	5.79263	16.54470	0.87369
H	7.23085	17.31413	1.55425
H	7.11496	17.05854	-0.19135
H	10.95155	14.85481	-3.22155
H	12.57376	15.23760	-2.64684
H	12.30270	13.77906	-3.62553
H	12.66693	12.29001	-0.19412
H	13.24811	12.20373	-1.86528
H	13.68463	13.60001	-0.87575
H	12.09861	14.77976	4.29175
H	11.55518	12.92449	5.49036
H	9.53165	12.46050	4.12062
H	9.71965	11.25528	5.40990
H	8.51440	12.54229	5.56530
H	11.35756	13.57590	7.89179
H	9.62961	13.19942	7.86324
H	10.81191	11.91027	7.62228
H	8.51267	14.85917	6.64361
H	7.15023	16.66822	6.67686
H	8.68438	18.02161	8.08448
H	8.76788	19.26449	6.82587
H	7.23612	18.94838	7.65351
H	6.65317	17.30667	4.32164
H	6.03447	18.50811	5.46820
H	7.50188	18.84311	4.54553
H	9.80008	18.38805	4.57304

H	15.14862	19.86228	4.31348
H	16.75759	20.93371	5.50379
H	15.35058	22.96008	5.41455
H	15.31951	23.04812	7.18335
H	16.84554	23.28330	6.31405
H	17.26702	19.80347	7.68840
H	18.01007	21.40785	7.56653
H	16.56898	21.17610	8.55624
H	14.33048	20.82563	8.39805
H	11.06266	18.93572	8.32552
H	12.95710	17.93015	9.58896
H	13.43352	19.53009	10.17472
H	11.87866	18.84378	10.65811
H	10.83187	21.40702	8.10445
H	10.63168	20.88875	9.78905
H	12.14333	21.64486	9.26553
H	11.51308	18.51520	6.16013
H	15.79101	19.80868	1.20009
H	14.87759	23.99464	1.39888
H	12.18886	21.12562	3.10826
H	11.15587	19.19988	-0.04275
H	10.10706	20.06170	-1.87231
H	11.66843	21.93284	-2.38692
H	11.99537	21.23908	-3.98008
H	10.37146	21.82377	-3.59289
H	9.93331	18.08304	-3.37297
H	9.34762	19.55473	-4.17236
H	10.93573	18.89602	-4.58297
H	13.20885	19.08686	-3.80354
H	15.06193	17.45499	-0.29620
H	15.86944	17.60040	7.14106
H	18.06640	16.67421	7.91108
H	16.78712	16.40009	9.10795
H	17.33212	15.07088	8.07024
H	13.93825	16.12860	6.67470
H	14.83591	14.71709	7.27103
H	14.40235	16.03050	8.36972
H	17.52727	19.12160	2.94043
H	19.98395	19.52161	2.95700
H	19.42695	18.91400	4.52595
H	20.26105	17.82862	3.40617
H	17.45376	17.70018	0.84812
H	18.74644	18.91006	0.83255
H	19.12688	17.21646	1.14199
H	18.82612	12.05494	5.43026
H	17.08356	10.96002	9.19046
H	13.60377	10.91127	7.71184
H	14.69308	8.68954	8.06319
H	15.37823	9.26033	9.58845
H	13.62408	9.11705	9.41460
H	14.15420	12.84485	9.18607

H	13.33026	11.56159	10.08955
H	15.07644	11.78165	10.25616
H	14.59290	11.56239	5.73637
H	18.14435	8.79405	2.87982
H	17.68399	5.98687	1.04154
H	19.01102	6.91732	1.74102
H	19.02031	5.15327	1.85658
H	13.01783	8.15666	6.07758
H	12.48255	9.57987	5.17485
H	11.37686	8.21971	5.40834
H	15.45149	10.06123	0.45157
H	18.01533	8.60320	-2.64910
H	19.59297	11.18674	0.38835
H	17.17457	13.85092	-0.58854
H	17.63246	14.96750	-2.57427
H	19.08323	17.01799	-2.42388
H	20.40089	16.12759	-3.20010
H	18.90369	16.41461	-4.08158
H	18.62878	12.76710	-3.16259
H	18.73546	13.89877	-4.52678
H	20.16810	13.55292	-3.54238
H	21.19157	15.14528	-1.36961
H	22.81904	15.01237	0.19945
H	22.89052	12.54977	0.56098
H	23.99484	13.39585	1.66012
H	22.45186	12.77340	2.25968
H	23.44181	15.72582	2.49590
H	21.97502	16.55443	1.94657
H	21.85932	15.21911	3.10222
H	20.14741	13.56725	2.47852
H	14.40124	13.13384	4.13075
H	15.34849	15.13671	1.42023
H	9.41243	16.76740	2.23616
H	12.86762	15.42027	0.11148
H	17.98828	15.62881	2.09807
H	9.00517	13.79567	-0.82859
H	16.99608	18.35754	5.26038
H	16.34192	14.14685	5.77621
H	18.06249	6.13937	5.36073
H	19.24892	5.24696	4.38847
H	19.23663	7.01732	4.37359
H	15.74007	6.69138	-0.65565
H	14.72397	6.48678	-2.09501
H	16.47480	6.67763	-2.26584
H	19.84355	10.35151	-3.80562
H	21.45106	9.62534	-3.63880
H	20.01872	8.60221	-3.58718
H	20.87764	10.70920	-1.53396
H	21.16478	8.79202	0.02347
H	22.17284	8.58475	-1.42092
H	20.66494	7.66805	-1.24747

H	14.99224	10.04733	-3.29704
H	14.25538	8.46710	-3.62438
H	15.98544	8.71141	-3.88938
H	12.81599	6.75870	4.02602
H	11.00277	8.00276	2.89377
H	12.38607	7.80076	1.80182
H	12.08935	9.36143	2.58426
H	14.19870	10.27545	3.63490
H	14.94194	6.04838	3.67985
H	17.01749	5.19336	3.30787
H	20.42392	13.07412	6.88202
H	21.19427	12.76160	8.44204
H	19.64702	13.62391	8.37178
H	21.30385	10.26531	7.96900
H	20.52881	10.48096	6.39204
H	19.82785	9.36462	7.56950
H	19.33654	11.26352	9.10363
H	10.86628	12.84360	-1.79489
H	16.25869	17.49368	-2.26380
H	14.81472	15.80530	-3.36548
H	16.05042	16.39042	-4.49444
H	14.38176	16.96568	-4.62649
H	17.00138	18.71612	-4.26804
H	16.33343	19.85696	-3.08718
H	15.38901	19.39363	-4.50778
H	12.63487	24.96211	0.84296
H	11.11244	25.21915	1.70774
H	11.37228	23.72567	0.78515
H	11.62234	23.32957	3.23092
H	13.45314	24.38795	4.53173
H	12.34220	25.60911	3.88840
H	13.91726	25.35968	3.12748
H	17.09884	20.46693	-0.59214
H	17.88405	21.88709	-1.29243
H	16.12913	21.67077	-1.44797
H	16.69515	23.37882	0.26487
H	17.85781	22.77025	2.36902
H	18.90506	22.50205	0.96232
H	18.12474	21.13025	1.76547
H	14.53484	8.78990	-1.18940
H	14.84747	14.08773	3.76360
H	13.32377	14.60858	2.49326

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Complex 3 - 2nd xyl. H2 lost prod

C	4.67711	-1.72212	-1.51652
C	3.32913	-1.56897	-1.87955
C	3.04064	-0.96639	-3.10929
C	4.05607	-0.54550	-3.97297
C	5.38730	-0.73244	-3.58351
C	5.71757	-1.31255	-2.35578

C	2.31055	-2.15268	-0.96135
C	2.12007	-1.82439	0.43808
C	1.43836	-2.95136	1.04486
C	1.12198	-3.88764	0.01085
C	1.67345	-3.40216	-1.21530
C	2.33074	-0.51139	1.04463
C	1.89816	-0.20030	2.37805
C	2.05385	1.05916	2.95070
C	2.64140	2.10367	2.18214
C	3.19413	1.81209	0.90896
C	2.99627	0.55466	0.34829
C	1.60007	1.37367	4.37215
C	0.77915	0.26597	5.03301
C	4.00706	2.88906	0.20546
C	4.16731	2.68447	-1.30110
La	-0.42913	-1.52780	-0.58658
La	0.29333	1.55961	0.71752
C	-1.47277	2.95746	-1.00909
C	-2.21491	1.89647	-0.35853
C	-2.40397	2.29815	1.02115
C	-1.73293	3.54172	1.21471
C	-1.15912	3.94380	-0.02986
C	-2.47978	0.57522	-0.92776
C	-3.18458	-0.43738	-0.19480
C	-3.46178	-1.69432	-0.71913
C	-2.93686	-2.04552	-1.98937
C	-2.32237	-1.05456	-2.79122
C	-2.08509	0.21237	-2.25490
C	-4.36404	-2.69320	-0.00730
C	-5.67773	-2.85318	-0.79397
C	-2.01209	-1.36781	-4.24873
C	-0.56286	-1.08600	-4.65120
C	-3.38471	1.75866	2.00406
C	-3.02796	1.21150	3.24283
C	-3.99209	0.81396	4.17286
C	-5.34320	0.98029	3.84616
C	-5.74192	1.52080	2.62082
C	-4.75005	1.89915	1.70962
C	-1.73117	4.38550	2.43428
C	-0.53788	4.93077	2.93238
C	-0.52294	5.79119	4.03242
C	-1.73780	6.10808	4.64803
C	-2.94783	5.58282	4.18443
C	-2.92769	4.72337	3.08303
C	-0.68716	5.32711	-0.31281
C	0.64315	5.66099	-0.58127
C	1.02576	6.98725	-0.83220
C	0.04135	7.97614	-0.82389
C	-1.30246	7.67912	-0.56740
C	-1.64468	6.35317	-0.31066
C	-1.48100	3.26072	-2.46465

C	-2.73519	3.43303	-3.07348
C	-2.86409	3.82243	-4.40738
C	-1.69723	4.03514	-5.14871
C	-0.43007	3.86766	-4.58224
C	-0.33665	3.47952	-3.24047
C	-3.57713	0.23139	5.51372
C	-3.88511	1.20238	6.66218
C	-7.21634	1.72693	2.31185
C	-7.65923	0.98981	1.04173
C	0.78507	6.38935	4.52273
C	1.05517	6.07393	5.99953
C	-4.27082	5.97273	4.82372
C	-4.62257	7.43624	4.51869
C	2.47651	7.37221	-1.07400
C	3.11124	6.59673	-2.23328
C	-2.36350	8.76603	-0.56539
C	-2.48969	9.44271	-1.93696
C	-4.24014	4.06879	-5.00462
C	-4.47471	3.29440	-6.30712
C	0.82090	4.12146	-5.40694
C	0.90374	3.19407	-6.62635
C	1.48810	-3.33522	2.47840
C	2.71298	-3.21358	3.15727
C	2.88273	-3.67488	4.46600
C	1.79357	-4.26587	5.11117
C	0.55694	-4.40757	4.47130
C	0.42383	-3.94330	3.16176
C	0.71310	-5.30575	0.23089
C	1.69715	-6.21602	0.64013
C	1.40411	-7.56415	0.85936
C	0.08694	-7.99398	0.67294
C	-0.92367	-7.12029	0.26509
C	-0.58919	-5.78036	0.03837
C	1.74061	-4.19193	-2.46991
C	0.58482	-4.67917	-3.09737
C	0.65042	-5.47427	-4.24511
C	1.90745	-5.78425	-4.77134
C	3.08325	-5.31898	-4.17460
C	2.98258	-4.52450	-3.03050
C	4.22881	-3.57389	5.16625
C	4.66687	-2.11800	5.36833
C	-0.61517	-5.07779	5.16846
C	-0.97949	-4.38786	6.48909
C	2.48521	-8.55070	1.26728
C	3.16218	-8.15818	2.58655
C	-2.35146	-7.62081	0.12049
C	-2.96613	-7.29145	-1.24462
C	-0.61854	-5.99136	-4.90210
C	-0.66161	-7.52528	-4.92857
C	4.44839	-5.70351	-4.72179
C	4.61683	-5.33670	-6.20098

C	3.71323	0.07298	-5.31789
C	3.97841	-0.91662	-6.46174
C	7.17229	-1.50403	-1.95809
C	7.53937	-0.67669	-0.71879
C	-4.67309	-2.35784	1.45123
C	-4.20456	-1.14409	5.77281
C	-7.56704	3.21952	2.22886
C	0.83653	7.90186	4.26385
C	-4.30096	5.70690	6.33374
C	3.31215	7.23856	0.20680
C	-2.11673	9.80028	0.54137
C	-4.48780	5.57085	-5.20857
C	0.92160	5.59243	-5.83468
C	2.81038	1.72931	5.25248
C	5.38324	3.01973	0.88049
C	5.31349	-4.37622	4.43457
C	-0.35508	-6.57585	5.38089
C	3.52206	-8.73685	0.15027
C	-3.23702	-7.10072	1.26231
C	4.43971	1.40073	-5.56370
C	7.51978	-2.98445	-1.75154
C	-2.99304	-0.61683	-5.16176
C	-0.80727	-5.41433	-6.31174
C	4.73722	-7.19402	-4.48978
H	-3.85161	-3.66725	-0.03393
H	-5.25561	-3.16680	1.90361
H	-3.76941	-2.21714	2.05034
H	-5.26459	-1.44041	1.53376
H	-6.31373	-3.61214	-0.32592
H	-6.23203	-1.90869	-0.80996
H	-5.50004	-3.15324	-1.83056
H	-4.03147	-0.83790	-4.89543
H	-2.84661	0.46512	-5.07995
H	-2.83992	-0.90186	-6.20845
H	0.13381	-1.72251	-4.09591
H	-0.41535	-1.29656	-5.71612
H	-0.29160	-0.03973	-4.47715
H	-1.97471	1.08466	3.47955
H	-2.48850	0.09569	5.48052
H	-3.96518	-1.84813	4.97015
H	-3.83590	-1.56384	6.71514
H	-5.29574	-1.08029	5.84682
H	-3.39098	2.16563	6.50386
H	-4.96204	1.38774	6.74386
H	-3.54248	0.79461	7.61982
H	-6.10896	0.68460	4.56113
H	-7.78143	1.30278	3.15305
H	-7.28981	3.74262	3.14934
H	-7.04085	3.70307	1.39848
H	-8.64205	3.35849	2.06825
H	-7.46384	-0.08433	1.11746

H	-8.73253	1.12704	0.86963
H	-7.13204	1.36460	0.15769
H	-5.02744	2.33128	0.75096
H	0.40006	4.68970	2.43540
H	1.58919	5.92793	3.93363
H	0.67810	8.12477	3.20449
H	0.06111	8.42537	4.83441
H	1.80626	8.31601	4.56277
H	1.04193	4.99543	6.18518
H	2.03320	6.46126	6.30592
H	0.30182	6.53223	6.64963
H	-1.74199	6.78434	5.50029
H	-5.04413	5.34350	4.36369
H	-4.07827	4.65954	6.55717
H	-3.57024	6.32572	6.86617
H	-5.28909	5.94052	6.74548
H	-4.64358	7.62158	3.44037
H	-5.60458	7.69582	4.93017
H	-3.88521	8.11692	4.95891
H	-3.86444	4.32248	2.70750
H	1.39572	4.87490	-0.58497
H	0.33560	9.00572	-1.02095
H	-2.68086	6.09840	-0.10216
H	-3.62832	3.27269	-2.47381
H	-4.97469	3.70999	-4.27102
H	-4.35818	6.12293	-4.27270
H	-3.78705	5.98814	-5.94035
H	-5.50400	5.75308	-5.57627
H	-4.33372	2.21911	-6.16336
H	-5.49465	3.45720	-6.67251
H	-3.78880	3.61892	-7.09724
H	-1.77554	4.34757	-6.18788
H	0.64363	3.33496	-2.79299
H	0.96771	2.27352	4.31320
H	3.38593	2.56318	4.84085
H	2.48282	2.01006	6.25917
H	3.48344	0.87037	5.34139
H	-0.08301	-0.02497	4.42483
H	1.38111	-0.63306	5.20309
H	0.41030	0.60616	6.00589
H	3.47841	3.84106	0.36418
H	5.95720	3.83796	0.43237
H	5.28898	3.21652	1.95254
H	5.95651	2.09448	0.75934
H	3.20077	2.56936	-1.80259
H	4.68344	3.54290	-1.74259
H	4.76281	1.79434	-1.52806
H	3.55167	-2.76633	2.62959
H	1.92186	-4.63254	6.12821
H	-1.48048	-4.98621	4.49833
H	-0.14069	-7.07431	4.43075

H	0.50226	-6.73582	6.04440
H	-1.22482	-7.06285	5.83662
H	-1.18992	-3.32497	6.33604
H	-1.86642	-4.85074	6.93610
H	-0.16566	-4.46478	7.21854
H	-0.52725	-4.07379	2.65852
H	2.70990	-5.84941	0.78445
H	3.04598	-9.05047	-0.78384
H	4.05836	-7.80237	-0.04747
H	4.26235	-9.49501	0.42961
H	-2.82295	-7.37221	2.23815
H	-3.31804	-6.00832	1.22850
H	-4.24959	-7.51421	1.19281
H	-0.38888	-4.43837	-2.67458
H	1.97165	-6.40677	-5.66140
H	3.88990	-4.16662	-2.55319
H	2.00407	-0.80473	-3.38706
H	2.63572	0.28311	-5.30705
H	4.24520	2.11658	-4.75938
H	5.52410	1.26082	-5.63156
H	4.10957	1.84859	-6.50698
H	3.41688	-1.84419	-6.31589
H	3.68645	-0.48643	-7.42645
H	5.04232	-1.17372	-6.51718
H	6.19159	-0.41944	-4.24674
H	7.78314	-1.13574	-2.79358
H	7.29073	-3.57358	-2.64501
H	8.58572	-3.10554	-1.52859
H	6.95600	-3.41223	-0.91539
H	8.59903	-0.79956	-0.46865
H	7.35172	0.38864	-0.88513
H	6.95286	-0.98771	0.15271
H	4.90071	-2.18702	-0.55920
H	-1.72530	-3.37506	0.91775
H	0.56975	0.45224	-1.23250
H	-3.54583	-0.19799	0.79387
H	-1.59350	0.95298	-2.87141
H	3.37158	0.36626	-0.64582
H	-3.16813	-3.01587	-2.42103
H	2.80117	3.08215	2.62789
H	1.41046	-0.97505	2.95089
H	2.43124	-8.05344	3.39371
H	3.89575	-8.91590	2.88409
H	3.68966	-7.20309	2.49304
H	-0.53766	-7.94147	-3.92436
H	-1.61518	-7.88070	-5.33493
H	0.13758	-7.93390	-5.55681
H	4.44394	-4.26957	-6.36731
H	5.62982	-5.57542	-6.54386
H	3.91741	-5.89277	-6.83498
H	5.19226	-5.12965	-4.15347

H	4.65700	-7.45235	-3.42954
H	5.74575	-7.45396	-4.83081
H	4.02649	-7.82182	-5.03898
H	-0.80404	-4.32010	-6.29682
H	-1.75618	-5.74859	-6.74623
H	-0.00318	-5.73831	-6.98178
H	-2.31493	-8.71528	0.20751
H	-3.96937	-7.72329	-1.33042
H	-2.35450	-7.68560	-2.06130
H	-3.06220	-6.20986	-1.39127
H	-1.35596	-5.08718	-0.30078
H	-0.15760	-9.04106	0.84813
H	1.99138	-9.51963	1.42374
H	4.78958	-1.60444	4.40865
H	5.62439	-2.06902	5.89902
H	3.92688	-1.56266	5.95278
H	6.25861	-4.34569	4.98837
H	5.50165	-3.96923	3.43500
H	5.01980	-5.42391	4.31889
H	4.10518	-4.02209	6.16163
H	-2.18758	-2.44322	-4.38574
H	1.68290	3.90289	-4.76305
H	0.86954	2.14151	-6.32943
H	1.83388	3.36354	-7.17984
H	0.07202	3.37151	-7.31715
H	1.86603	5.78246	-6.35694
H	0.86442	6.26070	-4.97050
H	0.10630	5.86194	-6.51533
H	-1.56742	9.96900	-2.20706
H	-3.30147	10.17873	-1.93285
H	-2.69624	8.70949	-2.72262
H	-3.32204	8.27516	-0.35002
H	-2.05952	9.32123	1.52341
H	-2.92423	10.54052	0.56714
H	-1.17764	10.34061	0.37738
H	3.15073	5.52290	-2.02373
H	4.13793	6.93663	-2.40941
H	2.54428	6.73416	-3.15841
H	2.47814	8.43471	-1.35289
H	2.88848	7.83689	1.01915
H	4.34247	7.57167	0.03811
H	3.34934	6.19752	0.54599
H	-1.46173	-5.64905	-4.28683
H	-1.72099	-2.74319	1.32872
H	-0.71552	-0.39288	1.34278

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Complex 4

C	12.43350	15.61344	1.87485
C	11.87358	14.53918	2.64414
C	11.65840	13.26735	2.12205

C	12.06206	12.98176	0.79026
C	12.53368	14.03440	-0.04016
C	12.73699	15.29732	0.50804
C	10.98713	12.16608	2.93061
H	11.54257	11.23894	2.72568
C	10.99738	12.38885	4.44359
H	10.60398	11.50360	4.95382
H	12.00638	12.58175	4.82183
H	10.36958	13.23825	4.73217
C	9.55006	11.95193	2.42591
H	9.07571	11.11783	2.95410
H	8.94793	12.85034	2.59680
H	9.52605	11.73282	1.35420
C	11.45073	13.56477	-2.24829
H	10.83452	12.78518	-1.79033
H	10.87836	14.49853	-2.22582
H	11.61880	13.29340	-3.29600
C	13.65797	14.77715	-2.22593
H	14.60070	14.95343	-1.69854
H	13.89087	14.43548	-3.23954
H	13.14536	15.74075	-2.31412
C	12.66520	16.94193	2.44199
C	12.55004	17.30409	3.84186
C	13.20186	18.55835	4.03422
C	13.69333	19.00806	2.77430
C	13.34101	18.04450	1.78335
C	11.64193	16.72973	4.86901
C	12.07921	16.33537	6.14035
H	13.14287	16.35757	6.36279
C	11.18453	15.92101	7.12915
C	11.69264	15.52909	8.50645
H	12.78152	15.41537	8.42376
C	11.12549	14.18982	8.99133
H	11.31490	13.39139	8.26780
H	11.58315	13.90245	9.94402
H	10.04350	14.24473	9.15419
C	11.42266	16.64146	9.53031
H	11.87151	17.58711	9.21201
H	10.34586	16.80479	9.65348
H	11.83549	16.37828	10.51093
C	9.81731	15.91098	6.82924
H	9.10205	15.60190	7.58902
C	9.33869	16.29640	5.57398
C	7.84463	16.31413	5.29366
H	7.34562	15.94635	6.20062
C	7.33526	17.73927	5.03610
H	7.57749	18.40296	5.87195
H	7.78487	18.16350	4.13161
H	6.24792	17.74449	4.90055
C	7.45584	15.37705	4.14345
H	7.76335	14.34782	4.35213

H	6.37113	15.38205	3.98851
H	7.92680	15.68394	3.20324
C	10.26361	16.69782	4.60436
H	9.92034	17.01687	3.62299
C	13.15331	19.39801	5.25734
C	14.31246	19.86405	5.89135
H	15.28510	19.57396	5.49819
C	14.25155	20.70201	7.00893
C	15.52537	21.18516	7.68230
H	16.36709	20.80363	7.08853
C	15.62578	22.71642	7.69126
H	15.53643	23.12526	6.68032
H	14.83254	23.16357	8.30047
H	16.58494	23.03973	8.11099
C	15.66660	20.61903	9.10224
H	15.63019	19.52519	9.09910
H	16.61628	20.92878	9.55284
H	14.85880	20.97520	9.75113
C	12.99574	21.08161	7.49097
H	12.93562	21.73918	8.35570
C	11.81581	20.64326	6.88098
C	10.45456	21.10704	7.37310
H	9.70199	20.55089	6.79857
C	10.22382	20.79450	8.85653
H	10.34127	19.72612	9.05944
H	10.92928	21.33700	9.49567
H	9.21332	21.08998	9.16033
C	10.24357	22.60104	7.08706
H	10.36827	22.82099	6.02231
H	9.23832	22.91847	7.38678
H	10.96579	23.21275	7.63931
C	11.91277	19.80007	5.77236
H	11.00463	19.45471	5.28619
C	14.14165	20.40080	2.49747
C	15.46054	20.83315	2.65986
H	16.21030	20.11811	2.99293
C	15.82985	22.16251	2.41056
C	17.26791	22.63644	2.54655
C	17.90642	22.24708	3.88429
C	18.12285	22.15616	1.36488
C	14.84388	23.05718	1.99205
H	15.12597	24.09125	1.79978
C	13.51232	22.66112	1.81727
C	12.44921	23.64938	1.36912
C	12.27893	24.79798	2.37239
C	13.18196	21.33101	2.07209
H	12.15445	20.99986	1.94315
C	13.34371	18.38363	0.33966
C	12.12306	18.38588	-0.35660
H	11.22665	18.05345	0.16260
C	12.02901	18.82222	-1.67945

C	10.68132	18.85649	-2.38217
H	9.96050	18.36393	-1.71567
C	10.20258	20.30018	-2.59319
H	10.15603	20.84329	-1.64440
H	10.88260	20.84666	-3.25616
H	9.20575	20.31834	-3.04820
C	10.68644	18.08364	-3.70703
H	10.99904	17.04499	-3.56245
H	9.68632	18.07834	-4.15437
H	11.36855	18.53797	-4.43395
C	13.19141	19.27130	-2.31618
H	13.13286	19.62864	-3.34199
C	14.42567	19.28109	-1.65897
C	15.67557	19.79801	-2.35169
C	15.61307	21.32057	-2.54094
C	14.48506	18.83234	-0.33646
H	15.43944	18.84158	0.18410
C	17.35682	14.59163	3.47345
C	17.04014	14.91355	4.83663
C	17.23537	16.18060	5.38023
C	17.72085	17.22743	4.55013
C	18.14116	16.93454	3.22582
C	17.92685	15.66162	2.70620
C	16.93775	16.49561	6.84142
H	16.36395	17.43500	6.85429
C	18.24880	16.75812	7.60199
H	18.83521	17.55731	7.13911
H	18.04067	17.04790	8.63752
H	18.86888	15.85580	7.61963
C	16.10744	15.43351	7.56254
H	15.17876	15.20876	7.02869
H	16.65997	14.49450	7.67135
H	15.84878	15.78168	8.56764
C	18.83308	18.02738	2.42407
H	18.29479	18.96353	2.63461
C	20.27248	18.21345	2.93329
H	20.76222	19.04279	2.41168
H	20.29699	18.42497	4.00652
H	20.85958	17.30602	2.75806
C	18.82142	17.81221	0.91005
H	17.80949	17.64095	0.52912
H	19.23365	18.69130	0.40411
H	19.43278	16.95175	0.61899
C	17.12459	13.26441	2.90184
C	16.44045	12.15963	3.54862
C	16.08984	11.20392	2.54831
C	16.59028	11.66207	1.29526
C	17.24860	12.90995	1.50063
C	16.42078	11.81688	4.99207
C	17.63346	11.79906	5.69958
H	18.53446	12.12470	5.18493

C	17.70594	11.35475	7.02380
C	19.03116	11.30576	7.76810
C	16.53078	10.92314	7.64471
H	16.58223	10.56714	8.67172
C	15.30173	10.92800	6.97448
C	14.03787	10.41488	7.64436
H	13.19459	10.71715	7.00913
C	14.03805	8.88012	7.70949
H	14.15235	8.44386	6.71274
H	14.86479	8.51728	8.33081
H	13.10346	8.50750	8.14436
C	13.81037	11.02210	9.03327
H	13.81767	12.11539	8.99585
H	12.84506	10.70066	9.43922
H	14.58274	10.70596	9.74300
C	15.26509	11.37794	5.65338
H	14.31806	11.37700	5.11936
C	15.60565	9.81802	2.79524
C	16.49711	8.88532	3.33891
H	17.49989	9.21712	3.59404
C	16.12689	7.55305	3.54181
C	17.10932	6.53590	4.09685
C	18.31325	6.34571	3.16404
H	17.99256	6.05844	2.15790
H	18.89518	7.26963	3.07623
H	18.98173	5.56619	3.54653
C	14.82865	7.16890	3.19803
C	13.90487	8.07067	2.66099
C	12.49496	7.59195	2.35155
C	11.56072	7.83723	3.54659
H	11.94356	7.35826	4.45292
H	11.46738	8.90927	3.75277
H	10.55778	7.44224	3.34829
C	11.90853	8.18501	1.06774
C	14.31193	9.39430	2.46324
C	16.66178	10.83736	0.06167
C	15.52745	10.47730	-0.67572
H	14.54841	10.82072	-0.34556
C	15.61934	9.67997	-1.82143
C	16.88077	9.23115	-2.22222
H	16.96573	8.60828	-3.11050
C	18.03529	9.55588	-1.50195
C	19.46130	7.49671	-1.83027
C	17.90785	10.36242	-0.36992
H	18.79517	10.62550	0.19940
C	18.17312	13.47669	0.48366
C	17.75266	13.88263	-0.78984
H	16.69077	13.87764	-1.02146
C	18.66203	14.28737	-1.76916
C	18.17257	14.69354	-3.14899
H	17.08230	14.80425	-3.08033

C	18.74417	16.03999	-3.60888
H	18.54055	16.82950	-2.87943
H	19.82898	15.98932	-3.75352
H	18.30204	16.33758	-4.56579
C	18.45935	13.59483	-4.18288
H	18.01278	12.64279	-3.88128
H	18.05565	13.86800	-5.16459
H	19.53814	13.43860	-4.29734
C	20.02664	14.27677	-1.45700
H	20.75281	14.57881	-2.20930
C	20.48840	13.88039	-0.19895
C	21.97922	13.84325	0.09607
H	22.49237	14.19521	-0.80927
C	22.46613	12.41383	0.37248
H	22.22163	11.74511	-0.45861
H	23.55205	12.39484	0.51772
H	22.00305	12.00517	1.27738
C	22.36927	14.78629	1.24108
H	23.45230	14.76905	1.40671
H	22.07682	15.81729	1.01973
H	21.88524	14.49418	2.17940
C	19.54917	13.48827	0.76059
H	19.87915	13.16084	1.74375
La	15.24438	16.64063	3.32581
La	14.54935	13.57213	1.99870
H	14.37491	14.65609	3.99038
H	15.42182	15.55630	1.33463
H	11.60861	14.72526	3.67406
H	13.14561	16.07387	-0.12100
H	18.20264	15.47080	1.67997
H	11.86399	12.00208	0.36231
H	17.91318	18.21015	4.97343
H	16.62356	14.13956	5.46395
C	12.79040	13.73974	-1.51231
C	12.72851	24.18291	-0.04247
C	15.94315	19.08958	-3.68522
C	20.03002	10.35456	7.09502
C	19.64371	12.70025	7.95086
C	17.56192	6.89397	5.51815
H	16.70773	6.97957	6.19626
H	18.23914	6.12867	5.91388
H	18.09151	7.85213	5.53404
C	14.37384	9.32228	-2.61537
C	14.38306	9.97535	-4.00467
C	14.17500	7.80476	-2.72584
H	14.16561	7.33178	-1.73916
H	13.22906	7.57224	-3.22755
H	14.97880	7.33981	-3.30712
C	19.39807	9.02784	-1.91829
C	19.80708	9.51762	-3.31346
H	19.80590	10.61030	-3.36339

H	20.81250	9.16421	-3.56843
H	19.12178	9.14605	-4.08351
H	20.12713	9.42980	-1.20225
H	19.20113	7.14694	-0.82658
H	20.46802	7.13506	-2.06836
H	18.76555	7.02962	-2.53626
H	14.48964	11.06217	-3.93175
H	13.45493	9.75772	-4.54524
H	15.21621	9.60097	-4.60970
H	12.55913	6.50453	2.20720
H	10.94701	7.71524	0.83467
H	12.57819	8.03400	0.21616
H	11.72550	9.26073	1.16513
H	13.62239	10.11538	2.02983
H	14.52784	6.13219	3.34650
H	16.57934	5.57496	4.15074
H	19.86778	13.16472	6.98420
H	20.57987	12.64254	8.51750
H	18.96131	13.36322	8.49158
H	20.95644	10.28993	7.67671
H	20.29314	10.70125	6.08972
H	19.61560	9.34617	7.00304
H	18.82018	10.90527	8.76907
H	13.31568	12.77395	-1.55905
H	16.52259	19.58254	-1.68700
H	15.99639	18.00473	-3.55494
H	16.89034	19.42891	-4.11864
H	15.15496	19.29975	-4.41661
H	16.54129	21.69668	-2.98623
H	15.45749	21.83033	-1.58552
H	14.78796	21.59868	-3.20650
H	13.66666	24.74815	-0.07423
H	11.92623	24.85356	-0.37016
H	12.80727	23.36470	-0.76455
H	11.49893	23.10007	1.33180
H	12.05380	24.41859	3.37381
H	11.46335	25.46267	2.06626
H	13.18973	25.40298	2.44287
H	18.18002	21.06244	1.34270
H	19.14488	22.54543	1.43632
H	17.69781	22.48442	0.41154
H	17.24332	23.73400	2.50549
H	17.30901	22.60419	4.72823
H	18.91074	22.67596	3.97087
H	18.00732	21.16061	3.98241
H	13.51449	9.72887	-2.06474

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