

Supporting Information for:

Group 13 Salphen Compounds (In, Ga And Al): A Comparison of their Structural Features and Activities as Catalysts for Cyclic Carbonate Synthesis

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[1] General experimental considerations

All solvents and reagents were purchased from Fisher Scientific or Cymit Quimica and were used without further purification. ^1H , $^{13}\text{C}\{^1\text{H}\}$ and COSY NMR spectra were recorded on a Bruker AV-400 spectrometer in CDCl_3 and referenced to the residual solvent peak at 7.26 ppm (^1H) or 77.16 ppm (^{13}C). Elemental analysis was performed by the Centro de Espectometría de Masas y Análisis Elemental (CEMAETA) at the Universidad de Alcalá. The Salphen ligand (6,6'-((1*E*,1'*E*)-(1,2-phenylenebis(azaneylylidene))bis(methaneylylidene))bis(2,4-di-*tert*-butylphenol)) was prepared according to a reported literature procedure.^[1] All syntheses of the **[MX(Salphen)]** compounds were carried out using a Schlenk line and with dry solvents in order to exclude air or moisture. All catalytic reactions were performed in Berghof High-pressure reactors (BR-40, PTFE liner, 70 mL volume) using high-purity carbon dioxide (>99.995 %) purchased from Linde (no further purification), with an initial starting pressure of 8.0 bar.

[2] General synthetic procedures for **[MX(Salphen)]** preparation

General method [A]

Ligand ($\text{H}_2\text{Salphen}$) was dissolved in toluene in a Schlenk tube under argon and cooled to $-78\text{ }^\circ\text{C}$. To the solution was slowly added 1.0 equiv. of dimethylaluminum chloride (AlMe_2Cl) solution (1.0 M in hexane). The reaction was allowed to warm to room temperature and stirred overnight. The next day, the solvent was removed under reduced pressure and the crude solid was washed with hexane (3 times) to remove residual unreacted ligand. The resulting solid was further dried under vacuum to provide analytically pure **[AlCl(Salphen)]** as a yellow powder.

*General method [B]:**

Ligand ($\text{H}_2\text{Salphen}$) was dissolved in THF in a Schlenk tube under an argon atmosphere. To the solution was slowly added 2.0 equiv. of $\text{K}[\text{N}(\text{SiMe}_3)_2]$ as a solid. The reaction was sealed and left to stir overnight. The next day, the solution was filtered into a solution of **MX₃** in THF using a filter cannula. The reaction mixture was stirred for a further 24 hours, during which time a white precipitate formed. The solution was filtered, and the solvent removed under reduced pressure. The crude residue was washed with hexane (3 times) to remove residual unreacted ligand. Finally, the solid was taken up into dichloromethane, filtered and the solvent removed from the filtrate under reduced pressure. The resulting solid was further dried under vacuum to provide analytically pure **[MX(Salphen)]** as a yellow powder.

This method is based on the procedure reported by Williams and co-workers for the synthesis of **[InCl(Salen)].*^[2]

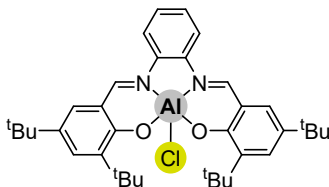
[3] General procedure for the catalytic conversion of epoxides and CO_2 to cyclic carbonates

A high-pressure reactor, equipped with a stirrer bar, was charged with catalyst, TBAI and epoxide. The reactor was then filled with CO_2 to 2 bar and partially vented, a procedure that was repeated 3 times, before being finally filled with CO_2 to a pressure of 8 bar. The reactor was left stirring for the required time at the required temperature. At the end of the reaction the reactor was cooled and slowly vented before a known amount of mesitylene was added. An aliquot was

then removed and dissolved in CDCl_3 . The percentage conversion and NMR yield of the reaction was obtained from the ^1H NMR spectrum of this crude sample using the mesitylene as internal standard and comparison to published spectra.^[3]

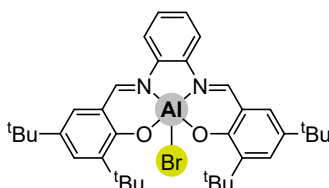
[4] Characterisation data for the $[\text{MX}(\text{Salphen})]$ compounds

$[\text{AlCl}(\text{Salphen})]$:^[4]



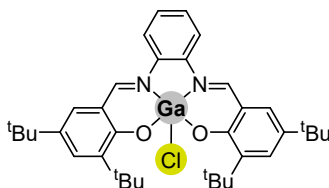
Prepared using general method A; yellow powder (82 %). ^1H NMR (400 MHz, 298 K, CDCl_3) δ 8.95 (s, 2H), 7.76 – 7.72 (m, 2H), 7.69 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 7.40 – 7.35 (m, 2H), 7.24 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 1.62 (s, 18H), 1.36 (s, 18H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, 298 K, CDCl_3) δ 164.4, 162.5, 141.6, 139.7, 137.8, 133.1, 128.3, 128.2, 118.5, 115.4, 35.7, 34.2, 31.3, 29.9 ppm. IR (ATR): 2946.5, 2903.6, 2868.2, 1613.9, 1584.1, 1537.5, 1386.6, 1358.6, 1200.2, 1183.4, 846.1, 592.6 cm^{-1} .

$[\text{AlBr}(\text{Salphen})]$:^[5]



Prepared using general method B; yellow powder (31 %). ^1H NMR (400 MHz, 298 K, CDCl_3) δ 8.98 (s, 2H), 7.79 – 7.75 (m, 2H), 7.69 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 7.44 – 7.41 (m, 2H), 7.25 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 1.60 (s, 18H), 1.36 (s, 18H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, 298 K, CDCl_3) δ 164.2, 162.5, 141.7, 139.9, 137.5, 133.2, 128.3, 128.3, 118.5, 115.5, 35.7, 34.2, 31.3, 29.9 ppm. IR (ATR): 2959.5, 2868.2, 1613.9, 1580.4, 1537.5, 1384.7, 1360.5, 1202.1, 1183.4, 848.0, 758.5, 568.4 cm^{-1} .

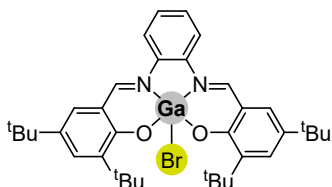
$[\text{GaCl}(\text{Salphen})]$:^[6]



Prepared using general method B; yellow powder (82 %). ^1H NMR (400 MHz, 298 K, CDCl_3) δ 8.93 (s, 2H), 7.77 – 7.73 (m, 2H), 7.64 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 7.43 – 7.38 (m, 2H), 7.16 (d, $^4J_{\text{HH}} = 2.6$

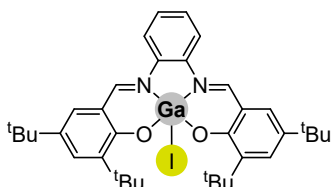
Hz, 2H), 1.59 (s, 18H), 1.35 (s, 18H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, 298 K, CDCl_3) δ 167.6, 162.2, 142.4, 139.2, 135.8, 132.8, 128.6, 128.2, 117.0, 115.2, 35.8, 34.1, 31.2, 29.8. IR (ATR): 2946.5, 2868.2, 1604.6, 1584.1, 1533.8, 1386.6, 1358.6, 1198.3, 1183.4, 743.6, 542.3 cm^{-1} .

[GaBr(Salphen)]:



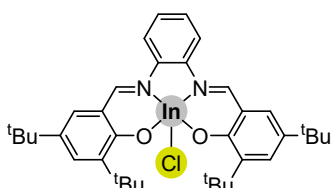
Prepared using general method B; yellow powder (91 %). ^1H NMR (400 MHz, 298 K, CDCl_3) δ 8.90 (s, 2H), 7.76 – 7.71 (m, 2H), 7.65 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 7.40 – 7.36 (m, 2H), 7.16 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 1.61 (s, 18H), 1.35 (s, 18H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, 298 K, CDCl_3) δ 167.4, 162.1, 142.4, 139.3, 135.5, 132.9, 128.7, 128.2, 117.0, 115.3, 35.8, 34.1, 31.3, 29.8 ppm. IR (ATR): 2952.1, 2905.5, 2868.2, 1602.8, 1582.3, 1531.9, 1388.4, 1358.6, 1196.5, 1179.7, 747.3, 538.6 cm^{-1} . Elemental analysis for $\text{C}_{36}\text{H}_{46}\text{GaBrN}_2\text{O}_2$. Calc. C: 62.81 %, H: 6.74 %, N: 4.65 %. Found: C: 62.64 %, H: 6.68 %, N: 4.40 %.

[GaI(Salphen)]:



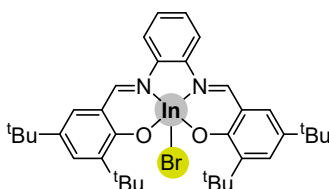
Prepared using general method B; yellow powder (88 %). ^1H NMR (400 MHz, 298 K, CDCl_3) δ 8.89 (s, 2H), 7.78 – 7.74 (m, 2H), 7.65 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 7.45 – 7.40 (m, 2H), 7.16 (d, $^4J_{\text{HH}} = 2.6$ Hz, 2H), 1.59 (s, 18H), 1.35 (s, 18H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, 298 K, CDCl_3) δ 167.1, 161.8, 142.5, 139.3, 135.2, 133.0, 128.7, 128.2, 117.0, 115.4, 35.8, 34.1, 31.2, 29.9 ppm. IR (ATR): 2953.9, 2903.6, 2866.3, 1600.9, 1582.3, 1531.9, 1358.6, 1248.7, 1196.5, 1179.7, 747.3, 538.6 cm^{-1} . Elemental analysis for $\text{C}_{36}\text{H}_{46}\text{GaIN}_2\text{O}_2$. Calc. C: 58.80 %, H: 6.31 %, N: 3.81 %. Found: C: 58.84 %, H: 6.13 %, N: 4.08 %.

[InCl(Salphen)]:^[7]



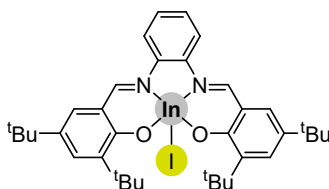
Prepared using general method B; yellow powder (72 %). **¹H NMR (400 MHz, 298 K, CDCl₃)** δ 8.79 (s, 2H), 7.72 – 7.67 (m, 2H), 7.59 (d, ⁴J_{HH} = 2.6 Hz, 2H), 7.44 – 7.40 (m, 2H), 7.09 (d, ⁴J_{HH} = 2.6 Hz, 2H), 1.53 (s, 18H), 1.33 (s, 18H) ppm. **¹³C{¹H} NMR (101 MHz, 298 K, CDCl₃)** δ 169.6, 165.4, 143.0, 138.6, 137.1, 132.3, 129.8, 128.4, 117.8, 116.3, 35.7, 34.1, 31.3, 29.6 ppm. **IR (ATR):** 2953.9, 2905.5, 2866.3, 1600.9, 1580.4, 1528.2, 1429.4, 1388.4, 1172.2, 749.2, 533.0 cm⁻¹.

[InBr(Salphen)]:^[7]



Prepared using general method B; yellow powder (93 %). **¹H NMR (400 MHz, 298 K, CDCl₃)** δ 8.78 (s, 2H), 7.71 – 7.67 (m, 2H), 7.59 (d, ⁴J_{HH} = 2.6 Hz, 2H), 7.43 – 7.39 (m, 2H), 7.10 (d, ⁴J_{HH} = 2.6 Hz, 2H), 1.54 (s, 18H), 1.34 (s, 18H) ppm. **¹³C{¹H} NMR (101 MHz, 298 K, CDCl₃)** δ 169.5, 165.2, 143.1, 138.5, 137.0, 132.3, 129.8, 128.4, 117.8, 116.4, 35.7, 34.1, 31.3, 29.6 ppm. **IR (ATR):** 2953.9, 2905.5, 2868.2, 1599.0, 1578.5, 1528.2, 1429.4, 1388.4, 1250.5, 1172.2, 751.1, 533.0 cm⁻¹.

[InI(Salphen)]:



Prepared using general method B; yellow powder (88 %). **¹H NMR (400 MHz, 298 K, CDCl₃)** δ 8.76 (s, 2H), 7.72 – 7.68 (m, 2H), 7.58 (d, ⁴J_{HH} = 2.6 Hz, 2H), 7.45 – 7.41 (m, 2H), 7.09 (d, ⁴J_{HH} = 2.6 Hz, 2H), 1.53 (s, 18H), 1.33 (s, 18H) ppm. **¹³C{¹H} NMR (101 MHz, 298 K, CDCl₃)** δ 169.2, 164.8, 143.1, 138.4, 137.0, 132.2, 129.7, 128.4, 117.9, 116.4, 35.7, 34.1, 31.3, 29.7 ppm. **IR (ATR):** 2952.1, 2903.6, 2868.2, 1597.2, 1578.5, 1526.3, 1425.7, 1386.6, 1250.5, 1172.2, 747.3, 531.1 cm⁻¹. Elemental analysis for C₃₆H₄₆InIN₂O₂. Calc. C: 55.40 %, H: 5.94 %, N: 3.59 %. Found: C: 55.18 %, H: 5.89 %, N: 3.82 %.

[5] Original NMR and IR spectra for the synthesised [MX(Salphen)] compounds

This section contains the original ^1H , ^{13}C { ^1H } and COSY NMR and IR spectra of the [MX(Salphen)] compounds.

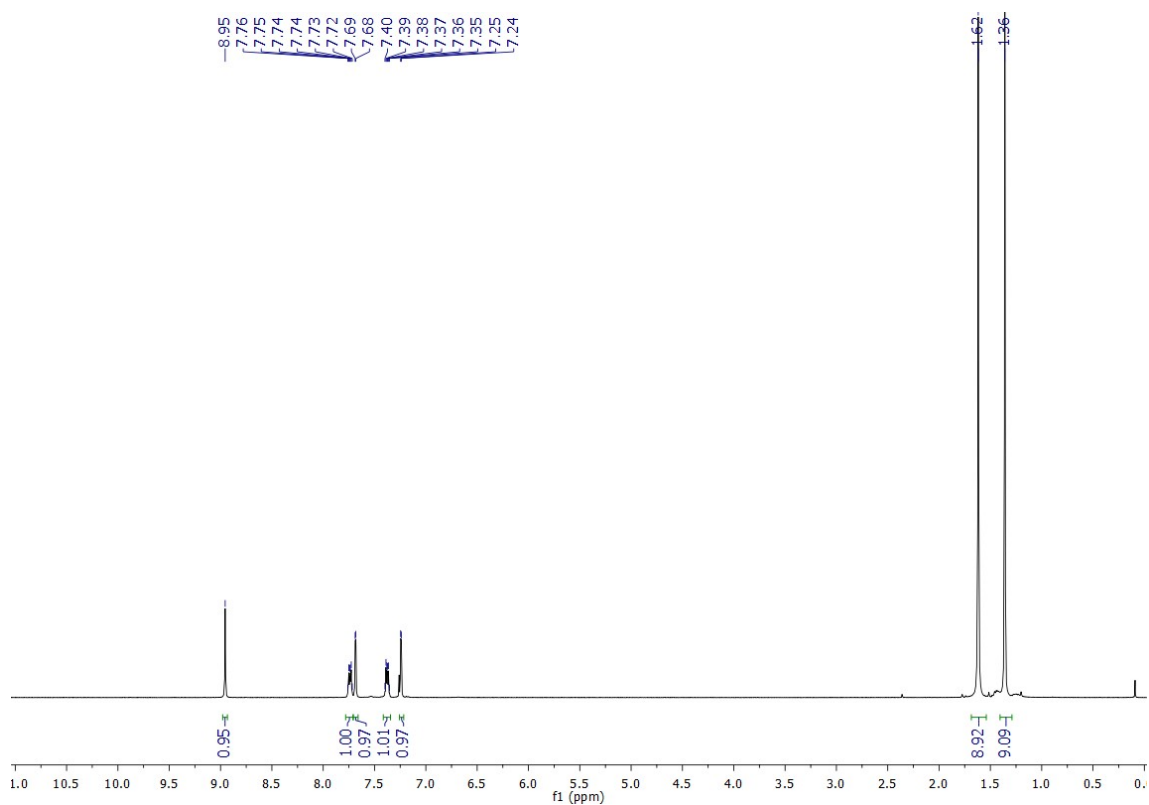


Figure S1. ^1H NMR spectrum of compound [AlCl(Salphen)] in CDCl_3 at 298K.

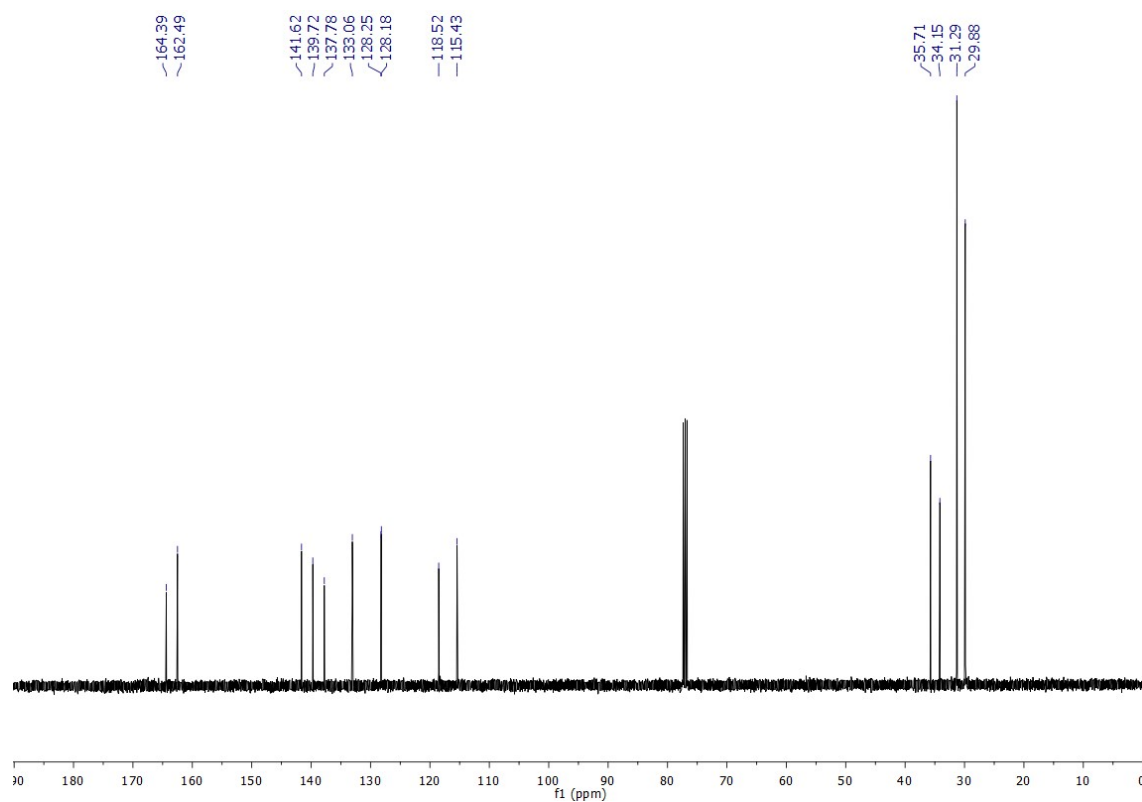


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound $[\text{AlCl}(\text{Salphen})]$ in CDCl_3 at 298K.

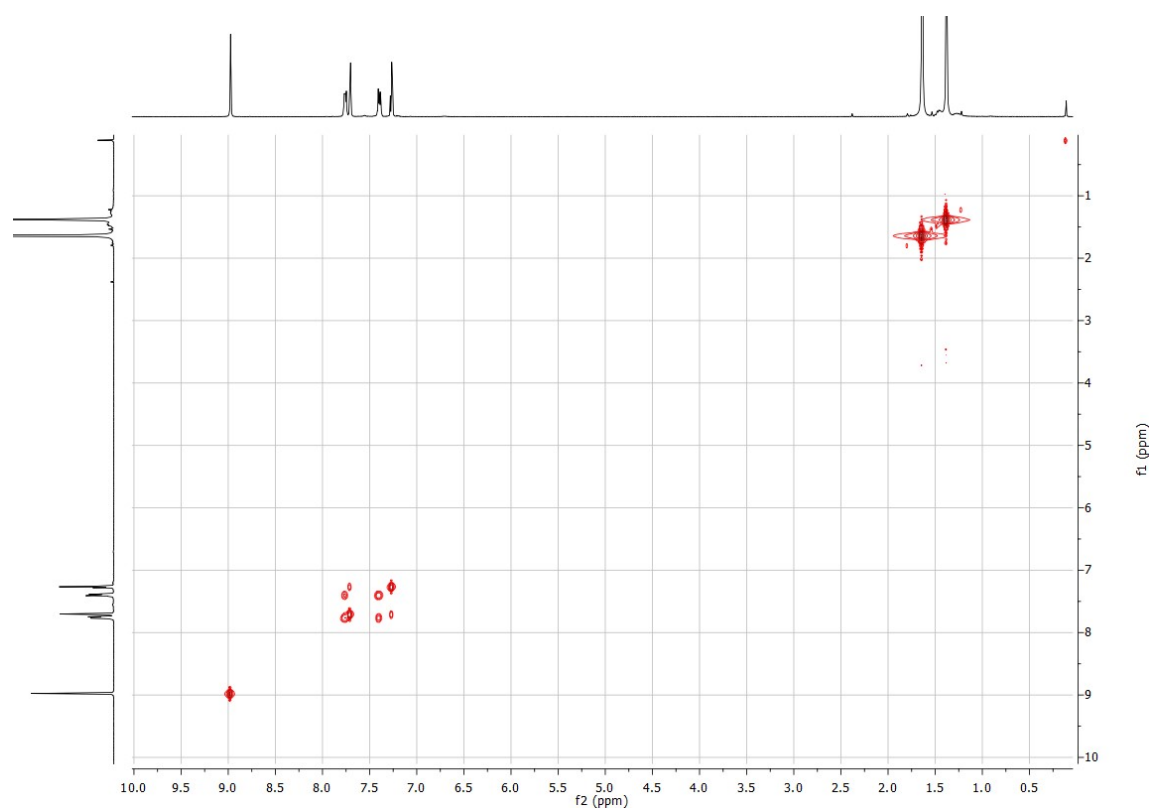


Figure S3. COSY NMR spectrum of compound $[\text{AlCl}(\text{Salphen})]$ in CDCl_3 at 298K.

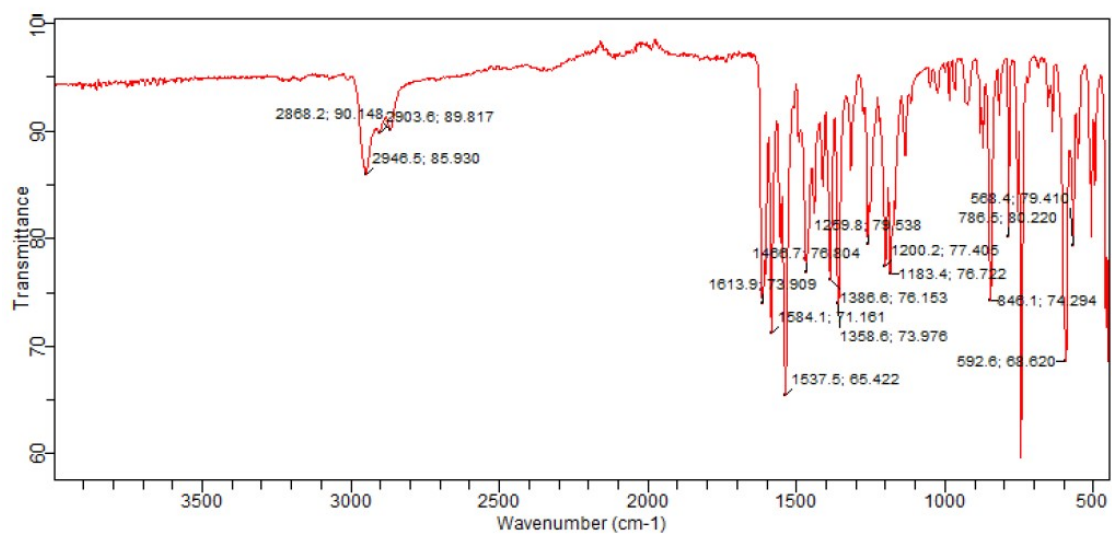


Figure S4. IR spectrum of compound $[AlCl(Salphen)]$ at 298K.

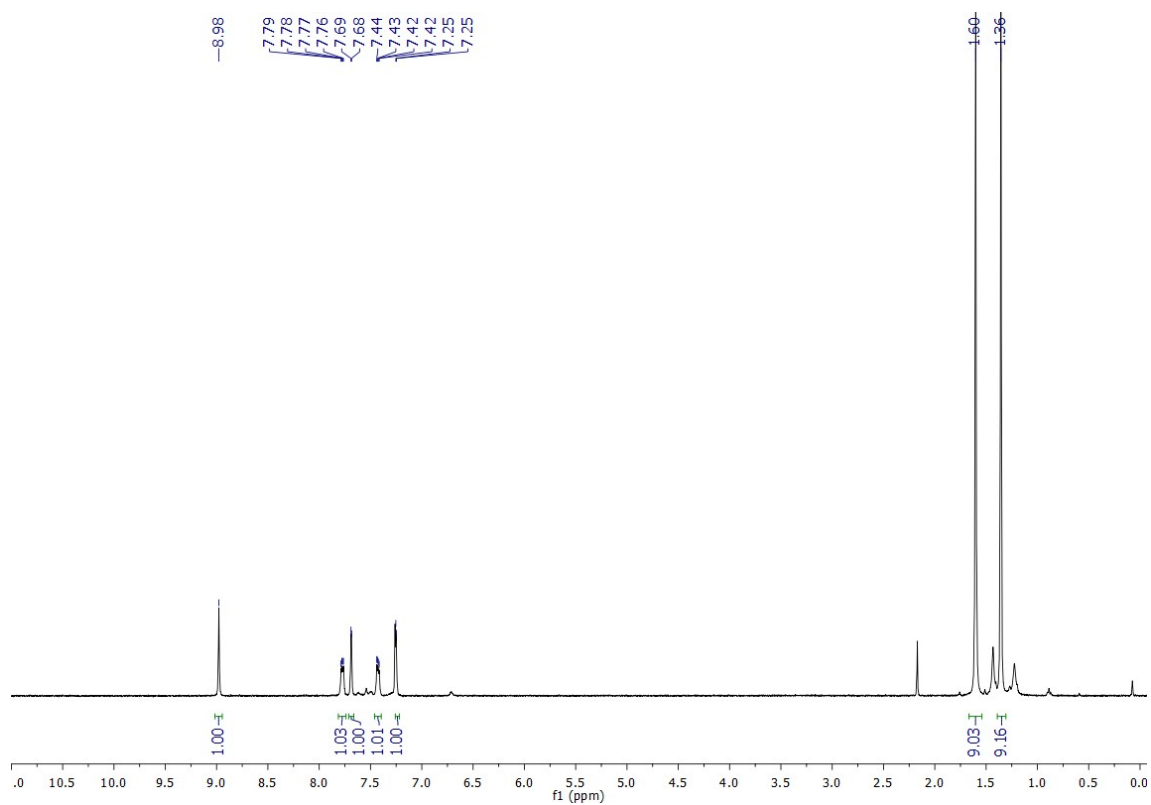


Figure S5. 1H NMR spectrum of compound $[AlBr(Salphen)]$ in $CDCl_3$ at 298K.

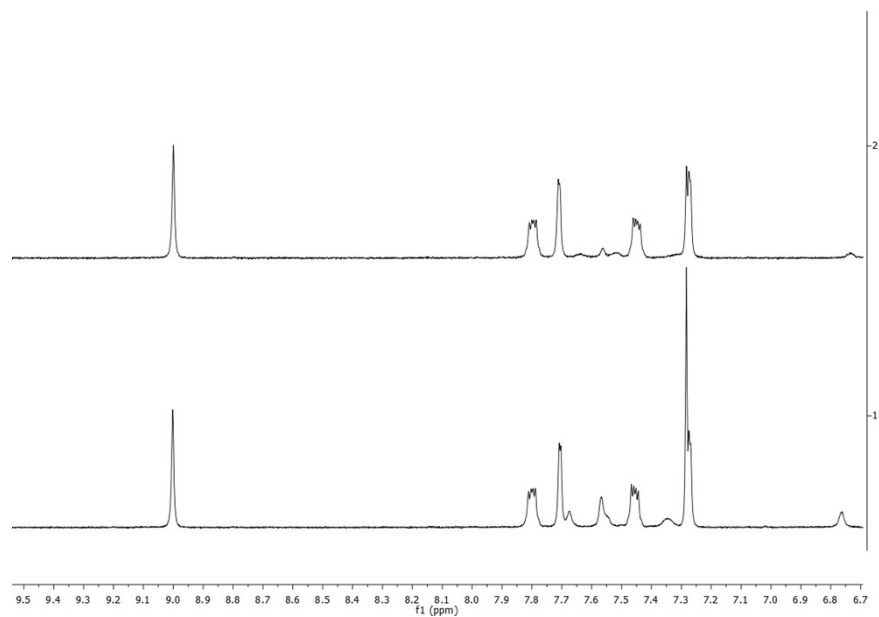


Figure S6. ^1H NMR spectrum of compound $[\text{AlBr}(\text{Salphen})]$ in CDCl_3 at 298K just after isolation (upper) and after two weeks of storage under air (as a solid). Small impurities appear, indicating that the compound is unstable.

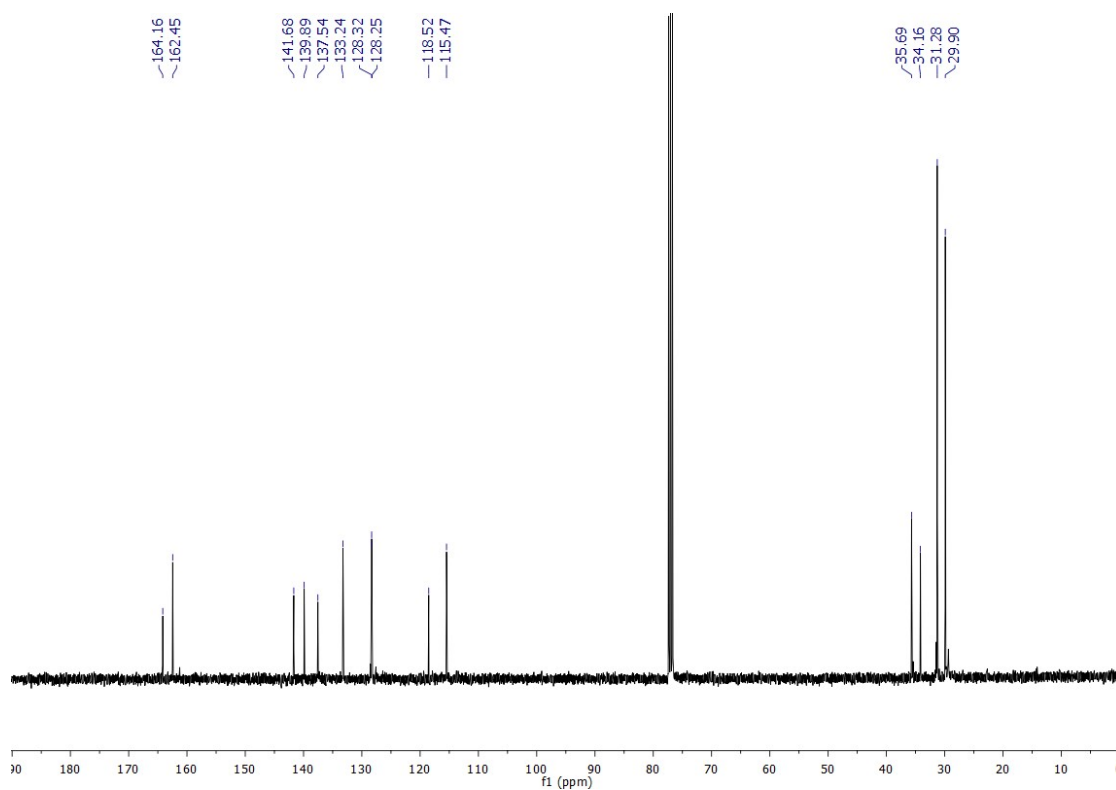


Figure S7. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound $[\text{AlBr}(\text{Salphen})]$ in CDCl_3 at 298K.

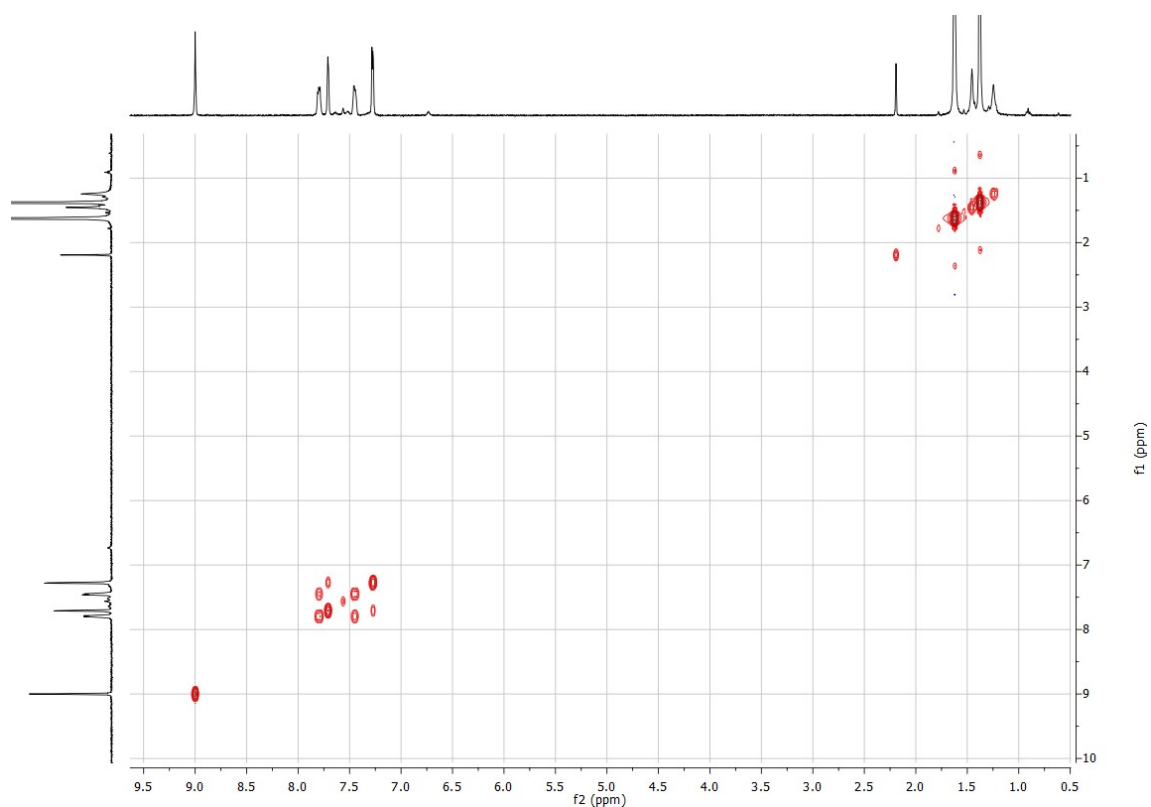


Figure S8. COSY NMR spectrum of compound $[AlBr(Salphen)]$ in $CDCl_3$ at 298K.

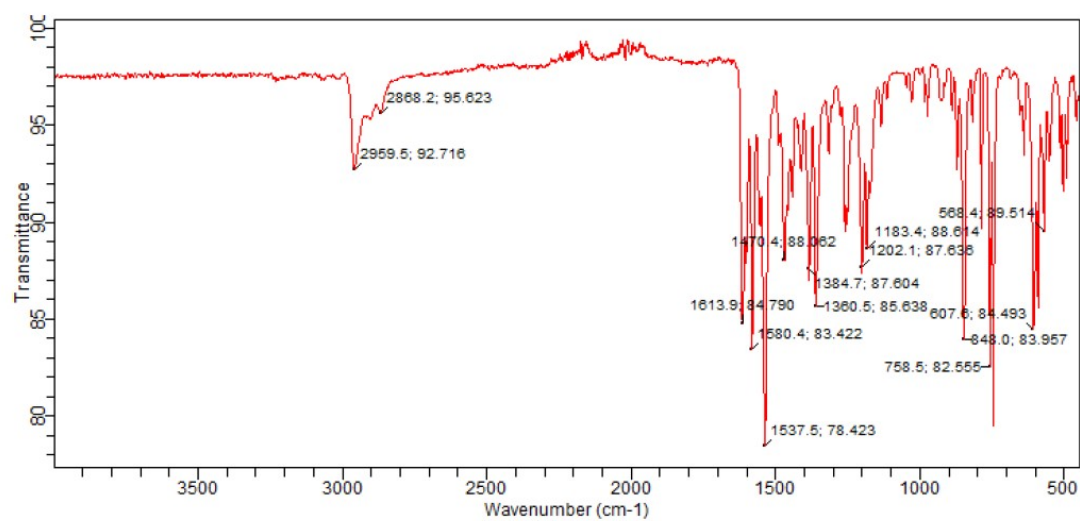


Figure S9. IR spectrum of compound $[AlBr(Salphen)]$ at 298K.

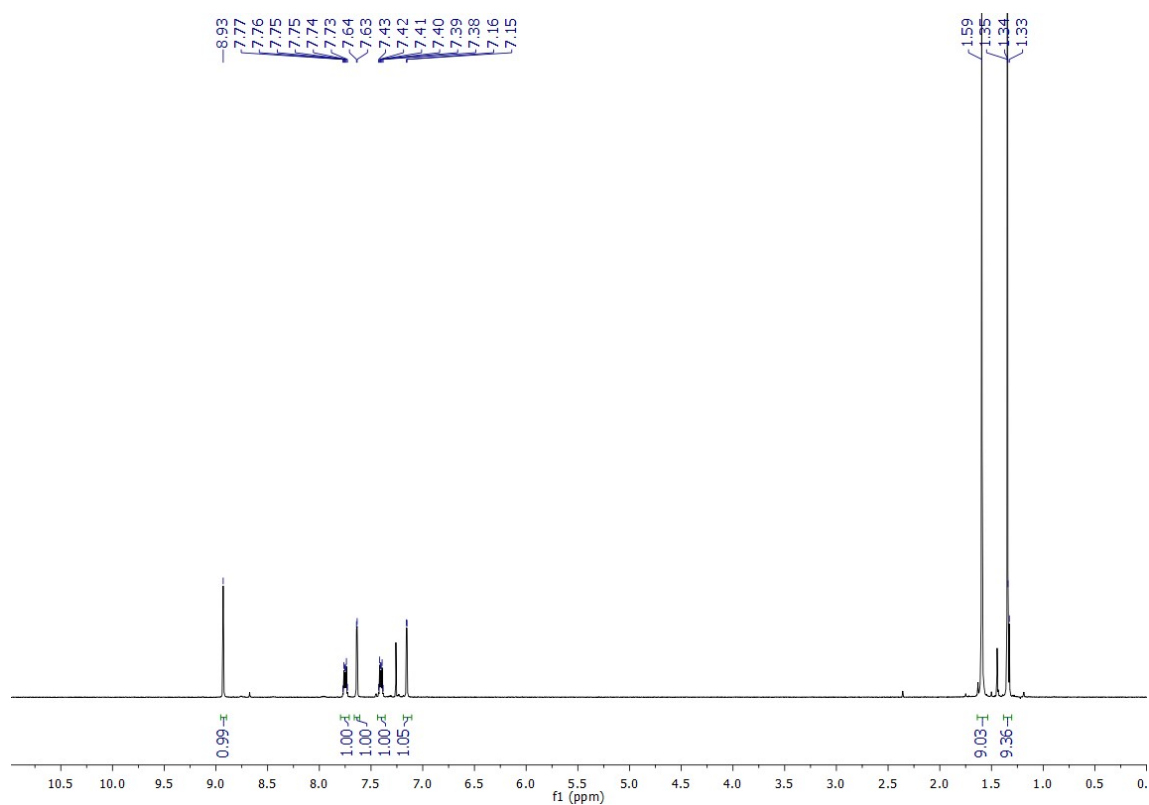


Figure S10. ¹H NMR spectrum of compound [GaCl(Salphen)] in CDCl₃ at 298K.

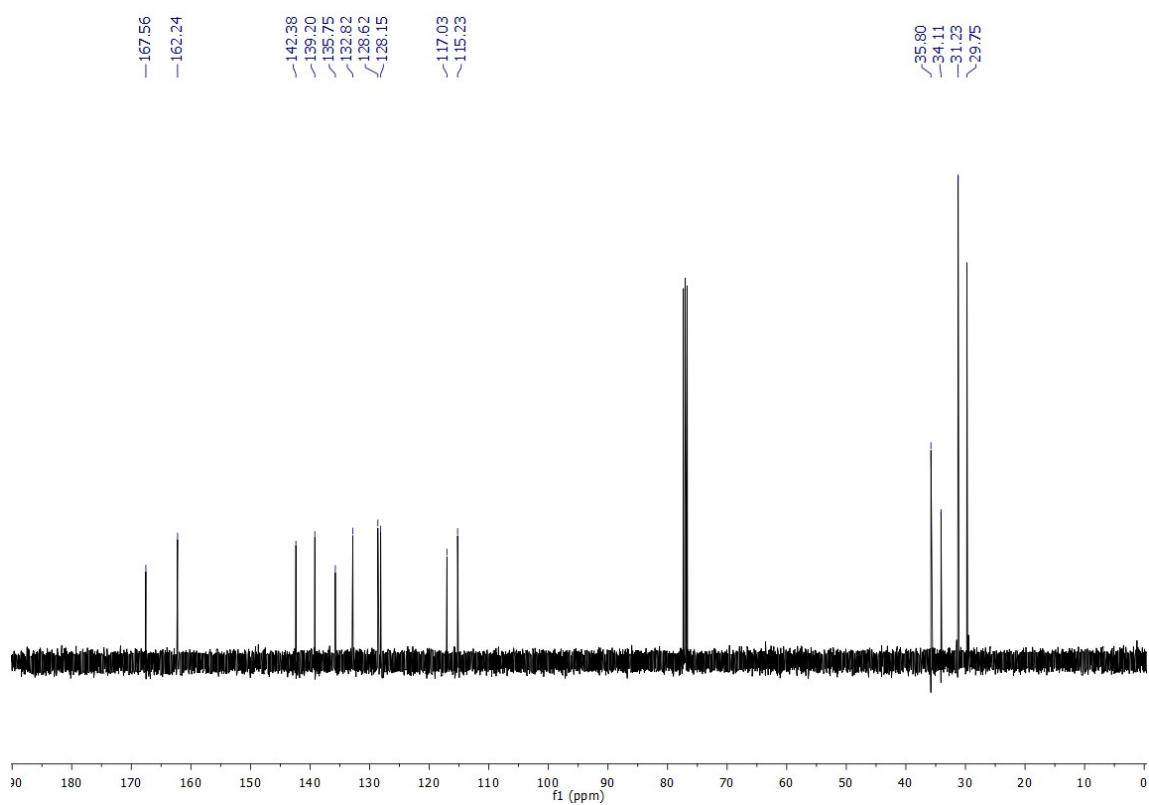


Figure S11. ¹³C{¹H} NMR spectrum of compound [GaCl(Salphen)] in CDCl₃ at 298K.

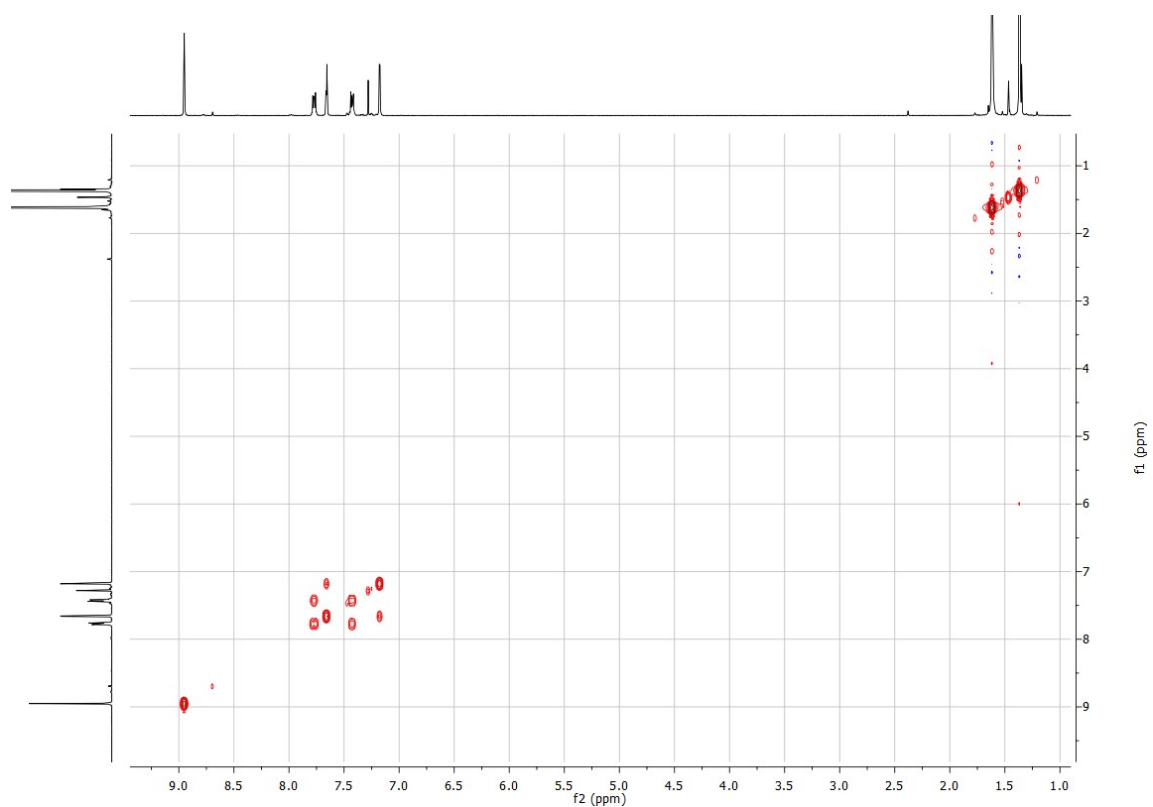


Figure S12. COSY NMR spectrum of compound $[\text{GaCl}(\text{Salphen})]$ in CDCl_3 at 298K.

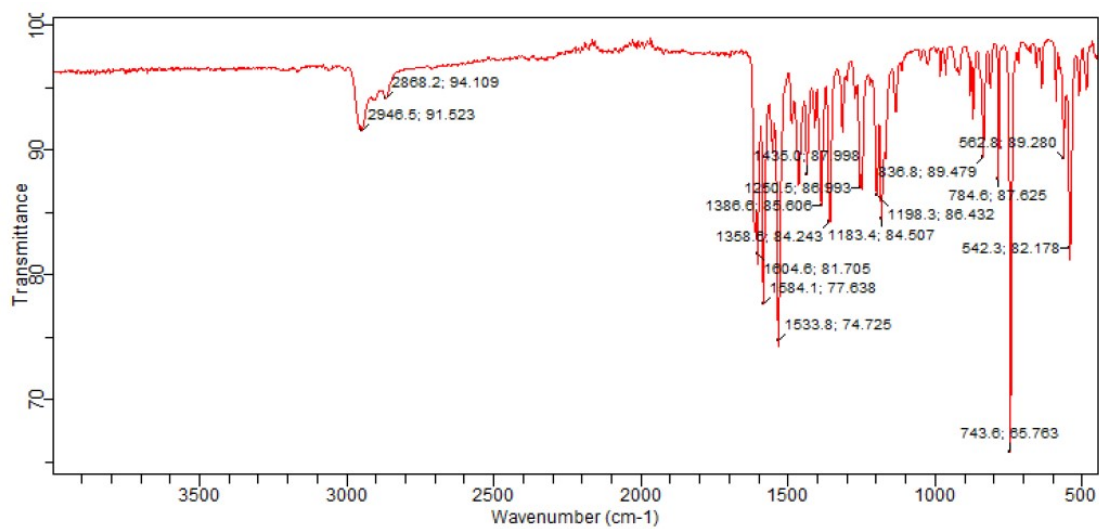


Figure S13. IR spectrum of compound $[\text{GaCl}(\text{Salphen})]$ at 298K.

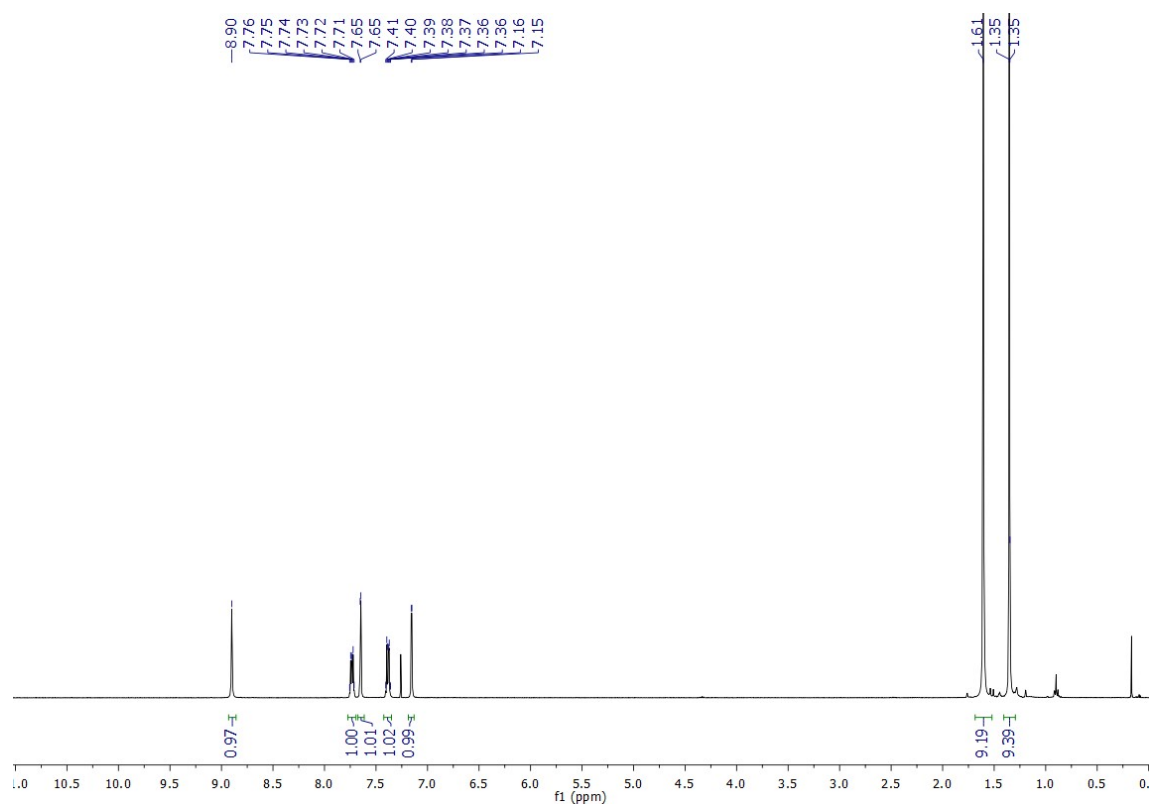


Figure S14. ¹H NMR spectrum of compound [GaBr(Salphen)] in CDCl₃ at 298K.

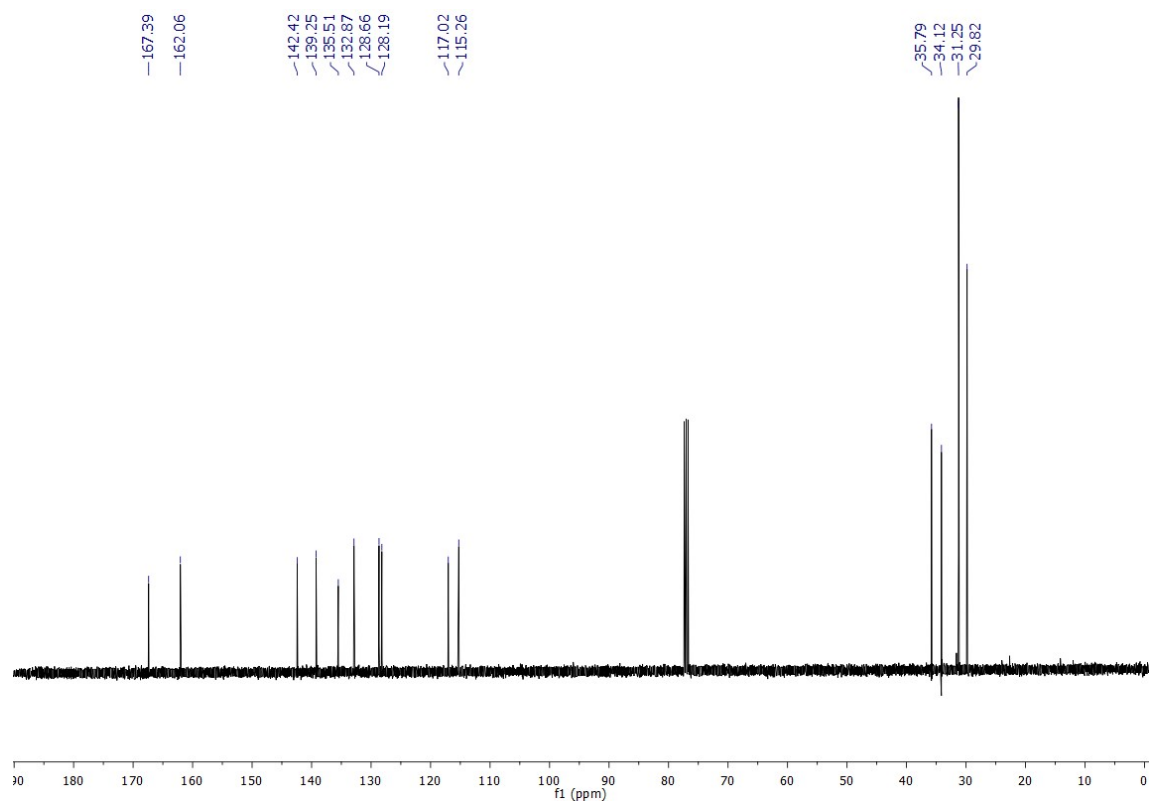


Figure S15. ¹³C{¹H} NMR spectrum of compound [GaBr(Salphen)] in CDCl₃ at 298K.

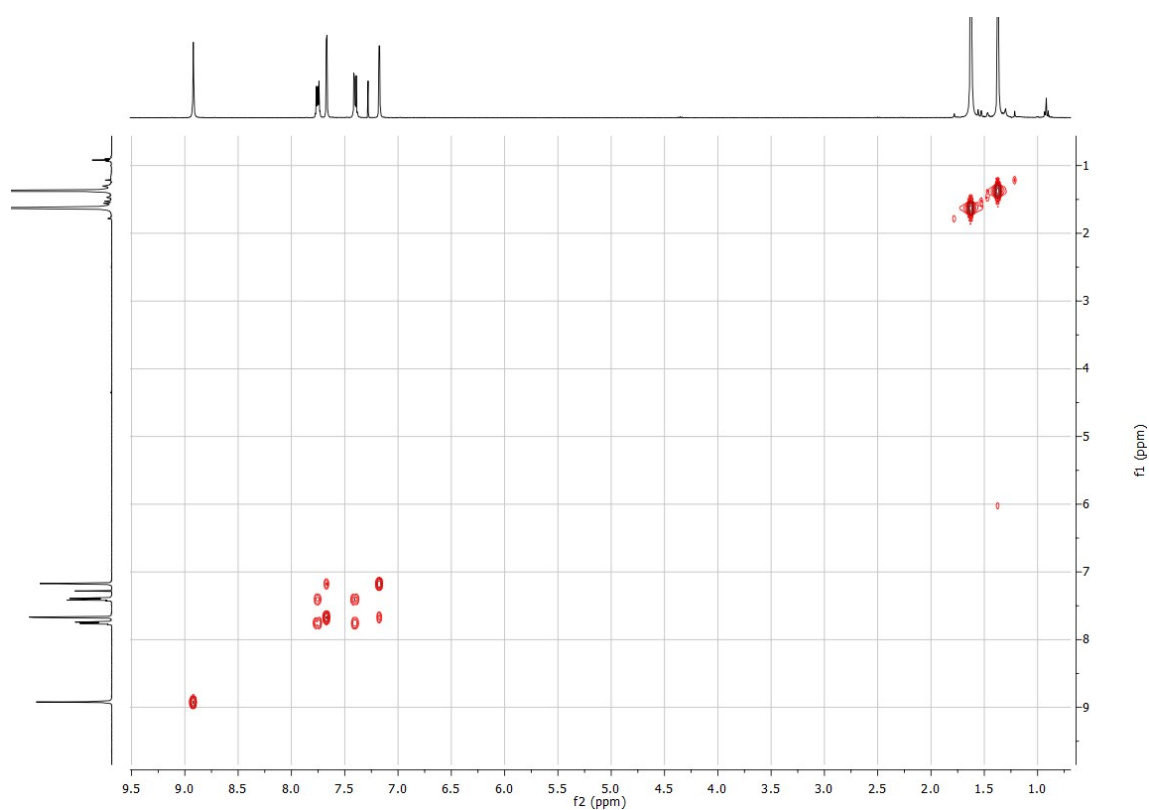


Figure S16. COSY NMR spectrum of compound $[\text{GaBr}(\text{Salphen})]$ in CDCl_3 at 298K.

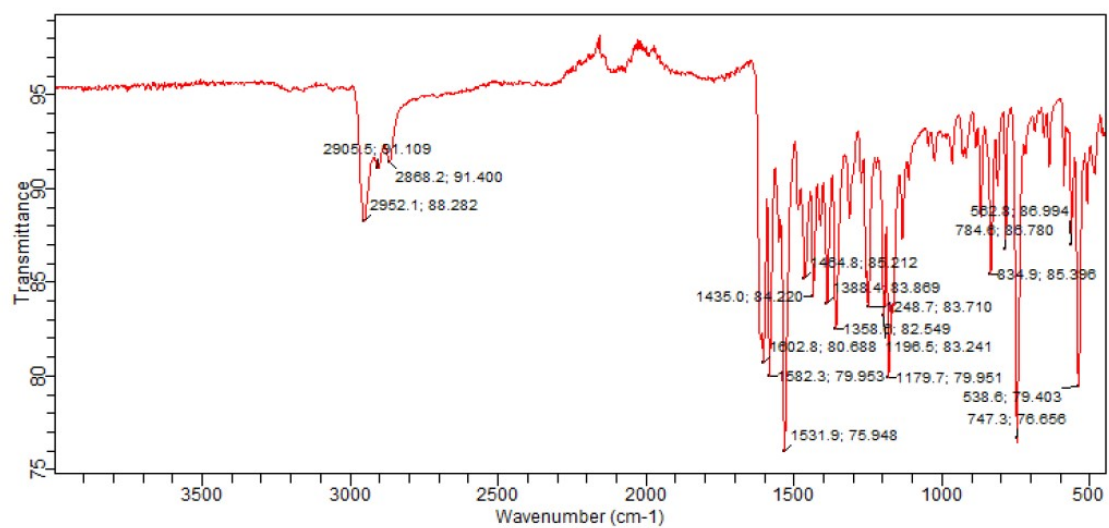


Figure S17. IR spectrum of compound $[\text{GaBr}(\text{Salphen})]$ at 298K.

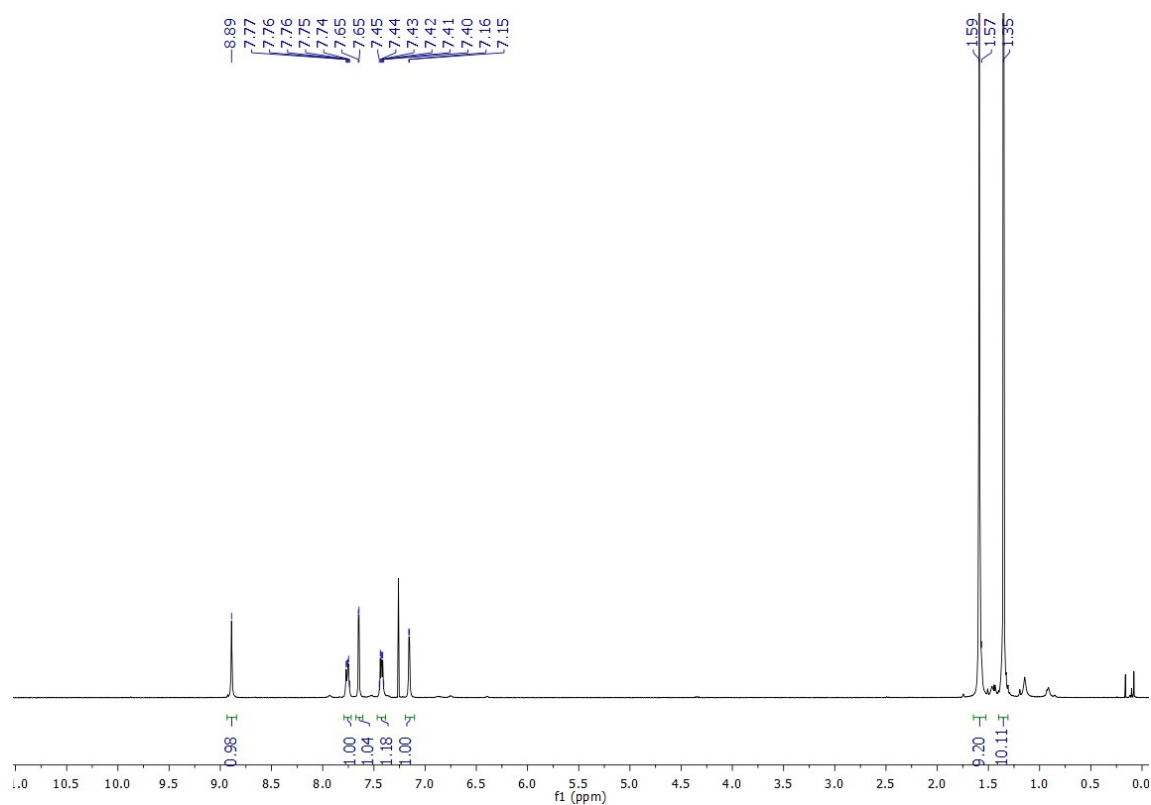


Figure S18. ¹H NMR spectrum of compound [Gal(Salphen)] in CDCl₃ at 298K.

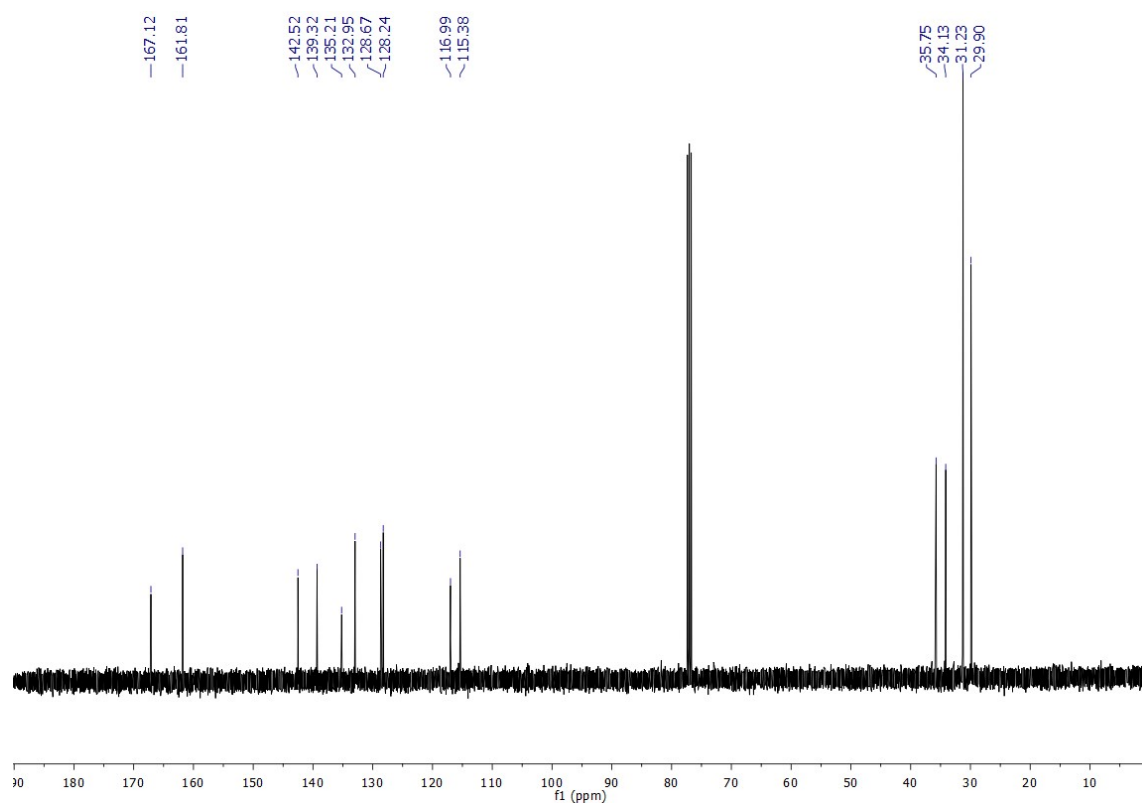


Figure S19. ¹³C{¹H} NMR spectrum of compound [Gal(Salphen)] in CDCl₃ at 298K.

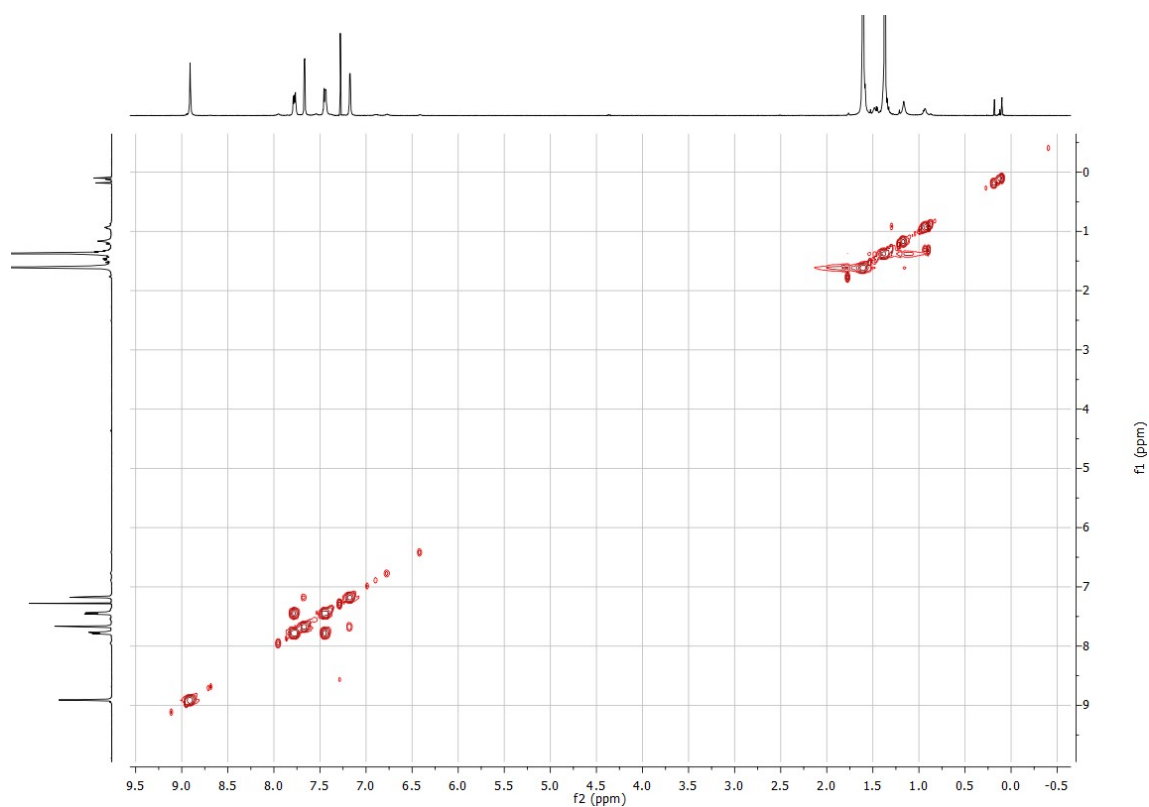


Figure S20. COSY NMR spectrum of compound *[Gal(Salphen)]* in CDCl_3 at 298K.

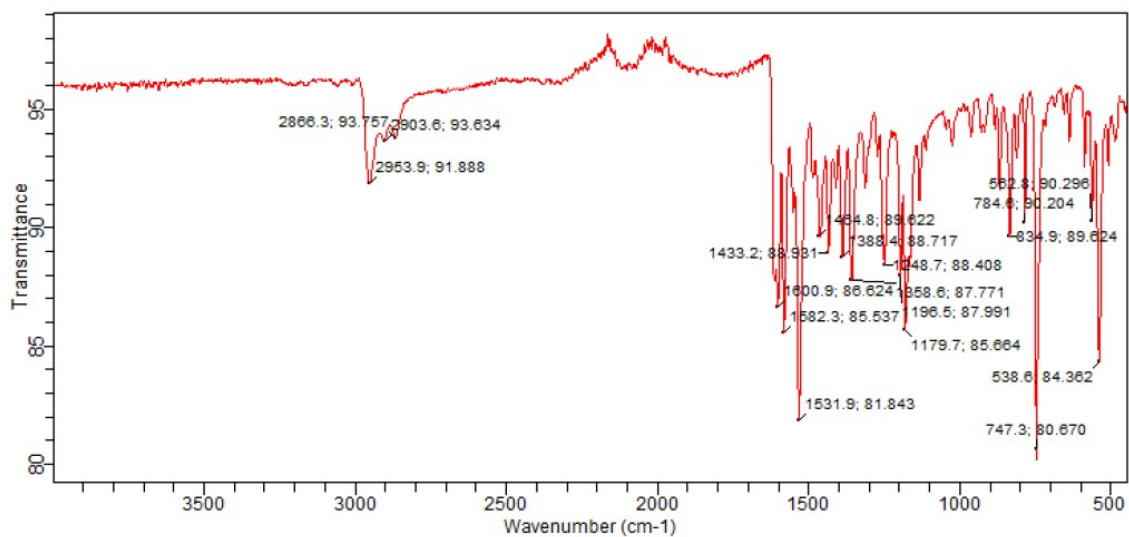


Figure S21. IR spectrum of compound *[Gal(Salphen)]* at 298K.

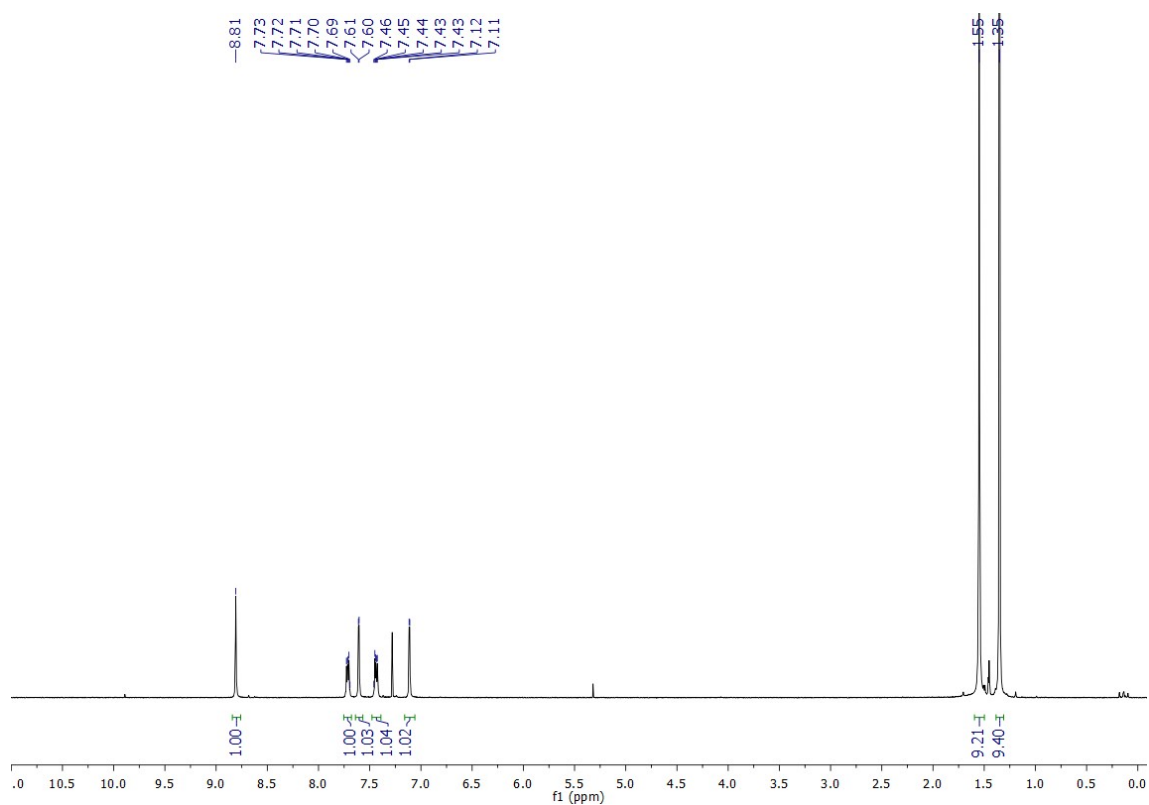


Figure S22. ¹H NMR spectrum of compound [InCl(Salphen)] in CDCl₃ at 298K.

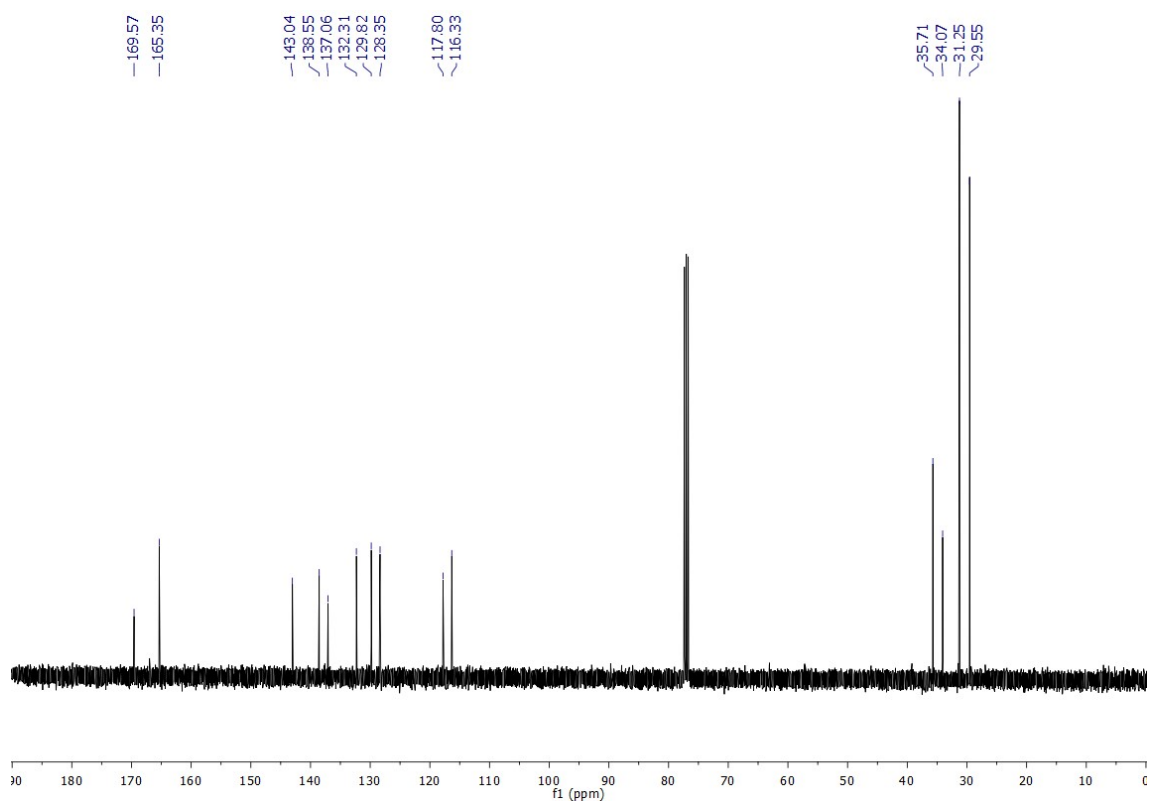


Figure S23. ¹³C{¹H} NMR spectrum of compound [InCl(Salphen)] in CDCl₃ at 298K.

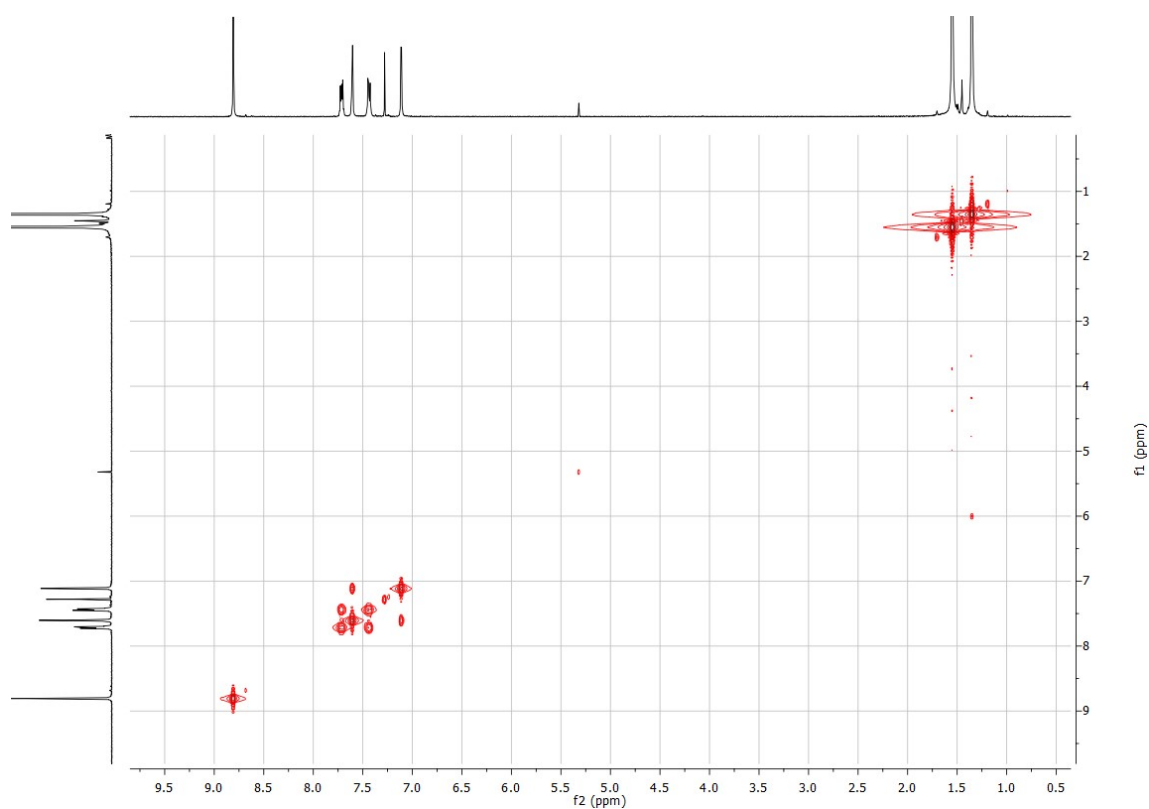


Figure S24. COSY NMR spectrum of compound $[\text{InCl}(\text{Salphen})]$ in CDCl_3 at 298K.

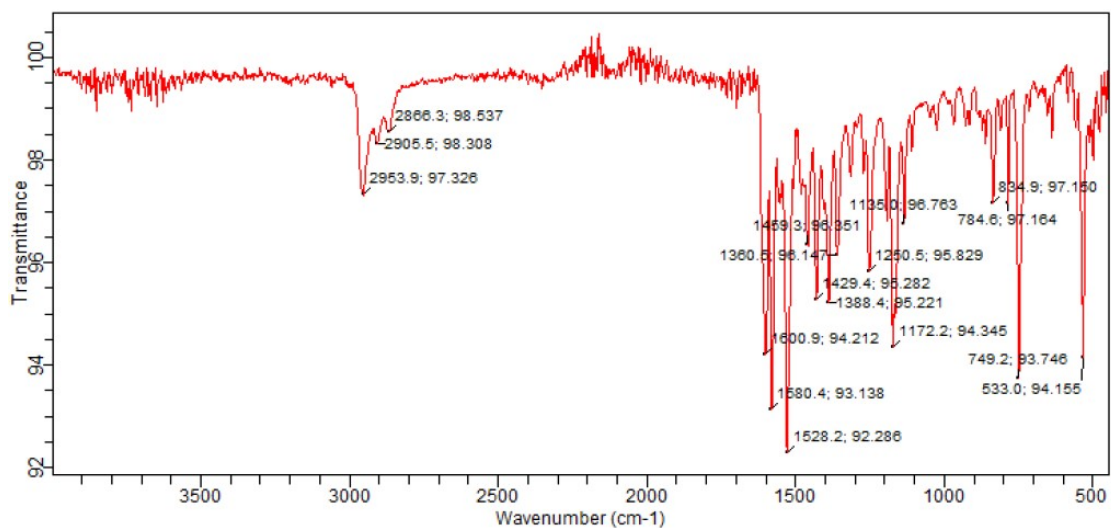


Figure S25. IR spectrum of compound $[\text{InCl}(\text{Salphen})]$ at 298K.

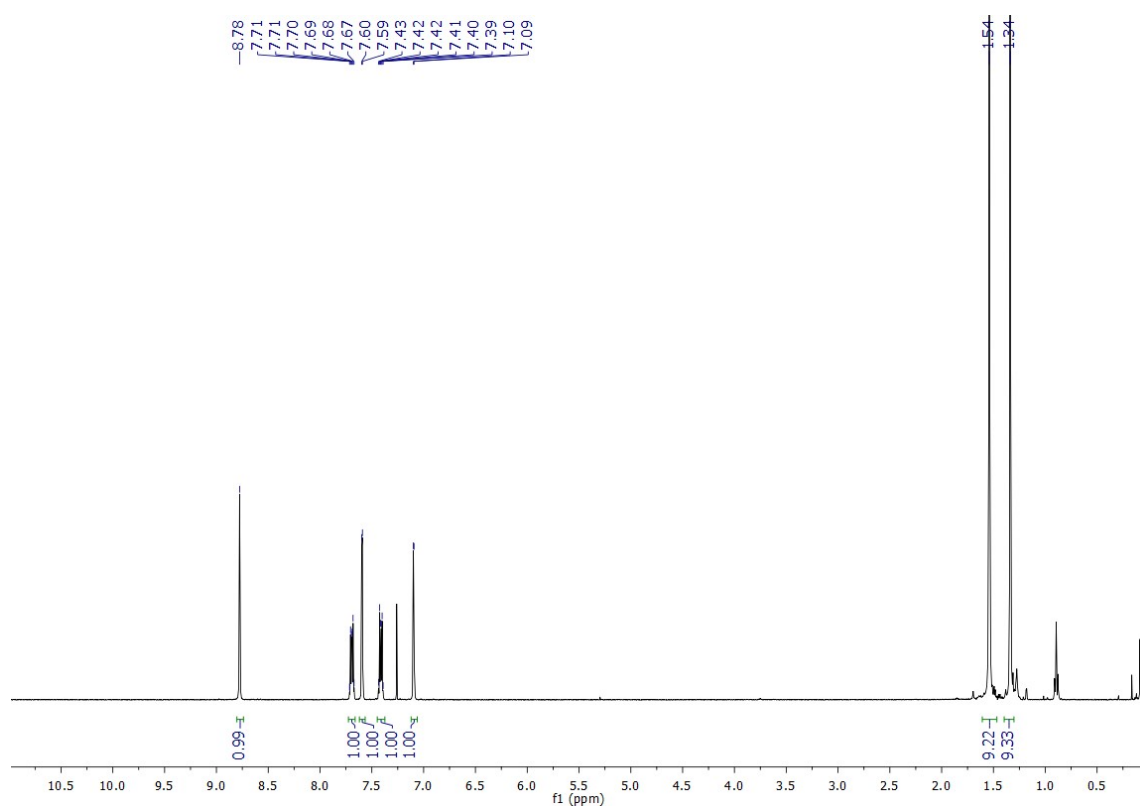


Figure S26. ¹H NMR spectrum of compound [InBr(Salphen)] in CDCl₃ at 298K.

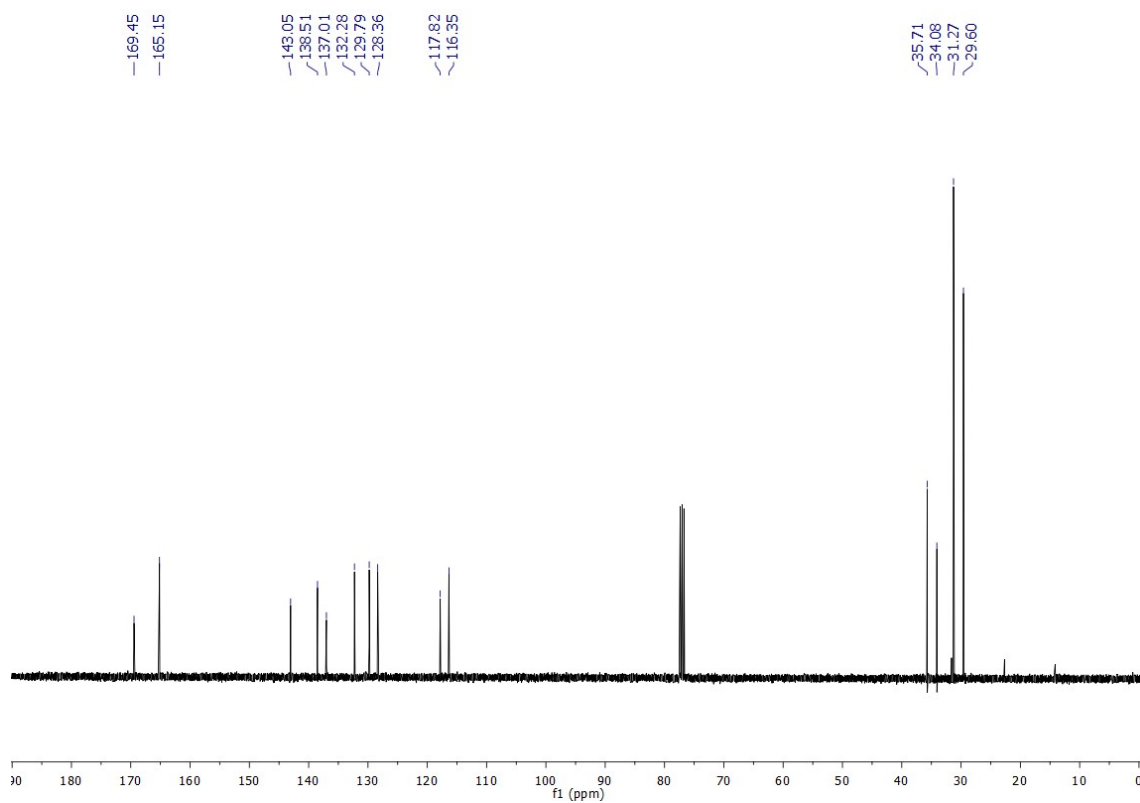


Figure S27. ¹³C{¹H} NMR spectrum of compound [InBr(Salphen)] in CDCl₃ at 298K.

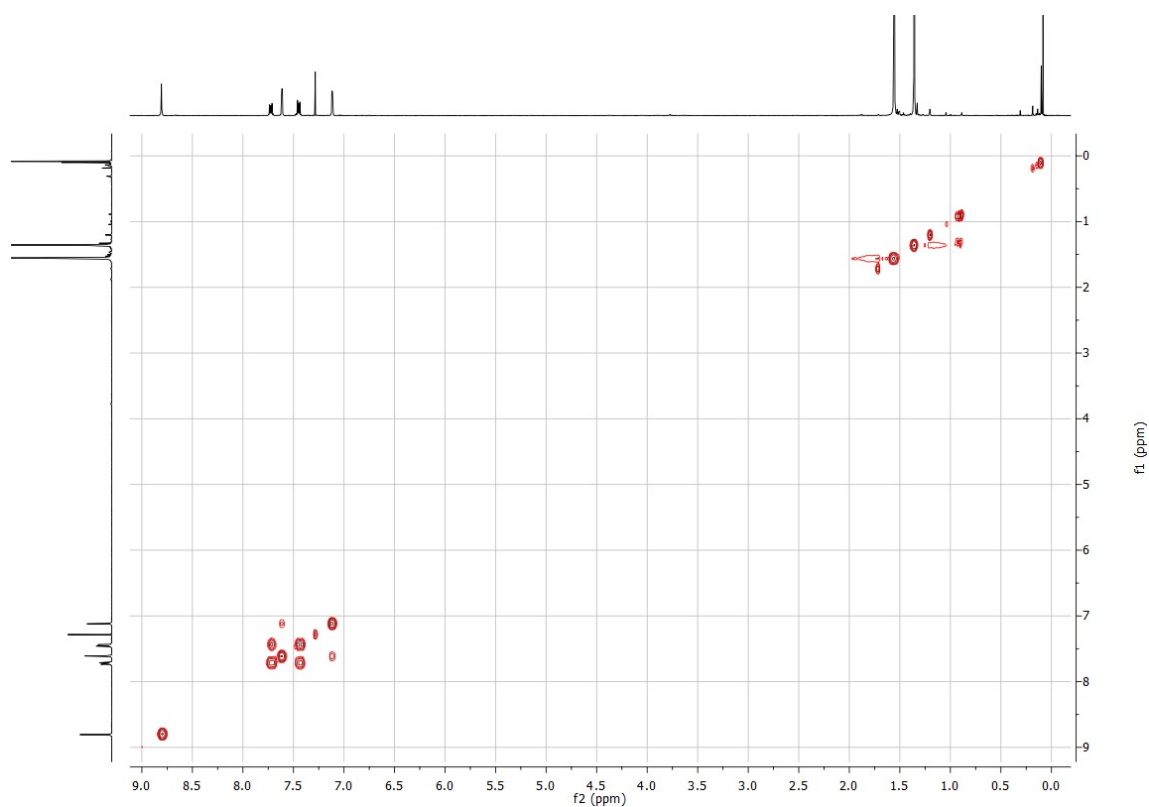


Figure S28. COSY NMR spectrum of compound $[\text{InBr}(\text{Salphen})]$ in CDCl_3 at 298K.

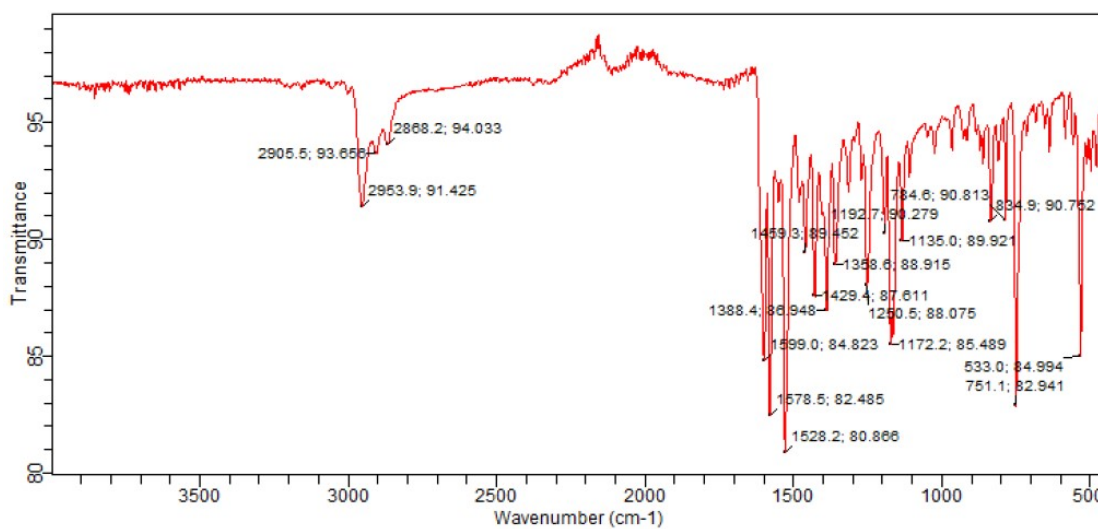


Figure S29. IR spectrum of compound $[\text{InBr}(\text{Salphen})]$ at 298K.

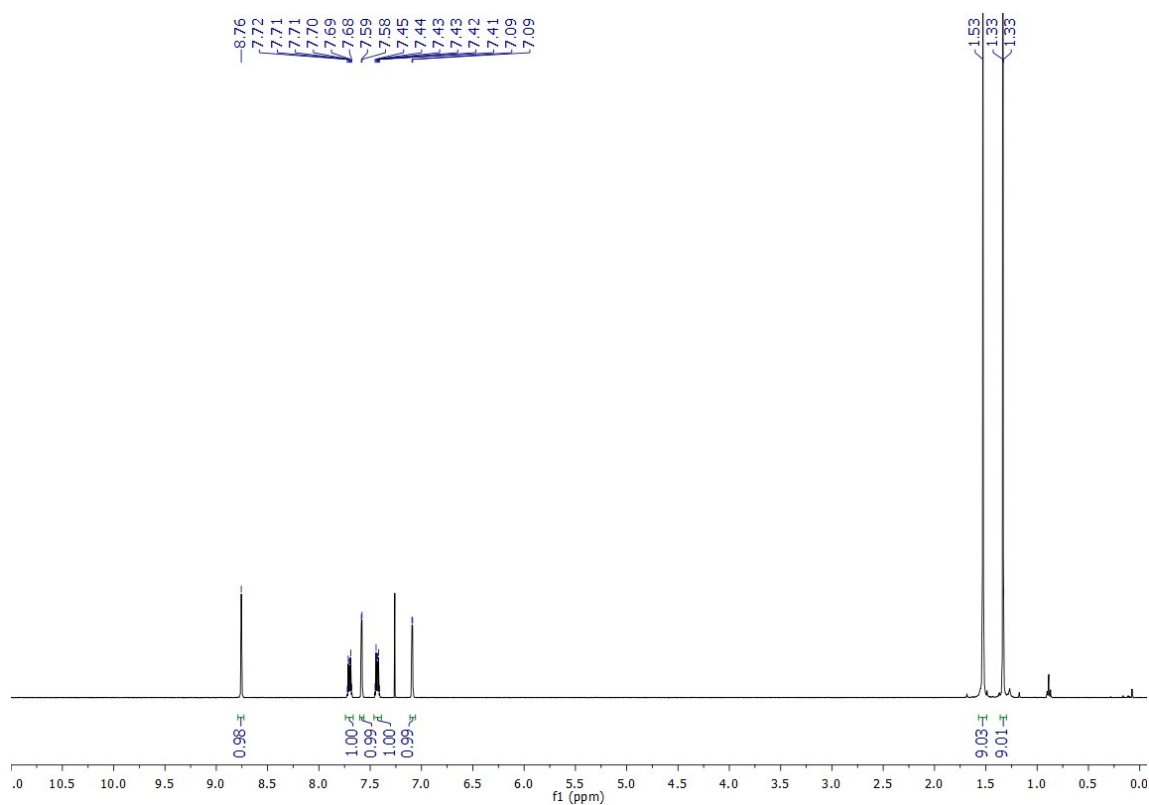


Figure S30. ¹H NMR spectrum of compound [InI(Salphen)] in CDCl₃ at 298K.

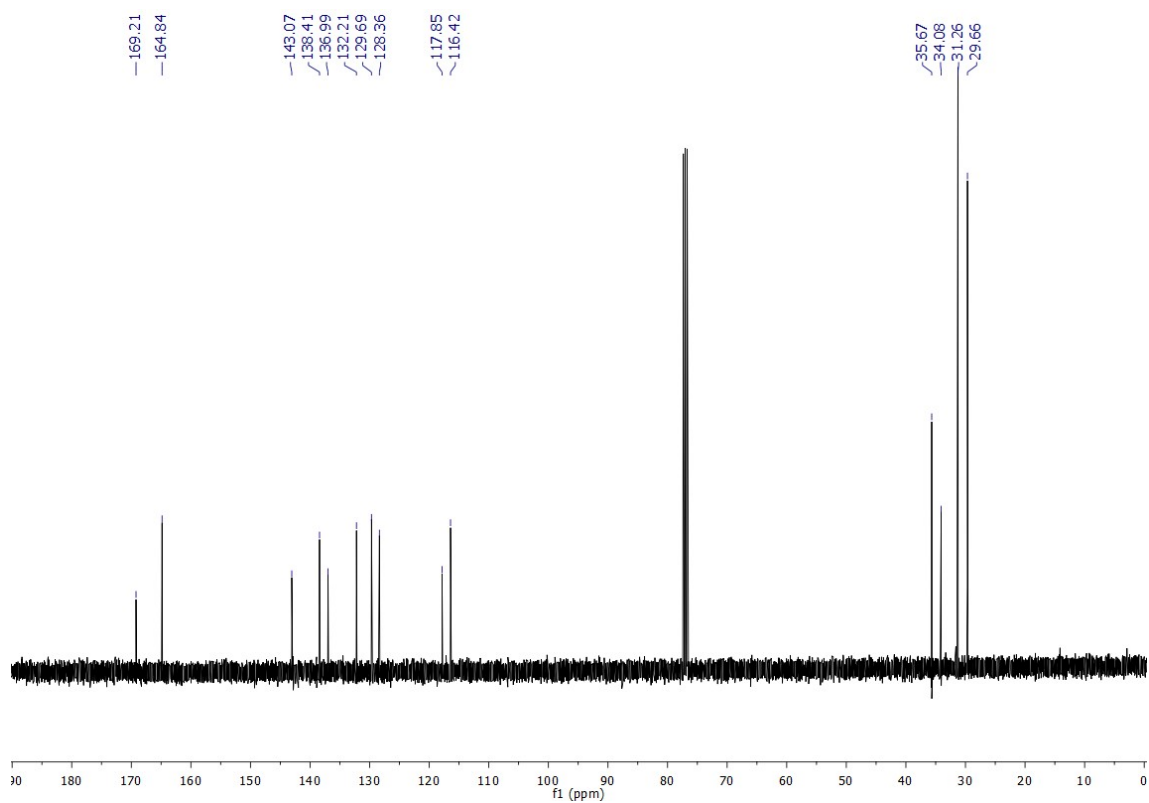


Figure S31. ¹³C{¹H} NMR spectrum of compound [InI(Salphen)] in CDCl₃ at 298K.

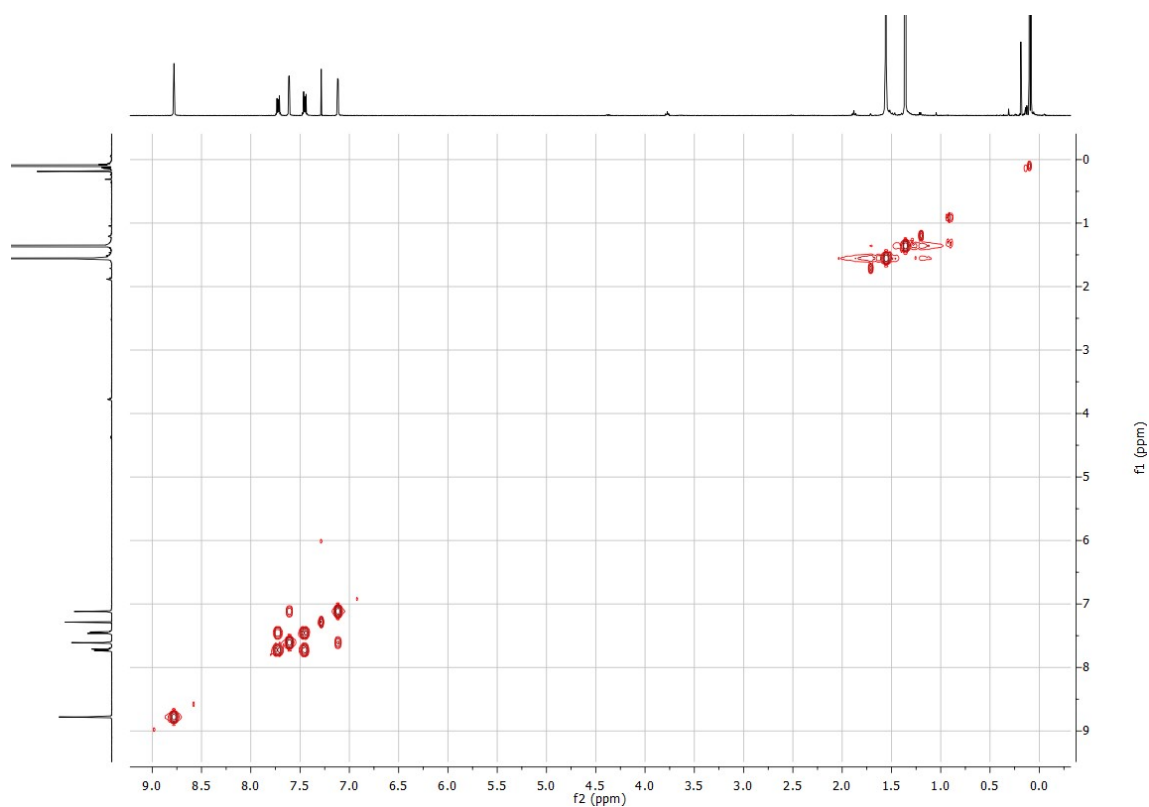


Figure S32. COSY NMR spectrum of compound $[InI(Salphen)]$ in $CDCl_3$ at 298K.

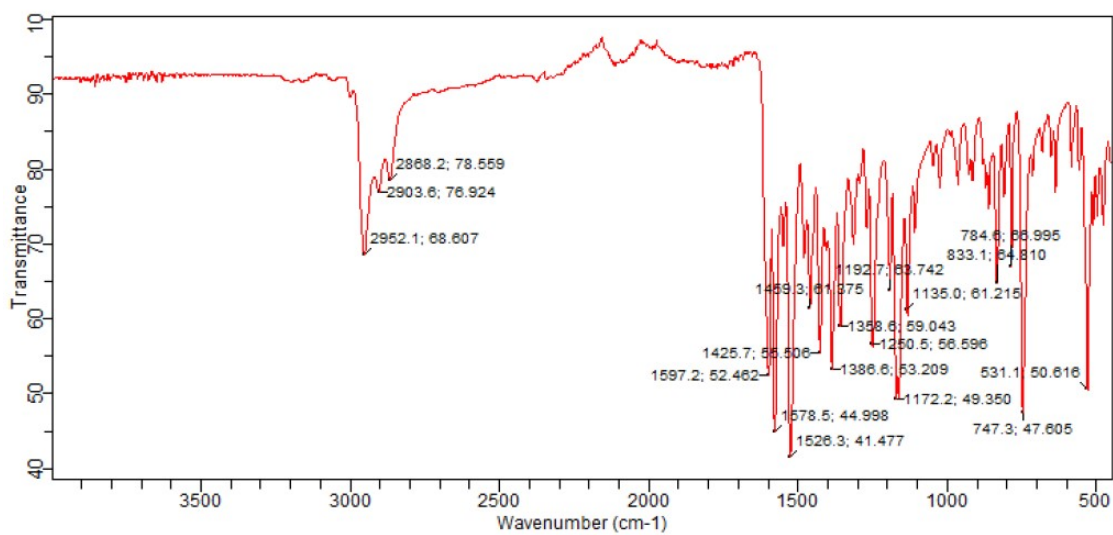


Figure S33. IR spectrum of compound $[InI(Salphen)]$ at 298K.

[6] X-ray crystallography data for [GaBr(Salphen)] and [GaI(Salphen)]

Diffraction data were collected using an Oxford Diffraction Supernova diffractometer, equipped with an Atlas CCD area detector and a four-circle kappa goniometer. For the data collection, Mo source with multilayer optics was used. Data integration, scaling, and empirical absorption correction were carried out using the CrysAlis Program package.^[8] The structures were solved using direct methods and refined by Full-Matrix-Least-Squares against F² with SHELX^[9] under OLEX2.^[10] The non-hydrogen atoms were refined anisotropically, and hydrogen atoms were placed at idealized positions and refined using the riding model. Graphics were made with OLEX2 and MERCURY.^[11] Crystal data, particular details, and CCDC reference numbers are given in the table. Crystallographic data (excluding structure factors) for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC) which have been assigned as entries 2173026 and 2177923.

Table S1 X-ray structure parameters obtained for [GaBr(Salphen)]:

	[GaBr(Salphen)]
Empirical formula	C ₃₆ H ₄₆ BrGaN ₂ O ₂
Formula weight	688.38
Temperature/K	200.0
Crystal system	triclinic
Space group	<i>P</i> -1
<i>a</i> /Å	9.7269(4)
<i>b</i> /Å	12.7417(6)
<i>c</i> /Å	14.5254(7)
α /°	84.461(2)
β /°	78.992(2)
γ /°	71.350(2)
Volume/Å ³	1673.11(13)
<i>Z</i>	2
ρ_{calc} g/cm ³	1.366
μ /mm ⁻¹	2.050
<i>F</i> (000)	716.0
Crystal size/mm ³	0.234 × 0.203 × 0.140
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection/°	4.506 to 55.838
Reflections collected	93585
Independent reflections [<i>R</i> _{int}]	7988 [0.0909]
Restraints/parameters	0/391
GOF on <i>F</i> ²	1.049, <i>R</i> _{sigma} = 0.0400]
Final <i>R</i> ₁ indexes [<i>I</i> > 2 σ (<i>I</i>)]	0.0398
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0646, <i>wR</i> ₂ = 0.0970
Largest diff. peak/hole / e Å ⁻³	0.68/-0.64

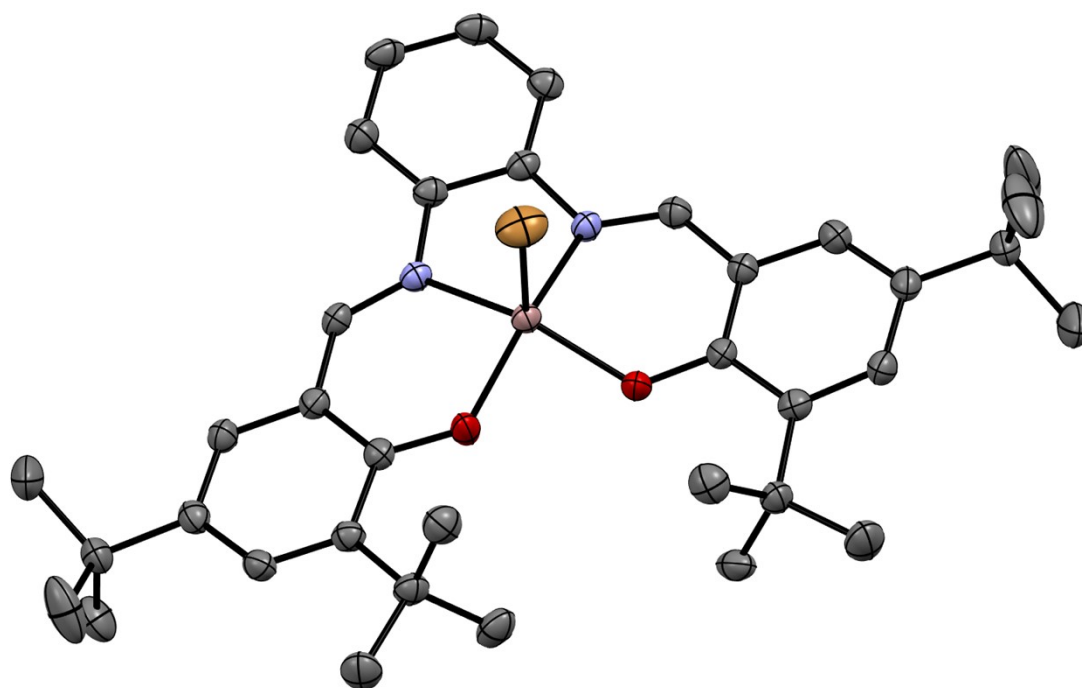


Figure S34 X-ray crystal structure of [**GaBr(Salphen)**].

Table S2 Selected bond lengths (Å) and bond angles (°) obtained from the X-ray of [**GaBr(Salphen)**]:

Selected bond lengths (Å)		Selected bond angles (°)	
Ga1-Br1	2.3419(4)	O1-Ga1-Br1	106.77(6)
Ga1-O1	1.8745(17)	O1-Ga1-N1	90.11(8)
Ga1-O2	1.8726(17)	O1-Ga1-N2	153.59(9)
Ga1-N1	2.034(2)	O2-Ga1-Br1	109.34(6)
Ga1-N2	2.048(2)	O2-Ga1-O1	87.60(7)
		O2-Ga1-N1	145.13(8)
		O2-Ga1-N2	88.24(8)
		N1-Ga1-Br1	104.63(6)
		N1-Ga1-N2	78.68(8)
		N2-Ga1-Br1	99.21(6)

Table S3 X-ray structure parameters obtained for [Gal(Salphen)]:

	[Gal(Salphen)]
Empirical formula	C ₃₆ H ₄₆ BrGaN ₂ O ₂
Formula weight	735.37
Temperature/K	200.0
Crystal system	Monoclinic
Space group	P2 ₁ /c
a/Å	7.6466(3)
b/Å	18.2837(7)
c/Å	25.0241(11)
α/°	90
β/°	96.779(2)
γ/°	90
Volume/Å ³	3474.1(2)
Z	4
ρ _{calc} g/cm ³	1.406
μ/mm ⁻¹	1.713
F(000)	1504.0
Crystal size/mm ³	0.289 × 0.232 × 0.092
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.748 to 63.128
Reflections collected	142440
Independent reflections [R _{int}]	11584 [0.0784]
Restraints/parameters	0/391
GOF on F ²	0.996
Final R ₁ indexes [I ≥ 2σ (I)]	0.0396
Final R indexes [all data]	R ₁ = 0.0663, wR ₂ = 0.0908
Largest diff. peak/hole / e Å ⁻³	0.44/-0.67

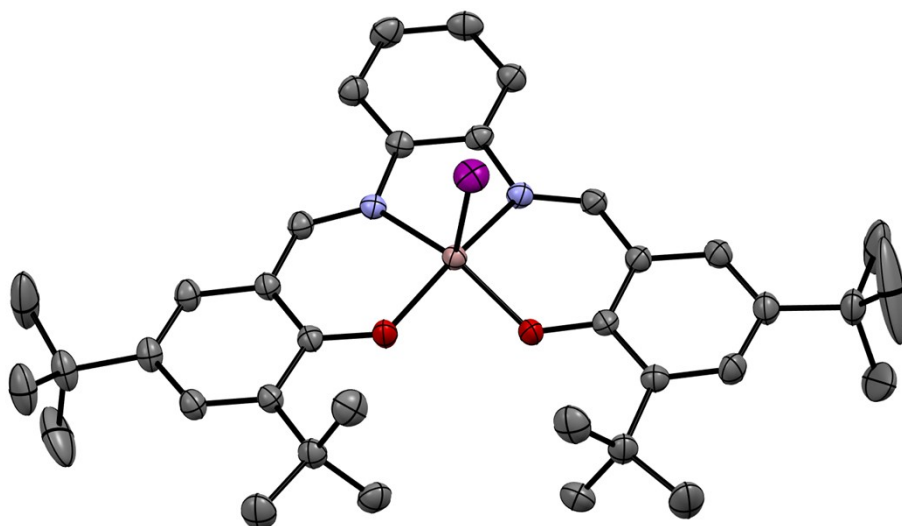


Figure S35 X-ray crystal structure of **[Gal(Salphen)]**.

Table S4 Selected bond lengths (Å) and bond angles (°) obtained from the X-ray of **[Gal(Salphen)]**:

Selected bond lengths (Å)		Selected bond angles (°)	
Ga1-I1	2.5499(3)	O1-Ga1-I1	104.77(5)
Ga1-O1	1.8791(15)	O1-Ga1-N1	90.15(7)
Ga1-O2	1.8701(16)	O1-Ga1-N2	155.55(8)
Ga1-N1	2.0250(18)	O2-Ga1-I1	107.80(5)
Ga1-N2	2.0500(17)	O2-Ga1-O1	88.11(7)
		O2-Ga1-N1	144.32(8)
		O2-Ga1-N2	88.37(7)
		N1-Ga1-I1	107.09(5)
		N1-Ga1-N2	78.83(7)
		N2-Ga1-I1	99.35(6)

[7] Computational study details

General comments: All DFT calculations undertaken using the ORCA 4.2.1 computational software.¹² Optimisations and analytical frequency calculations were performed at the RI-B97-D3/def2-SVP level of theory¹³⁻¹⁵ and single-point energies and solvation corrections calculated at RIJCOSX- ω B97M-D3BJ/def2-TZVPP.¹⁵⁻¹⁷ Solvation correction was implemented with the CPCM model¹⁸ with a dielectric constant value of 16 to represent the epoxide solvent environment. Analytical frequencies were calculated for inclusion of the Zero Point Energy (ZPE) correction and entropic contributions to the free energy term (ΔG_{298K}), as well as confirming all intermediate were true with no imaginary modes and all transition states had the correct critical frequency of decomposition (imaginary mode). All thermodynamic parameters were calculated in the standard state (298.15 K and 1 atm). Numerical precision integration grids were increase beyond the default settings, to *Grid4* for the SCF step and *Grid5* for the final energy evaluation. Concentration correction for the individual species was applied as a free energy correction based on $RT \ln(c_i/c_{atm})$ ¹⁹ where c_i is the experimental concentration of the relevant species. This is particularly important in systems such as this, given the dual role of the epoxide, as both reagent and solvent. Graphical visualisation and structural analysis performed from the DFT calculations using Avogadro 1.2.0.²⁰ Quantum Theory of Atoms in Molecules (QTAIM) analysis was conducted with the Multiwfn software package.²¹ Comparison of the metal-to-ligand bonding descriptors are given in Table S5.

Fluoride Ion Affinity calculations: FIA calculations using the method developed by Krossing²² and updated by Greb²³ have been calculated on the full ligand system for all experimentally studied catalysts. The TMS-anchored isodesmic reaction scheme method is shown in Figure S36 and the “level of choice” for our calculations was RIJCOSX-PW6B95/def2-qzvpp,²⁴ based on the previously optimised structures. This method is the recommended DFT method for these calculations.²³

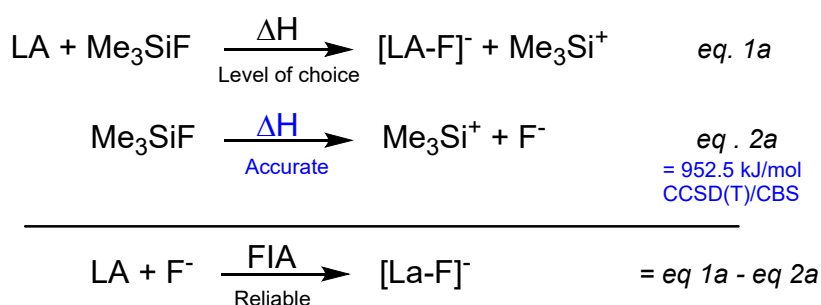


Figure S36 Isodesmic reaction scheme, with revised anchor, for reliable calculations of Fluoride Ion Affinity.¹³

Model vs. full ligand structure: When exploring the effect of varying the metal on the reactivity a model ligand structured was used, omitting the *p*-*tert*-butyl groups, to reduce computational costs. Comparison of this model to the full ligand is given in Figure S37 for the [InCl(Salphen)] system. For the majority of the mechanism the model system is in excellent agreement with the full ligand system energies, differences less than 2 kcal mol⁻¹. For TS3R2 β there is larger difference, 4.4 kcal mol⁻¹, however it does not change the overall conclusions of the reaction.

Due to the small experimental reactivity differences observed on exchange of the halide it was deemed important to calculate the full ligand system, as shown in the main manuscript.

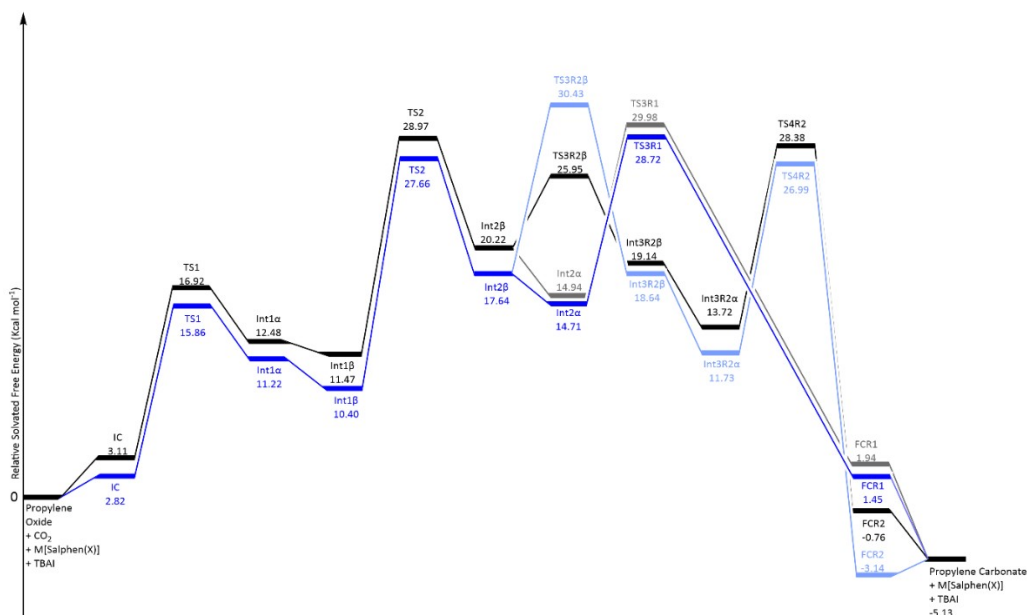


Figure S37 Free energy pathway for the addition of CO_2 and epoxide with the $[\text{InCl}(\text{Salphen})]$ catalyst. The black line presents the model ligand and the blue the full ligand system with $t\text{Bu}$ groups.

QTAIM Analysis: Table S5 highlights the metal-to-ligand bond critical point (bcp) descriptors for each $[\text{MCl}(\text{Salphen})]$ catalyst. The Al catalyst shows an expected lower electron density (ρ) and the bcp , compared to Ga and In. What is particularly interesting to note is the positive sign in the energy density term (H) for the Al-O bonds. This implies a more ionic bonding character to the metal-to-ligand interaction compared to Ga and In, which both show negative energy density terms, and therefore covalent-like interactions.

Table S5 QTAIM descriptors for metal-to-ligand bcp s for $[\text{MCl}(\text{Salphen})]$, where $M = \text{Al}, \text{Ga}, \text{In}$:

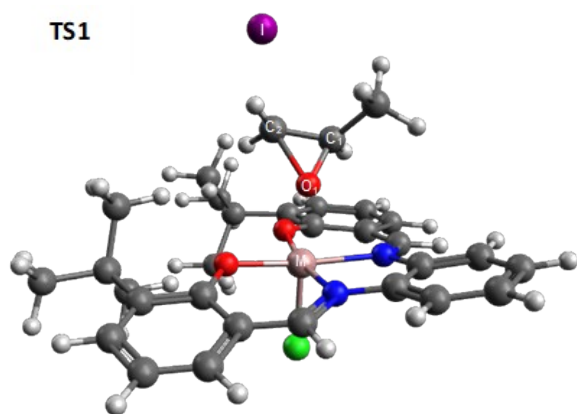
Catalyst	Bond	(ρ)	$V(r)$	$G(r)$	$H(r)$	$\nabla^2\rho(r)$
$[\text{AlCl}(\text{Salphen})]$	Al-Cl	6.04×10^{-2}	-8.71×10^{-2}	7.64×10^{-2}	-1.06×10^{-2}	2.63×10^{-1}
	Al-O(A)	6.85×10^{-2}	-1.20×10^{-1}	1.27×10^{-1}	6.88×10^{-3}	5.35×10^{-1}
	Al-O(B)	6.76×10^{-2}	-1.18×10^{-1}	1.25×10^{-1}	6.79×10^{-3}	5.28×10^{-1}
	Al-N(A)	5.20×10^{-2}	-7.49×10^{-2}	7.37×10^{-2}	-1.21×10^{-3}	2.90×10^{-1}
	Al-N(B)	5.34×10^{-2}	-7.74×10^{-2}	7.64×10^{-2}	-1.04×10^{-3}	3.01×10^{-1}
$[\text{GaCl}(\text{Salphen})]$	Ga-Cl	8.15×10^{-2}	-9.75×10^{-2}	7.21×10^{-2}	-2.54×10^{-2}	1.87×10^{-1}
	Ga-O(A)	9.02×10^{-2}	-1.38×10^{-1}	1.28×10^{-1}	-9.38×10^{-3}	4.75×10^{-1}
	Ga-O(B)	8.84×10^{-2}	-1.34×10^{-1}	1.25×10^{-1}	-8.97×10^{-3}	4.65×10^{-1}
	Ga-N(A)	7.56×10^{-2}	-9.72×10^{-2}	7.97×10^{-2}	-1.75×10^{-2}	2.49×10^{-1}
	Ga-N(B)	7.78×10^{-2}	-1.01×10^{-1}	8.33×10^{-2}	-1.79×10^{-2}	2.62×10^{-1}
$[\text{InCl}(\text{Salphen})]$	In-Cl	7.00×10^{-2}	-7.52×10^{-2}	6.37×10^{-2}	-1.15×10^{-2}	2.09×10^{-1}
	In-O(A)	7.52×10^{-2}	-1.05×10^{-1}	1.05×10^{-1}	-4.40×10^{-4}	4.18×10^{-1}
	In-O(B)	7.53×10^{-2}	-1.05×10^{-1}	1.04×10^{-1}	-6.41×10^{-4}	4.15×10^{-1}
	In-N(A)	6.54×10^{-2}	-7.74×10^{-2}	7.16×10^{-2}	-5.83×10^{-3}	2.63×10^{-1}
	In-N(B)	6.44×10^{-2}	-7.55×10^{-2}	6.99×10^{-2}	-5.66×10^{-3}	2.57×10^{-1}

Charges on metal centre: Table 6 gives the Mulliken and Lowdin charges of each of the catalyst species, highlighting trends within varying both the metal centre and halide. The charges on the metal decrease as the halide varies down the series. In agreement with the decrease in τ_5 value. Interesting the Ga catalysts have lower Mulliken charges compared to the equivalent In species. This is in agreement with the expressed higher barriers for the Ga species.

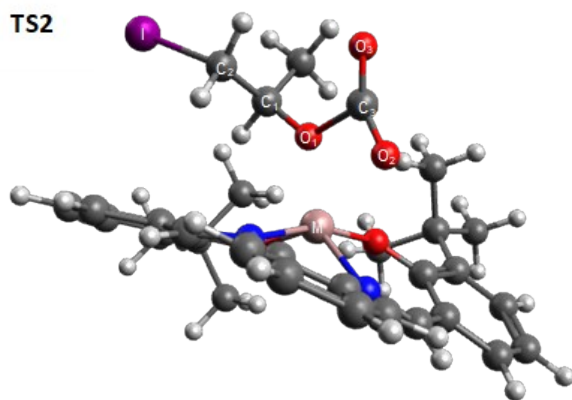
Table S6. Mulliken and Lowdin charges for each catalyst system.

	[AlCl(L)]	[AlBr(L)]	[AlI(L)]	[GaCl(L)]	[GaBr(L)]	[GaI(L)]	[InCl(L)]	[InBr(L)]	[InI(L)]
Mulliken	0.973	0.946	0.938	0.806	0.760	0.769	0.822	0.804	0.743
Lowdin	0.212	0.167	0.156	0.254	0.220	0.209	0.201	0.160	0.040

Transition state comparisons: Bond length comparison of the metal to ligand binding interactions of the transition states for each metal salen is presented below. The structures provided are of the GaCIL pathway.



Bond	Bond Length (Å)		
	AlCIL	GaCIL	InCIL
M-O ₁	1.991	2.083	2.239
O ₁ -C ₁	1.443	1.439	1.449
O ₁ -C ₂	1.681	1.705	1.681
C ₁ -C ₂	1.455	1.456	1.455
C ₂ -I	3.023	2.997	3.028



Bond	Bond Length (Å)		
	AlCIL	GaCIL	InCIL
M-O ₁	1.860	1.959	2.125
M-O ₂	2.361	2.425	2.522
O ₁ -C ₃	1.850	1.739	1.841
O ₂ -C ₃	1.213	1.222	1.217
C ₃ -O ₃	1.185	1.193	1.187
O ₁ -C ₁	1.425	1.436	1.431

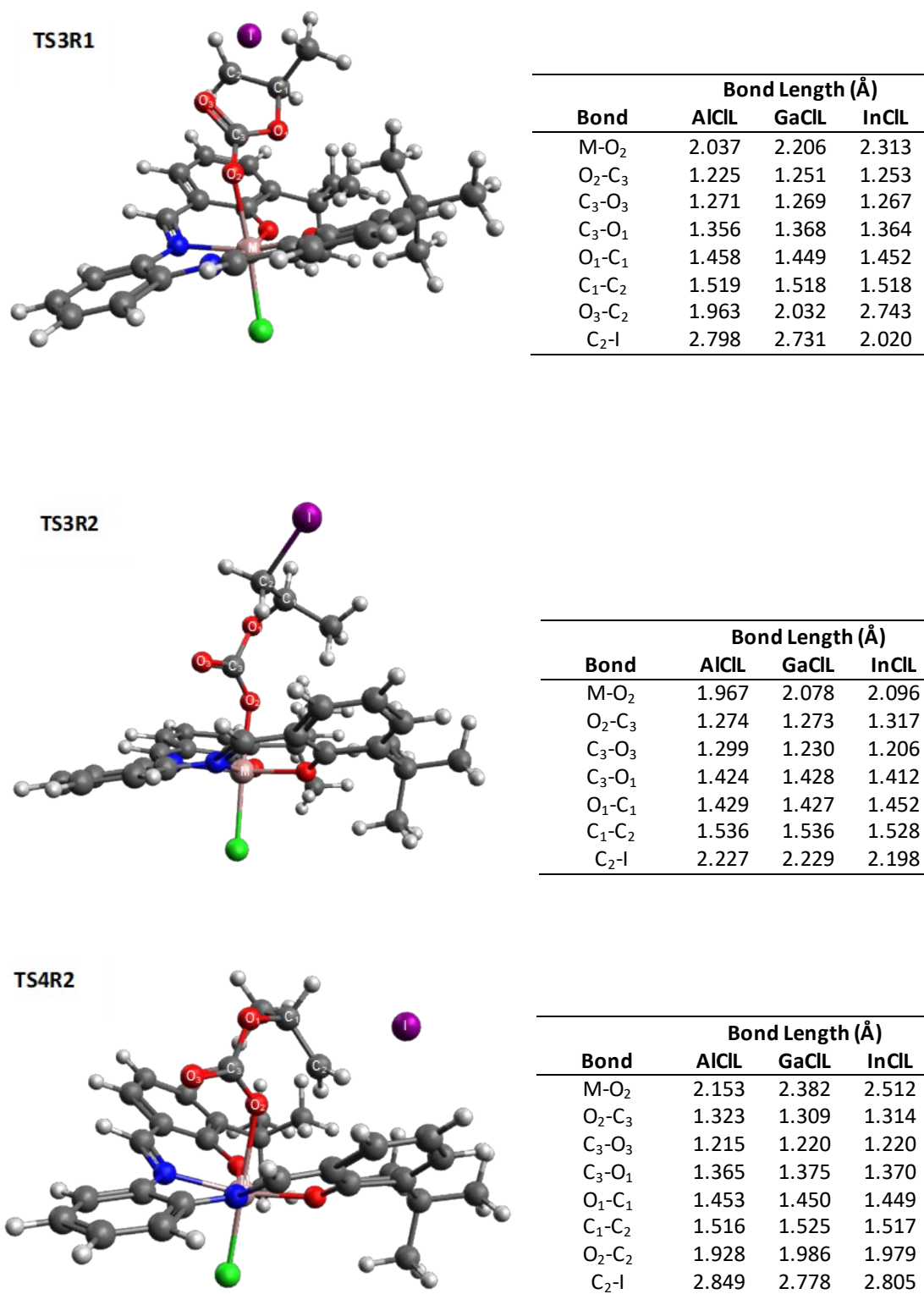


Figure S38. Structure and bond distance comparison for each transition state along the free energy surface. For visual representation the GaCl catalysts has been used.

Solvent corrected energy surface: Given the catalytic conditions, where the propylene oxide acts as both a substrate and solvent, an understanding of how the solution environment changes over the course of the reaction is important. The polarity of the bulk solution will increase as the product (propylene carbonate) is formed. As can be seen in Figure X below, this reduces the overall energy cost of the reaction by approximately 2 kcal mol⁻¹.

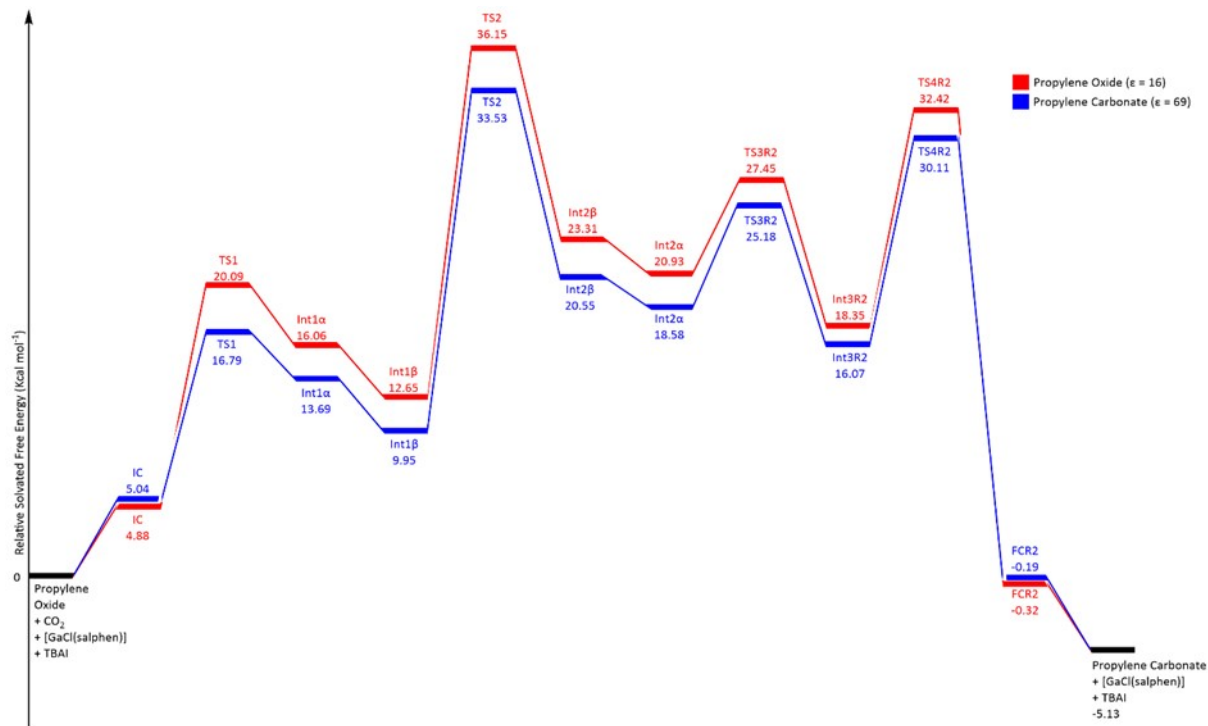


Figure S39. Comparison of the **GaCIL** free energy pathways with varying bulk conditions. Red line represents a propylene oxide environment (start of the reaction) and the blue line represents a propylene carbonate environment (end of the reaction). Computational details discussed in general comments.

[7] Computational study data

CO₂

C	-0.00000000005176	-0.00000000004508	0.00000000010100
O	0.00000000002588	0.00000000002254	1.17087949673272
O	0.00000000002588	0.00000000002254	-1.17087949683373

TBAI

N	-0.07183532984163	-0.01053092424696	0.05624219935141
C	1.38237006137525	-0.48633956986966	0.14079524500052
C	2.17886469701709	-0.04135886616498	1.35853920743602
C	3.60723975101423	-0.60617057119513	1.26365619203804
C	4.50299675935988	-0.15183069738845	2.41774390803723
H	1.33155367834990	-1.58458580043411	0.10240445110034
H	1.86925213124984	-0.15750421931099	-0.80374985051912
H	2.24380884952239	1.06058207446753	1.40298484357058
H	1.71403400190633	-0.37284065720127	2.30826310029469
H	3.55977379190402	-1.71266561544331	1.23642048957713
H	4.04329600607420	-0.29841670821040	0.29425866781359
H	5.51918375460244	-0.57350240303584	2.32420444347673
H	4.09618809443964	-0.46905870897956	3.39679722687479
H	4.59978477631149	0.94973743415285	2.43872888256784
C	-0.17325340677126	1.49005699179029	0.30738973168563
C	0.69248018180412	2.37702782858805	-0.57800294055979
C	0.55954072016107	3.85131591850499	-0.17274144656081
C	1.40635394227572	4.76903501273682	-1.05935994126623
H	-1.23535892184256	1.74746319646479	0.17137685326816
H	0.06753043188399	1.63855665938981	1.37307789482009
H	1.75153850690831	2.07332087596525	-0.53423653461376
H	0.42102592190903	2.25550656044609	-1.64031481896192
H	-0.50544051904852	4.15771579524284	-0.22350328113810
H	0.85879047911819	3.97340472432634	0.88878306819194
H	1.30402305264498	5.82669209033099	-0.75797818755497
H	1.10720615943214	4.68214470081856	-2.11918884242689
H	2.47574626475875	4.49727197211427	-1.00309803046822
C	-0.58885722395258	-0.29592668781851	-1.35719065306491
C	-0.65021130968526	-1.75905227814459	-1.76804905021343
C	-1.14079605167907	-1.85874213279440	-3.22206508557809
C	-1.17525495539789	-3.30016260573767	-3.73313564392405
H	-1.57721504624703	0.18575059406322	-1.42445080472371
H	0.12121452002512	0.21378221972739	-2.03944835499834
H	0.36253798182983	-2.19720741826267	-1.72428657874335
H	-1.30964053174836	-2.35611083279186	-1.10785248652715
H	-2.14876573437081	-1.40317584472922	-3.30357800423751
H	-0.46079792712181	-1.25309287998911	-3.85122007107862
H	-1.53569674030165	-3.34464730281855	-4.77604003011193
H	-1.84107024268245	-3.93694795143034	-3.11921175859575
H	-0.16511104096757	-3.74839080868260	-3.71070393630207
C	-0.88222651547943	-0.74745397714137	1.11013013539631
C	-2.39049638149229	-0.52255921948021	1.09855885222691
C	-3.07313623088651	-1.34793804900321	2.20106389965984
C	-4.59240203985698	-1.16211616025256	2.22520424815737

H	-0.66039168003847	-1.81627499946148	0.96906028991324
H	-0.45942409167574	-0.45166372612286	2.08319143075140
H	-2.63115051403791	0.54554554780630	1.24879976273393
H	-2.81515852168478	-0.80973424385195	0.12024512157389
H	-2.82961790491454	-2.41911330986010	2.05621212498644
H	-2.64575782536673	-1.06991248603584	3.18496244830496
H	-5.05756382563533	-1.76648138637168	3.02348568869750
H	-5.04771964323004	-1.46606716362295	1.26463516924270
H	-4.86403293198035	-0.10499161494323	2.40222560615950
I	2.50621257205959	0.29554862389125	-3.31183485073998

TBA⁺

N	0.00137644742828	-0.00124159136935	-0.00027296196092
C	1.45801264376290	-0.46252351211750	0.09542028816805
C	2.21028995476054	-0.09385978390506	1.36911847853146
C	3.65451434789290	-0.62416171366763	1.31178827366791
C	4.45754342949986	-0.27688224463321	2.56765083882553
H	1.43264560333299	-1.55549449257227	-0.02692010484666
H	1.96518229841008	-0.04329529489799	-0.78719861485280
H	2.23842054816123	1.00179710607741	1.50713487037476
H	1.71015689709607	-0.51645003282042	2.25911832101839
H	3.63387729155475	-1.72240280640409	1.16943232391402
H	4.15809614607587	-0.20928824207740	0.41651547519479
H	5.48689365423863	-0.66770441404027	2.49907928622284
H	3.99422749492114	-0.70914398976223	3.47323323513542
H	4.52302039000578	0.81689906095110	2.71301299859967
C	-0.11648510313806	1.50579249887219	0.24238809397191
C	0.75534941583499	2.40922245166150	-0.62266255201257
C	0.53749596329861	3.88585643590995	-0.24525196198177
C	1.38986776352877	4.83884025620104	-1.08660840508161
H	-1.17862716075658	1.74977145363961	0.09295846491591
H	0.11016986266371	1.65781724849445	1.30896054011701
H	1.82505382763647	2.16377061970616	-0.49684512812975
H	0.51983689275737	2.27602533927738	-1.69401257237232
H	-0.53487580934590	4.13759388625749	-0.36153568033447
H	0.76893817578473	4.02318460704915	0.82933843019412
H	1.21546790156263	5.88796783841058	-0.79351869737600
H	1.15243141401154	4.74717946230971	-2.16215705573474
H	2.46812595724076	4.63040042802450	-0.96143331978011
C	-0.52071352665953	-0.31272267162127	-1.40503360417451
C	-0.63580415945040	-1.78543805554135	-1.78264256060651
C	-1.18840152697767	-1.93037163023786	-3.21234925818672
C	-1.32770940492136	-3.39256141763107	-3.64269725041281
H	-1.50160478865134	0.18170705660524	-1.47801341661097
H	0.16094070267605	0.20333770479550	-2.09719830468443
H	0.34830879921266	-2.28494201281207	-1.72779403341508
H	-1.30603592823828	-2.32029351461448	-1.08617759861345
H	-2.17225333033690	-1.42487827486701	-3.27353312651238
H	-0.52396424315230	-1.39214771279806	-3.91638576524034
H	-1.72781403171017	-3.46603314069220	-4.66813157761683
H	-2.01394755684426	-3.94431160211065	-2.97455104835350
H	-0.35205561592927	-3.91157645348472	-3.62536985990576

C	-0.81595216598593	-0.73445888288065	1.06658962270755
C	-2.32635820952106	-0.52999288946567	1.03383285948566
C	-3.00147924540740	-1.34024179429874	2.15545665106488
C	-4.52266374539872	-1.17156743182173	2.16750669593344
H	-0.56940189532790	-1.80151160018068	0.95417919416464
H	-0.40962214656171	-0.40240725645848	2.03337837829740
H	-2.58326728618080	0.53720110007524	1.16026099770964
H	-2.74656984198996	-0.84779094788387	0.06288011657046
H	-2.74243141641045	-2.41068943217033	2.03586860333013
H	-2.58065753802380	-1.03133535436357	3.13235668869427
H	-4.97933918402484	-1.76342065272054	2.97876497068655
H	-4.97168828691115	-1.50611251637471	1.21450172526582
H	-4.80859967549358	-0.11505719102110	2.32113903603477

Propylene Oxide

C	-0.15214411413766	-0.03926466034198	0.48654797824856
C	1.04969528035586	0.61054343815283	-0.06421126355753
O	0.82683758116683	-0.78725491357684	-0.24143920711725
H	-0.15862217183399	-0.25118248986085	1.57182882474977
H	1.88419512800858	0.88560780872154	0.60332888694096
H	0.95981920905430	1.23008290919251	-0.97314882506718
C	-1.51536136805361	0.10121526922720	-0.14698295674211
H	-2.09167562818228	-0.83629719176746	-0.04165557512697
H	-2.09186086425819	0.90920991659728	0.34069306011115
H	-1.42565605211984	0.32973791365577	-1.22308792243938

Propylene Carbonate

O	0.16458705464277	0.23691136029425	1.90164933841989
C	0.50373164283083	1.24710472135809	2.76198895340251
O	0.05829075496344	2.35506024203305	2.72442627642482
O	1.42507524547321	0.79840742277861	3.66512217848013
C	1.86670084191040	-0.52754469771065	3.30400503956410
C	0.74818371197185	-0.98837585490260	2.34999106444281
H	2.82262595645688	-0.41755808441565	2.75283193510496
H	1.11948510880252	-1.55632682092686	1.48119544044118
H	-0.01955066144817	-1.58924641729556	2.87691689014338
C	2.06259149868045	-1.38351860274188	4.53966486885885
H	2.37854455711852	-2.40099233131432	4.24661027858987
H	2.84093592154020	-0.95545812810224	5.19318202818774
H	1.12214536705708	-1.45585480905425	5.11355170793973

[AlCl(Salphen)Cl] (2 x ^tBu) Pathway

[AlCl(Salphen)] (2 x ^tBu)

Al	-0.02504273890694	0.67051615715621	-0.53994935907874
O	1.28094213899815	-0.54770090448790	-0.11717805727075
N	1.25215654597818	2.15495538677936	0.00657078172904
C	2.56617764359111	-0.51282657247620	0.09480534584733
O	-1.30892291831589	-0.48193210571854	0.07725211930347
N	-1.32807460132779	2.20356089520939	-0.16953380659912
C	3.35884785263965	-1.71676926721483	0.04353277184810
C	4.71712961040230	-1.60723914954125	0.35411075828078

C	5.34805197215242	-0.38692727788409	0.70248432104438
C	4.60606581691400	0.77718159591950	0.71724916890391
C	3.21727081645202	0.74273922031330	0.39585891211607
C	2.51262839367387	1.97765673996181	0.35627072094254
C	0.69684605811569	3.44399287870639	-0.10576287562006
C	1.42044128675484	4.65153952748508	-0.16538738647407
C	0.74783307113810	5.87013549507518	-0.29799130250652
C	-0.65524105941655	5.89745608961630	-0.39276849151089
C	-1.38596267778415	4.70610581797939	-0.35756118717182
C	-0.72420546957069	3.47129929679036	-0.20851561601014
C	-2.63047108944843	2.04748922415192	-0.06337058495926
C	-3.32291275946720	0.80322559100599	-0.00195037864093
C	-4.74692084509591	0.83600652403400	0.02595199122493
C	-5.46585934721556	-0.33950549026402	0.12215167091761
C	-4.77113110348021	-1.56928649952602	0.21546833529378
C	-3.37632237867405	-1.67293090931643	0.21410717717381
C	-2.61737481277004	-0.45484026296655	0.08769402739938
H	-5.25596766528793	1.80604845716771	-0.03808184497071
H	-5.36877058262618	-2.48127136678695	0.29387022078371
H	-3.26608384997271	2.94589726402484	0.00076413642765
H	-2.47418874354496	4.74102628043787	-0.46532301599819
H	-1.17955481383916	6.85174334772447	-0.51582365414173
H	1.32088261959427	6.80263507613827	-0.35035324834758
H	2.51416568567675	4.64263388606049	-0.13539137509251
H	3.10274259541890	2.86619278515628	0.63426810738197
H	5.07136398513087	1.74154143490495	0.95778754840178
H	5.33948713120802	-2.50576309054559	0.32691108048670
H	-6.56115047200790	-0.32963114788446	0.13154239565063
H	6.41713979065560	-0.37514480045152	0.94070184845707
C	-2.66573134590581	-3.03309685580715	0.35063891625040
C	-1.75416089832748	-3.28080834224205	-0.87709651938876
C	-1.84390062882312	-3.03287587144344	1.66384562880988
C	-3.66696031852122	-4.20373940034399	0.42742764054167
H	-2.35179865470827	-3.27493006180780	-1.80634692299006
H	-0.97092823786159	-2.51743492063579	-0.96554770663795
H	-1.26632103895675	-4.26820999336525	-0.79050235155108
H	-2.51467355455182	-2.91440472640407	2.53421951946371
H	-1.30242076210287	-3.98924929287077	1.77638765303956
H	-1.10855854634548	-2.21570790262372	1.67753557040664
H	-3.10861847771321	-5.15099879376441	0.52748643469232
H	-4.33822410938911	-4.12301335462482	1.30118737553108
H	-4.28705617579094	-4.27925180728585	-0.48387360179065
C	2.72078379934107	-3.06099781403594	-0.35472950873063
C	1.62218515918916	-3.42920152160995	0.66946934370958
C	2.12052729585726	-2.94497212382073	-1.77933374766171
C	3.75187797598096	-4.20712252693693	-0.37449392073606
H	2.05302703533640	-3.53266151522354	1.68204652681579
H	0.83869872824759	-2.66278265252229	0.69898348826345
H	1.15461215725418	-4.39240361444428	0.39667288726216
H	2.91740061027085	-2.73752506057989	-2.51623983947206
H	1.63525087593499	-3.89730001618223	-2.06073684410837
H	1.37238160727682	-2.14300704070942	-1.85131720537577

H	3.24728949722717	-5.14258748874969	-0.67343165536121
H	4.56426757571183	-4.02300498284273	-1.10030105012860
H	4.20321190043275	-4.37807258306863	0.61951369269447
Cl	-0.06149655480586	0.71281013721066	-2.70699505876939

[AlCl₂(Salphen)] (2 x ^tBu)

Al	0.00048488232048	0.64695239280357	-0.00408383126021
O	1.38588512661611	-0.60420697131988	-0.00831722983192
N	1.32763641813944	2.20105580478205	0.00751565322360
C	2.66543991359382	-0.50348200672704	0.03593474990493
O	-1.38665179774888	-0.60166814337296	0.03825511860707
N	-1.32587296625701	2.20076933697081	-0.06871966770631
C	3.47975400023075	-1.70322052041280	-0.02195829855377
C	4.86308816567377	-1.56763766194224	0.08309558630586
C	5.51015317249403	-0.31309011474516	0.22273952545256
C	4.74812971699675	0.84149326321889	0.23653318841596
C	3.32894384942397	0.78585078484982	0.13507551909898
C	2.62382977673990	2.03216627843640	0.10996292416964
C	0.71861402255606	3.46045961861692	-0.03063752016469
C	1.40155585582061	4.69559213250890	-0.04512645989211
C	0.70440188078155	5.90695298715946	-0.07056426272859
C	-0.70143980371253	5.90705338392199	-0.08168372776385
C	-1.39892083303443	4.69563267596184	-0.07716691748014
C	-0.71625872942409	3.46035316764628	-0.06237909688968
C	-2.62117765413166	2.02970962459391	-0.17860864604248
C	-3.32709365170637	0.78364013321301	-0.17103267690786
C	-4.74510155089102	0.83641148955914	-0.28882027209191
C	-5.50791565972659	-0.31695089026621	-0.24552196673131
C	-4.86307601684989	-1.56661324014120	-0.05940497937039
C	-3.48094807098288	-1.69911339320051	0.06397091309910
C	-2.66552004953556	-0.50201479125044	-0.02336234926824
H	-5.22355702388016	1.81805500684457	-0.41104811107741
H	-5.49337140053765	-2.46019551052164	-0.00770102064151
H	-3.26872579870589	2.91757812927290	-0.28609553515416
H	-2.49316156305641	4.71226994577493	-0.08030892981158
H	-1.25488005582721	6.85407152370550	-0.09352404307098
H	1.25814227230049	6.85381467772481	-0.08080137970321
H	2.49577824972543	4.71226585190285	-0.04013667934457
H	3.27317390522707	2.92226985925528	0.18201584931400
H	5.22806059416565	1.82629978486865	0.32195353220919
H	5.49263313905496	-2.46273282759272	0.05296306251258
H	-6.59946414141934	-0.27318206317132	-0.34011768950287
H	6.60262427110025	-0.26695439109147	0.30471132315898
C	-2.79755522347669	-3.05767996598574	0.31451737568334
C	-1.79573555211438	-3.37262973568571	-0.82554477128261
C	-2.06269971160776	-3.01001102530379	1.68017189804933
C	-3.81749659017013	-4.21285614750488	0.37148190230454
H	-2.31965507525900	-3.41515821273543	-1.79836458040368
H	-1.01078410318152	-2.60803339150785	-0.88902283357230
H	-1.31780489420060	-4.35473058051084	-0.64830081922668
H	-2.79328403784608	-2.88894229781184	2.50158299282475
H	-1.51078661026989	-3.95442760090272	1.84701637021177

H	-1.34892779401599	-2.17465117149199	1.73262525559953
H	-3.28428883106722	-5.16101071362024	0.56699450815777
H	-4.55677326324758	-4.07438690591530	1.18173393674481
H	-4.36564303451656	-4.32890279510190	-0.58181506943017
C	2.79401965388543	-3.06858968107122	-0.22509650286225
C	1.80111107132185	-3.34859360777432	0.93181135622321
C	2.04925365116004	-3.06134972974255	-1.58610051975314
C	3.81303985366420	-4.22562188090217	-0.25457244544881
H	2.33325533857269	-3.36356779015141	1.90098907546651
H	1.01768143982067	-2.58128800353801	0.97970177375215
H	1.32058098294253	-4.33475781853042	0.78728650699651
H	2.77389948365728	-2.96492912989049	-2.41597912010925
H	1.49592071925904	-4.00998249729360	-1.72110935604163
H	1.33567540538773	-2.22733122553721	-1.65813646943646
H	3.27772797346648	-5.17903145707167	-0.41581606647386
H	4.54556069812762	-4.11324752220011	-1.07492451157458
H	4.36909633301414	-4.31207304910176	0.69729509608035
Cl	0.00581331784019	0.68278070812473	-2.31832199451408
Cl	-0.00453364668000	0.75743790092157	2.30645135755225

IC

Al	0.29642185971182	-0.21865527167764	-1.23745284596200
O	1.48436605345615	-1.61119234352234	-0.97621854614245
N	1.74095460005978	1.12859776882912	-0.75733506289796
C	2.78625053106842	-1.67465359885262	-1.01838617551402
O	-1.17771694245070	-1.32112754736609	-1.20947923794879
N	-0.86938615077057	1.38443420478620	-0.80314532638705
C	3.44991099982830	-2.94421702105315	-1.18677714698566
C	4.84826124332842	-2.95386313959399	-1.18900258317247
C	5.63690963508049	-1.78980422855923	-1.03019815188362
C	5.01096724001839	-0.56790619026712	-0.87060176411067
C	3.58929979352371	-0.47875742114527	-0.87031967847276
C	3.01797185709521	0.82341740040788	-0.71600312666558
C	1.26894355305653	2.44918555338242	-0.66073128725707
C	2.06831877307862	3.60538514188638	-0.55169455705641
C	1.48174533570468	4.87281965044458	-0.49293292368689
C	0.08362545548402	5.00882485278607	-0.55976187311188
C	-0.72546865072125	3.87463978380115	-0.67160872902787
C	-0.15244550596112	2.58733743562964	-0.70417749803323
C	-2.15283953683678	1.30913521318629	-0.53406214400300
C	-2.97274562212196	0.14095384101590	-0.61485017760394
C	-4.35396148162025	0.28254576927449	-0.29616301181172
C	-5.21028979468998	-0.79820076027371	-0.39711242858925
C	-4.70627310126761	-2.04044481237783	-0.85424990333929
C	-3.36447575867826	-2.25269368147435	-1.18285767513852
C	-2.45057816793046	-1.14905281931804	-1.01367164929740
O	0.09205096989427	-0.33291102698908	1.05376573880690
C	0.93595887043581	-0.98604003035716	2.01795851823782
C	-0.40679919597047	-1.51649773709178	1.72688498019859
C	-1.60523806768282	-1.30771967394969	2.61098844032133
H	1.81582695083492	-1.48976953273796	1.59551417712111
H	1.10513544169213	-0.39974266973488	2.93373895662674

H	-0.45532184280598	-2.38460182035807	1.05625178226317
H	-1.48838552932696	-0.40749222469671	3.23837151081866
H	-1.74961341782489	-2.18504564758904	3.26738233444171
H	-2.51298483206618	-1.19217096538340	1.99245610395272
H	-4.72452683450405	1.26592764081545	0.02066424741361
H	-5.41560299025637	-2.86621131074646	-0.95810328503615
H	-2.67391819914963	2.22382294640437	-0.20480159645633
H	-1.80980550656624	3.99335508862330	-0.75919814272946
H	-0.37456463568579	6.00412557110509	-0.54157856856797
H	2.11797495007545	5.76153998732301	-0.41329271765301
H	3.15882441535991	3.52275027587752	-0.52365311209076
H	3.75050888651813	1.63337639627469	-0.56570223596551
H	5.59734395397937	0.35240947066519	-0.75302656098976
H	5.37228240831257	-3.90430308437725	-1.32180820175478
H	-6.27303484473243	-0.69771485780964	-0.15129704081096
H	6.72969212722648	-1.86450330736239	-1.04059542539015
C	-2.86181600354306	-3.59890860806037	-1.74174822137597
C	-2.27547337335906	-3.37103452622267	-3.15932155803695
C	-1.77803960310602	-4.19700878029519	-0.81321458398896
C	-4.00026887913146	-4.63169236624968	-1.85934663386979
H	-3.06136120540086	-3.00846110582628	-3.84613613804979
H	-1.45742220511402	-2.63559351975847	-3.15290123047747
H	-1.88298620127074	-4.32317352878237	-3.56124198596083
H	-2.16755949854641	-4.32559887853166	0.21376078485454
H	-1.46544720236474	-5.18968976635724	-1.18449437745931
H	-0.89153576855950	-3.55209847965012	-0.78242460348988
H	-3.59869740497086	-5.57005914658475	-2.28043785608732
H	-4.44554932460074	-4.87277674304140	-0.87688748909828
H	-4.80619512906018	-4.28666996454474	-2.53130012928837
C	2.63010667391634	-4.23978434383644	-1.35016294074908
C	1.82341441421011	-4.48950840808818	-0.05216368863643
C	1.68242475524467	-4.11982189091595	-2.57026133228863
C	3.53171118753062	-5.46945115558569	-1.58020383696092
H	2.50581111846348	-4.62338616557631	0.80718416497643
H	1.15187956453687	-3.64736041475384	0.16236203139209
H	1.20997364489208	-5.40328879328318	-0.14967430441395
H	2.26689038653616	-3.97152309558510	-3.49576929179586
H	1.09285284846873	-5.04809698993127	-2.68201291792737
H	0.98697237825776	-3.27679569100913	-2.46833797535924
H	2.89914883345893	-6.36689633970736	-1.69742544163800
H	4.13926059576079	-5.36953216224534	-2.49732768049826
H	4.21233870428063	-5.65429326630394	-0.72963265052094
Cl	0.48227739826764	0.08094286287294	-3.41508651190945

TS1

O	-0.08119299827948	-0.08864566302818	1.57126568740864
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O	2.28309871795099	-0.97348092082574	0.37270406249636
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C	-1.76793991599688	-0.32163379393226	3.22682613923074
C	-2.71995529420681	0.33063521673856	4.01176915850228

C	-2.95751935951756	1.72633871761387	3.94911630273442
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C	-1.23283795039326	1.90382181919341	2.23208987256092
C	-0.55916539727295	2.76237541477219	1.30696660976884
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C	0.40367989412822	4.54005511466956	-0.83358774426614
C	1.01622184367311	5.32942924598522	-1.81199060121235
C	2.17872752644717	4.87295430720804	-2.45770266606504
C	2.72364936668635	3.62947325756313	-2.12212628481217
C	2.13315816908239	2.82631209240239	-1.12367745191833
C	3.72579566429393	1.04804900130562	-1.12794677541958
C	6.02331195703236	-1.86766898800653	-1.17823316941284
C	5.30349361172638	-2.80523731907343	-0.39563059670730
C	4.05942929527492	-2.53593367497040	0.17561726191503
C	3.46535955595650	-1.24240562755220	-0.07834383124117
H	5.76264906962617	-3.78441001508857	-0.23253439704942
H	4.39997599087490	1.67133751405159	-1.74051799281076
H	3.60806569826754	3.27109065157140	-2.65790238756271
H	2.64974254509220	5.47913596127922	-3.24066065866835
H	0.57382637037456	6.29395852311960	-2.08831734671276
H	-0.52272469468380	4.88815733489874	-0.36602870272270
H	-0.90095653953279	3.81216711232163	1.31424458384130
H	-2.39446615217810	3.57856113031480	2.98997477783615
H	-3.31849798692304	-0.25261173042543	4.71789059211194
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H	-3.71865467435658	2.18093398968970	4.59382472961718
C	3.35933468103659	-3.53591391819148	1.11756009792513
C	3.37445739226744	-2.92441406039971	2.54296460255772
C	1.90313530276603	-3.82874184311347	0.67290016042037
C	4.10256209414007	-4.88670802854349	1.16878473993455
H	4.41323810148257	-2.83426208054322	2.91118226832186
H	2.92171100001628	-1.92133041975520	2.56046911621025
H	2.81479304879464	-3.57202853945840	3.24307617017911
H	1.85011895227380	-4.11517846753220	-0.39302018907652
H	1.49476090206878	-4.66244867113926	1.27381800088500
H	1.25920818211196	-2.95435789241667	0.82692579572657
H	3.57641867943856	-5.56319690472209	1.86569476652588
H	4.12632332208177	-5.37790055244307	0.17913994536150
H	5.14044082359598	-4.78240449052921	1.53450041898624
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C	-0.06989335510641	-2.10527801367801	3.77687146728214
C	-2.46508147648673	-2.50798722646567	4.35255749715903
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H	0.11558723163511	-3.19349133580073	3.84090382047025
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H	-2.25705210248196	-3.59245453787550	4.38318522131587
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C	0.73206029026898	-0.41279087595852	-2.27633054291330
C	-0.15064778699210	-1.35286333908892	-1.60198278591135
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H	0.26437408264841	-2.07777323083340	-0.90479974667877
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C	4.21599686896544	-0.26473503023859	-0.84748588824129
C	5.48935023917439	-0.61121068455420	-1.38640201352054
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O	-0.07975932729808	-0.08711600657972	1.59305988395752
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N	2.58577843916786	1.54479016189065	-0.77169755673049
C	-1.79291225985746	-0.30896284043086	3.21207547647659
C	-2.73990018370943	0.34546880349100	3.99883576674862
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C	-2.18733920749702	2.51648429663817	3.09349057227145
C	-1.20100226650027	1.92253212528962	2.25634083646794
C	-0.50494485358818	2.78630732660617	1.34957565832151
C	1.00786381166261	3.31990084549129	-0.41547633739596
C	0.50630266263686	4.60082459595282	-0.73057760937447
C	1.13373432298407	5.40682309459927	-1.68588951780426
C	2.27252151205293	4.93635952305806	-2.36222099899441
C	2.77572899992117	3.66221089696386	-2.07999120590836
C	2.16845920322241	2.83771654051688	-1.10921923280641
C	3.68559499911024	0.99971977447443	-1.23115645050073
C	5.95151717443095	-1.94808741334481	-1.31610189285281
C	5.27505280253662	-2.85017232319065	-0.45768327767601
C	4.05627812754946	-2.55512797050818	0.15349049019910
C	3.43365123038808	-1.28113568685097	-0.14430466602451
H	5.75009364006570	-3.81681401083680	-0.26430977628096
H	4.34714323093029	1.59779962219291	-1.88314139456156
H	3.64585576666438	3.29784217906826	-2.63498049265193
H	2.75922480673703	5.55724841586172	-3.12427449663570
H	0.72273468213851	6.39705243823217	-1.91764634113653
H	-0.40064944293178	4.96366764319492	-0.23667152280679
H	-0.82026643152719	3.84454632848614	1.38976874479032
H	-2.33702189781870	3.60346002204188	3.03502480673397
H	-3.35911321367870	-0.23769000045996	4.68781533480876
H	6.90469860843461	-2.23832147409132	-1.77346153156457
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C	3.43272636082876	-2.78053043576118	2.56335197630352
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H	4.47649475547393	-2.64181350292464	2.90082487040542
H	2.96092626099752	-1.78660374136459	2.51752377137319
H	2.90261104103496	-3.38721181351769	3.32148928232346
H	1.90878415512523	-4.27810556476269	-0.22118579421401
H	1.56037749438577	-4.62518761655619	1.50091824532649
H	1.29930400235715	-2.98265844278445	0.85163244381884
H	3.70245104971312	-5.45357909766241	2.08938268775061
H	4.20231402085433	-5.39046948028581	0.37730436390491
H	5.23324521626149	-4.65880827161885	1.64833545082730
C	-1.57938287899923	-1.83443347453457	3.27554720655494
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C	-0.13517444108755	-2.13484853672619	3.74976537798683
C	-2.55011550831760	-2.51284981942552	4.26278373671027
H	-2.86486673500937	-2.28690819755754	1.55327817048516
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H	-1.64689285828919	-3.55014515555708	1.91301530186331
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H	0.03490126109791	-3.22761847329124	3.78364234630009
H	0.60701362147833	-1.68739975183464	3.07582837095959
H	-2.36243791901848	-3.60191135718387	4.26894634102047
H	-2.41295805026304	-2.14663862535691	5.29675957296369
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O	0.21478770091613	0.24347780019256	-1.03684314645827
C	0.57315945024936	-0.43826536005128	-2.18410599599740
C	0.03523793026896	-1.85596931072429	-1.95936188674946
C	-0.00466782336808	0.25005484517359	-3.42667936631761
H	1.67837714458984	-0.51857895627185	-2.31952867068198
H	0.45391481279836	-2.28971871231299	-1.04400678684442
H	-1.06562417885704	-1.88988634119061	-1.94758827770921
I	0.63035103205244	-3.35844187307243	-3.53137579737809
H	-1.10470619819502	0.32351090173896	-3.33374968153954
H	0.24170764021624	-0.29426219998284	-4.35637761218118
H	0.39827289325361	1.27661491418123	-3.49339210943224
Cl	2.56300122954022	1.18679469824323	2.28644994307311
C	4.16145060064691	-0.32556753025136	-0.96251615876720
C	5.40651832983165	-0.69746421493681	-1.54353258747406
H	5.92698973021213	0.03269804331105	-2.17834500420600

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O	0.05659223173013	-0.00512425028244	1.63663013029234
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O	2.32593181368647	-0.75762553324178	0.59875455205527
N	2.54196110908081	1.55606196129684	-0.76942955017838
C	-1.71428254338186	-0.30660907075177	3.20866101519410
C	-2.66025879423370	0.33546288279903	4.01203491621658
C	-2.84632129948557	1.74047566045556	4.03475633831955
C	-2.07876879342101	2.53821219260049	3.20951934566059

C	-1.10325593824359	1.94993037556169	2.35201167324967
C	-0.38446410095854	2.80655584320794	1.47193657793368
C	1.06625740542229	3.36776146795664	-0.33027179521715
C	0.59386263179359	4.67363083513985	-0.56898092373113
C	1.23381767661135	5.49704596859039	-1.50066200584713
C	2.34503752885870	5.02169602827943	-2.21935607861396
C	2.81359805451550	3.72122839929544	-2.00992947173068
C	2.18674611213872	2.88191676875224	-1.06741551353922
C	3.61472692777895	0.98074113382865	-1.27157287746116
C	5.67768501251333	-2.09657679424008	-1.46977987907518
C	5.05102106394942	-2.89973709967447	-0.48843129446165
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C	3.39586424988270	-1.18558423631264	-0.02540574977867
H	5.46557086551221	-3.89575883546388	-0.31350091228609
H	4.25947287591423	1.56112272574470	-1.95169774025839
H	3.66405551287941	3.35834198991508	-2.59475835175860
H	2.83725490256661	5.66335576284463	-2.95877191632426
H	0.85343364029308	6.50860820259194	-1.68164951866613
H	-0.29235558536869	5.04542506887090	-0.04605720898923
H	-0.61749950681119	3.87978865022914	1.56535135008149
H	-2.21567100632144	3.62688719448798	3.18881170384921
H	-3.29959592011427	-0.26772791569518	4.66242301919301
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H	-3.60341160870923	2.17864332460899	4.69404856928454
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C	3.40479934884474	-2.66885735794470	2.70651114938549
C	1.84326830777036	-3.71140960610818	0.98319538835885
C	4.06124819992967	-4.73463092549587	1.46923156652917
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H	2.93760720526127	-3.28580858897601	3.49515112226898
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H	1.41129918015270	-4.38954448877406	1.74070980967807
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H	3.58793490377183	-5.33627560498849	2.26487945011816
H	4.01630979623576	-5.32498143294347	0.53663989871328
H	5.12207477668679	-4.59733751161738	1.74526231896024
C	-1.55122319301442	-1.83846509865032	3.20376217848825
C	-1.78892352633740	-2.38194891522904	1.77111563216744
C	-0.12940144417814	-2.20054435496973	3.69504861813102
C	-2.56345156759967	-2.52974659290890	4.13881412381175
H	-2.82381396826624	-2.16988427861403	1.44696050261798
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H	-1.64345739331445	-3.47747308443103	1.75582921463079
H	0.03138366065002	-1.82909312492939	4.72340430552705
H	0.00198681989830	-3.29755678101782	3.70339841910813
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H	-3.60847512028683	-2.32589631412079	3.84381876165766
Al	1.06456065147206	0.52343593609321	0.19943057566367
O	0.10876429982416	0.05832648327959	-1.20942067959010

C	0.54865969307107	-0.47377820684413	-2.42991748664689
C	0.71075021803868	-1.98675226455707	-2.21911341902131
C	-0.44294920930669	-0.12552937931065	-3.53939265399917
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H	1.28008583203271	-2.19862218246237	-1.30721622652162
H	-0.25617966957390	-2.51366449423170	-2.18748881173983
I	1.89401432718688	-2.98248717857371	-3.79794330765678
H	-1.44468941397729	-0.51334154472498	-3.27938169480166
H	-0.13234742515822	-0.55548768244191	-4.50765282972903
H	-0.51599810799391	0.97104516533358	-3.64288609804451
C	4.05077217211816	-0.35093289345744	-1.00726927812342
C	5.19063785341464	-0.82794680075509	-1.71477431082668
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TS2

Al	-2.06356442025397	-0.58751556762337	-0.30349825019460
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N	-2.13992398410200	-2.61019316087494	-0.54198609236164
C	-0.48952931849846	-1.81661795557747	1.77277923006291
O	-2.46859743532733	1.16833272438109	0.03918332836948
N	-4.06040301582083	-0.92780662870264	-0.58583177836387
C	0.34435791347738	-1.59201818382245	2.92703531070477
C	1.22940061937849	-2.61087232462187	3.29755965680157
C	1.33258322965934	-3.84636882317836	2.61904361089455
C	0.51416075486380	-4.08860370804321	1.53314188314127
C	-0.39947391295257	-3.09227128962659	1.08877955146103
C	-1.32663326524026	-3.44655361700416	0.05986120430679
C	-3.23268915431770	-3.03695676805586	-1.31354351772646
C	-3.32417714298927	-4.22848905566465	-2.05062276345170
C	-4.49811981297941	-4.51774517592689	-2.75832759007100
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C	-4.31890774274740	-2.11634670417722	-1.29476337454107
C	-5.02295537519316	-0.08795052047551	-0.26528513211795
C	-4.85246870032547	1.25773748299979	0.17176294023023
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H	-7.00030017447133	1.52128556101652	0.41731145487914
H	-4.60738551238547	5.06347327067386	0.89783641296716
H	-6.06714086684168	-0.42430695880901	-0.38456654193654
H	-6.30969942319851	-1.69520263232739	-2.06570364189439
H	-6.48196770177584	-3.83268994917158	-3.31539401307574
H	-4.56595332479935	-5.44127600854176	-3.34412858907577
H	-2.47301140482242	-4.91646563949410	-2.09050785954697
H	-1.40608522029718	-4.52241564440624	-0.17520055281019
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H	1.89051914283596	-2.45109114619799	4.15299026719883
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H	-1.22579989215038	2.70427547404698	-1.12950365873468
H	-1.24351767926987	6.01245897207858	0.54445070854509
H	-2.85984781989353	6.00025368035250	-0.20565456745820
H	-2.68430695727959	5.80884512450053	1.56776745552095
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C	0.91323603803338	0.83769318209714	2.72017912936502
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C	-3.51340050765936	-3.84481288873814	-3.49162394659294
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C	-4.30182221745932	0.68703923408249	-1.29222402085450
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C	-5.29435516388683	2.87914838246773	-0.86974212305842
C	-5.24294433658485	4.13604196815528	-0.30031172360094
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H	-1.89829367141706	-4.47556153308744	-2.21247763687439
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H	-6.03790613841795	4.86736175311813	-0.48201169218550
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C	1.24119878399115	1.03517693224129	2.87057360938676
C	-0.57101835702320	-0.02330626324669	4.32857297318506
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H	2.28388534178171	0.93276677951475	2.52197675435945
H	0.59255686383091	1.16104038553391	1.99442496567677
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H	-1.33696066582242	0.06312261946356	3.54536770203126
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C	3.19372453853368	-0.95369746154026	0.06866988273285
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H	3.22890666740876	-1.75990425397885	-0.67321895151149
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C	-3.72584499633641	-4.03780590609516	-3.20878958740255
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C	-4.10630147541606	0.79137713483748	-1.56965042996167
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C	-0.46584693473639	-0.26521525575736	4.41960210611584
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H	2.32826019913846	0.91591115115261	2.65806653531510
H	0.61933297527944	1.08687802740959	2.16130909662364
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H	3.13883066539123	-1.51830443321877	-0.81566597223025
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H	-0.37555467089553	2.80423280990914	0.67783644275596
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C	1.37592581557009	0.93957861294639	2.87004087433681
C	-0.37850999192583	-0.12626022128681	4.37992874925114
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C	2.85715158883288	-0.78323410516397	-0.30367809089880
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FCR1

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C	-0.37453258557761	-0.54307385255415	4.49634918921000
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C	-4.64208957765541	1.21175636993341	-2.45381488804880
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C	0.71213581189051	-2.95621505846095	3.13089203293042
C	1.65231482718810	-2.13330315759485	2.21063764359415
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H	2.14086343115022	-4.63969007762251	3.22385980657419
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Cl	-3.76884460325432	0.12155122207841	1.99060067067288

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O	-0.99162944454212	-1.39472062949120	1.34680659241649
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H	1.80981265244355	3.96395175307952	4.40846707412748
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C	1.78763846738166	-1.79304510459520	2.47036674549982
C	-0.15798646713432	-2.00952787534226	4.09684839143332
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Cl	-3.55681492186757	0.09488516013534	1.98995994189500

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O	-0.97992202899024	1.47158021250364	1.12225373952799
N	-2.84175738081777	1.25282730454082	-0.89523492436728
C	0.03389722028271	-3.34753204721523	1.96656744015155
C	0.12383548821346	-4.72225875112195	1.73505521775781
C	-0.61151703197660	-5.39321159609159	0.72875249660367
C	-1.48892813004837	-4.66946656573091	-0.05847431862330
C	-1.64104693297478	-3.26633667491990	0.12275152755962
C	-2.62520670994438	-2.60837839733173	-0.68583879833977
C	-3.96703582292978	-0.78042625982758	-1.41457261000663
C	-5.02452596822211	-1.49051589316913	-2.00954186868297
C	-6.00117394536247	-0.81494540338372	-2.75221935026453
C	-5.94467877011093	0.58272655766462	-2.88944149248815
C	-4.91143022664138	1.30731665633127	-2.28233916829223
C	-3.91204087357985	0.63974424349264	-1.55206504120461
C	-2.34939394556588	2.41537296851057	-1.25150455691709
C	-1.30017152176872	3.12218743056224	-0.58250411516466
C	-0.86507362258362	4.35650246179070	-1.14503981674641
C	0.08024722613803	5.12768738328736	-0.49481693519359
C	0.56133507472995	4.71413977626194	0.77278967571816
C	0.16740958818352	3.52759693161868	1.39360795030555
C	-0.71659322104348	2.65265475674337	0.66060430401808
H	-1.29503065488375	4.67934164905388	-2.10255430323433
H	1.27643548879387	5.36773744585849	1.27960244071861
H	-2.76482603087191	2.90843457030382	-2.14833959611627
H	-4.89298384181325	2.40004576177782	-2.35238174846575
H	-6.72330401946536	1.11253552459882	-3.45127947210771
H	-6.82372021526822	-1.37951391514859	-3.20745208866187
H	-5.09755915587443	-2.57479630805130	-1.87661658904594
H	-3.15886241365856	-3.25834510628199	-1.40041089923333
H	-2.09205733424809	-5.16706066795012	-0.82982577329951
H	0.79417541239457	-5.32275039649063	2.35698669249019
H	0.44165282369780	6.06375182980554	-0.93536540446440
H	-0.49172212181847	-6.47400690810764	0.59111624960031
C	0.59689831180435	3.16517964199090	2.83105289611878
C	-0.67963866184000	3.08100374888695	3.70881437133525
C	1.34664849425969	1.81376020300502	2.88638697979234
C	1.52945275623387	4.23827502307863	3.42708227923703
H	-1.21649768053694	4.04812576482077	3.71420409617858
H	-1.36648326483844	2.29983568572357	3.34534260033941
H	-0.40161612681738	2.83742495013184	4.75188882786842
H	2.22773218495711	1.82028235736310	2.22140185006512
H	1.69385536755395	1.62432754543901	3.91982778421104
H	0.68596152776124	0.98893176678016	2.59422581627936
H	1.79328302295105	3.95669670651576	4.46229327767478
H	2.46982690328044	4.31957094893437	2.85310924234076
H	1.05073095967515	5.23426421074315	3.46548710929910
C	0.85474336676431	-2.65561472083882	3.07420974513759
C	1.88585468798460	-1.70551554184416	2.42145234836152

C	-0.08242632987981	-1.86790753132874	4.02579602832777
C	1.63544910397536	-3.67151983838452	3.93312812142747
H	2.59827913182829	-2.27242672749328	1.79728125704806
H	1.38627421305887	-0.96271780765289	1.78810165493275
H	2.45998775518991	-1.16236734491545	3.19299657437278
H	-0.79219242931349	-2.55562489464741	4.52171554362599
H	0.51689880863464	-1.36845425716740	4.80963438054617
H	-0.66375753752179	-1.10300736491515	3.49243010626945
H	2.19142454217571	-3.12962284429418	4.71889777876556
H	0.96334419922764	-4.39258520560388	4.43364488377000
H	2.37511258853217	-4.23910037782200	3.33973082459838
Al	-1.93301442575213	0.04123704668794	0.45498569865867
O	-0.41583099481789	-0.02829870259499	-1.07125005737122
C	-0.45253722890699	-0.37565666882289	-2.34717581946024
O	-1.43870081280443	-0.56656970655953	-3.03080916948289
O	0.79948390603516	-0.49268250315254	-2.87795539995776
C	1.86230171773205	-0.36085112253552	-1.89538144762577
C	1.38884652179070	0.60654682640594	-0.82875912028466
C	2.24893781987116	-1.72744242406639	-1.34366038543682
H	2.70010543561765	0.08402017540143	-2.45221900739728
H	1.15612296286221	1.63671481783643	-1.10004581419332
H	1.41059918050401	0.36025927652072	0.22847371617265
I	3.96514694019076	1.67904100368884	-0.25475251474583
H	1.41778007090912	-2.16653298960188	-0.76679299182945
H	2.50847575818995	-2.40934686939524	-2.17126375496970
H	3.12208305530755	-1.61559717676919	-0.67939812927398
Cl	-3.55816495380038	0.12837786056025	2.00953469538906

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O	1.46997226650935	-0.88644857017610	-0.87093613491576
N	1.72821082173536	1.77331235666845	-1.37714853118542
C	2.74458327170702	-1.01451384537225	-1.14635830323949
O	-1.09220687325866	-0.56872264507957	-0.41512058524686
N	-0.72811868546423	2.10454626735156	-0.65269690996190
C	3.37135772328624	-2.31281214771901	-1.15938605024856
C	4.74419065985393	-2.37020973654617	-1.42546180907071
C	5.54307126150080	-1.22937687590027	-1.66845851516461
C	4.95123501340235	0.01957695329181	-1.66127570387758
C	3.55418654936196	0.15000858844639	-1.42278949901819
C	3.00188711374336	1.46607099828697	-1.46045322529022
C	1.26770522381004	3.09686304015567	-1.48388471522712
C	2.00194175924511	4.19812857908267	-1.96345351125986
C	1.40694594230503	5.46224881428785	-2.02949850732175
C	0.06726199109682	5.63810954976788	-1.63868342566061
C	-0.67963952858682	4.54906122302351	-1.17882536488795
C	-0.08583425278061	3.27735330204157	-1.08596469041436
C	-1.78077375349155	2.15660716873607	0.13081628499974
C	-2.53293515854366	1.03795240942334	0.60248940882314
C	-3.64502636620074	1.29472648419676	1.45195185693467
C	-4.43740698056609	0.25079660905562	1.89406208849566
C	-4.15643061220869	-1.06525654673522	1.45435802761844
C	-3.07536561934105	-1.38833942757937	0.62682509935638

C	-2.19216275198541	-0.31703286495097	0.23757813499691
H	-3.85880613248318	2.32986392235992	1.74483711624823
H	-4.82897310973052	-1.86249620776817	1.78239913708551
H	-2.11796190945708	3.14366152930628	0.48382658930465
H	-1.73350746099081	4.68375690241256	-0.91635100109664
H	-0.40227863527989	6.62516782362406	-1.71489432364323
H	1.98380555980748	6.31275446771552	-2.40988777943264
H	3.03282970060119	4.06953292029574	-2.30715725103004
H	3.73207508725006	2.28360331289293	-1.57821181978482
H	5.54139905471760	0.92444979936201	-1.85390775599768
H	5.23776181159453	-3.34536120030156	-1.44809939719323
H	-5.29188803504335	0.43494991729234	2.55406293696034
H	6.61468359501707	-1.34375036006466	-1.86430019577427
C	-2.83574323983252	-2.82517017470708	0.12369006441482
C	-2.84991870969151	-2.83128963789913	-1.42687445873818
C	-1.47511696697927	-3.34700926165671	0.63791448904125
C	-3.93021172251169	-3.79487384725293	0.61163395250510
H	-3.83489695973537	-2.50278442447123	-1.80447117889305
H	-2.07992030669166	-2.16816424143454	-1.84815528922218
H	-2.66592442338729	-3.85550857845750	-1.79965230231996
H	-1.43651697830284	-3.32663265289727	1.74313041311038
H	-1.31878819382818	-4.39165617457408	0.31426391222385
H	-0.65171396861291	-2.74265177489527	0.24003865549638
H	-3.72943267461085	-4.80254040387819	0.20778964496834
H	-3.95096150490931	-3.87885253810937	1.71343933460695
H	-4.93535119240744	-3.49369069113081	0.26661153324926
C	2.55836918778353	-3.58997597801215	-0.86864123980042
C	2.08164680949336	-3.53625556229849	0.60295915266909
C	1.35713134339178	-3.69993865270970	-1.84106556350137
C	3.40311703647475	-4.86945417377915	-1.03772486963846
H	2.94952527358527	-3.53432115196587	1.28716854069015
H	1.49274192022801	-2.62897540468427	0.78917886121376
H	1.45528112399058	-4.41474388689053	0.84085456769018
H	1.71448247787445	-3.76057072642789	-2.88454117037293
H	0.78029133126273	-4.61702628973587	-1.62323435742869
H	0.68183379919014	-2.83855548569310	-1.76255226095801
H	2.77155429729821	-5.75069696907754	-0.82847073588534
H	3.79042815988049	-4.97463381502354	-2.06688354044493
H	4.25736072195018	-4.90411547771288	-0.33819163795198
Al	0.22157688845725	0.40944929385615	-1.25120539289934
O	0.70946590278675	0.77097504646595	1.78163574979175
C	0.16041192168901	1.80276192768693	2.49253232762709
C	0.43264089107214	-0.47364819560146	2.44395447817246
O	0.32119330083980	2.96237371971858	2.23346726591326
O	-0.59124249661637	1.32086813475622	3.51265807160315
H	0.16088872263219	-1.22022945060464	1.68772406423830
H	1.34150326559809	-0.79801919036174	2.98512271767084
C	-0.72344484108651	-0.12114183009872	3.39402089184440
C	-0.67194141268217	-0.77970023999901	4.75632434574681
H	-1.69681465347101	-0.30935807911528	2.90614817019793
H	0.27969483302177	-0.55263878819137	5.26821421145440
H	-1.50716853337330	-0.43521285930777	5.38870037212276

H	-0.75818139857796	-1.87497645277579	4.63856372282578
Cl	-0.27185757232529	0.22993242806293	-3.35839718791379

[GaCl(Salphen)] (2 x ^tBu) Pathway (β Pathway structures included under the "[GaCl(Salphen)] (2 x ^tBu) Pathway" heading)

[GaCl(Salphen)] (2 x ^tBu)

Ga	-0.02845785497975	0.69064446087440	-0.57526427813700
O	1.30881645133991	-0.60600627129462	-0.09852230827829
N	1.27785120753719	2.19188090818358	-0.02458093987541
C	2.59919848948920	-0.52068367879691	0.04848648118334
O	-1.33196057367486	-0.52085441844117	0.13735171267251
N	-1.34766425031163	2.23908127197457	-0.14691830247546
C	3.40350801239118	-1.72120601054858	0.01627629003516
C	4.77281512005812	-1.58943112861416	0.25438241495272
C	5.40815080019921	-0.34896976927093	0.51470256640961
C	4.65556729477271	0.80716324490707	0.51744150754589
C	3.25036567143023	0.75524881650177	0.26966070598989
C	2.55159840813004	1.99521197691277	0.25301696125211
C	0.69774219976247	3.46988712792649	-0.07914443728940
C	1.41145007701935	4.68549113699137	-0.10274152766289
C	0.73378019076531	5.90590852940846	-0.16666961879218
C	-0.67129086139437	5.93185911893353	-0.22265483578021
C	-1.39561335639696	4.73709192428990	-0.21989750278270
C	-0.73049980737356	3.49607934081275	-0.14715693308454
C	-2.64887180432060	2.05894396979821	-0.08662224087871
C	-3.32945017665612	0.80591812649644	-0.05272909168533
C	-4.75490730569602	0.84055986999665	-0.08826922282368
C	-5.48466655841532	-0.32876632281430	-0.01339058549421
C	-4.80260882588862	-1.56261347903954	0.12111357540238
C	-3.41104895390624	-1.67354443644315	0.18079854968995
C	-2.63645775415728	-0.45989831354162	0.07780190512894
H	-5.25646203968321	1.81211626270928	-0.18234002544506
H	-5.40899918572473	-2.47032862935514	0.18023431256266
H	-3.30042550359503	2.94811331426904	-0.04363649747211
H	-2.48705724576425	4.77302660806442	-0.28681924194017
H	-1.20226519409816	6.88833284774718	-0.28493913214797
H	1.30316178750538	6.84178961712386	-0.19008671990972
H	2.50552144920635	4.68136695084891	-0.09290912738731
H	3.16548921233844	2.87822012278575	0.49698356246369
H	5.12367392054797	1.78343526416143	0.69704278313879
H	5.40202109407777	-2.48350151791638	0.23816871729147
H	-6.57919108171767	-0.31177881901743	-0.05204634911392
H	6.48745218230917	-0.31743107054595	0.69869967352166
C	-2.71219315479592	-3.03789609038245	0.34940152697317
C	-1.76069614426203	-3.29917374325576	-0.84518118466106
C	-1.92730091287292	-3.04373222813960	1.68542036021488
C	-3.72515639745266	-4.19981863720956	0.39891612685957
H	-2.32328012052270	-3.29076467565023	-1.79606595139265
H	-0.96624458009580	-2.54450327619083	-0.90511602700602
H	-1.28599094972889	-4.29108685487833	-0.73703963152577
H	-2.61850704869376	-2.91156095930909	2.53771773931158

H	-1.40505681494679	-4.00893594387353	1.81440658509154
H	-1.17819147628429	-2.23982334269465	1.71467871643880
H	-3.17874956778341	-5.15101103580254	0.52409151625483
H	-4.42509997738511	-4.10721771128920	1.24873616580291
H	-4.31437614798214	-4.27645828758524	-0.53257204708543
C	2.75701326985003	-3.08601074989741	-0.29463248897520
C	1.69218506361782	-3.42019390879896	0.77826291456485
C	2.11214080424985	-3.03866866474242	-1.70387841262589
C	3.79497338134857	-4.22639167741553	-0.29558810650488
H	2.15406665736147	-3.46901554965901	1.78126934465853
H	0.89379556239586	-2.66799392294110	0.79548766643265
H	1.23683577963705	-4.40412563651155	0.56411589669747
H	2.88444584080676	-2.86273502127128	-2.47435517186954
H	1.62234887230990	-4.00435983069973	-1.92558684614875
H	1.35795798469462	-2.24358490005821	-1.78726460398619
H	3.28752710637205	-5.17789800043851	-0.53245167122694
H	4.58097436445237	-4.07276921988764	-1.05666770610909
H	4.28120656991324	-4.34667056863534	0.68936756414538
Cl	-0.09822119932882	0.66730149113984	-2.78140607511322

[GaCl₂(Salphen)] (2 x ^tBu)

Ga	-0.01775635323456	0.60151077179808	-0.26091112008311
O	1.49346099139195	-0.66062533569655	-0.35125430381106
N	1.32552044343398	2.19901374610480	-0.06896191025358
C	2.71221124603092	-0.51330724998390	0.02708429048094
O	-1.51279159836653	-0.67961730394280	-0.27917263399000
N	-1.34948968245950	2.21448121002247	-0.14285984219947
C	3.57062316629915	-1.68628121934126	0.08478475561255
C	4.88539778732068	-1.52661175365494	0.51606202950096
C	5.43010313589448	-0.27212519241990	0.89277429389089
C	4.63523238932851	0.85621263459605	0.81861174045474
C	3.28012500260022	0.78073849304800	0.38405349108961
C	2.57081838163895	2.02213199376406	0.29357876157364
C	0.71749437048913	3.44442077283305	-0.20718127507524
C	1.41513705195001	4.66281780394050	-0.35091051357042
C	0.73078942280210	5.87248529023343	-0.50596865185743
C	-0.67451382942464	5.88300543681138	-0.54548407390549
C	-1.38651809415763	4.68471254644794	-0.43131430406101
C	-0.71963007496279	3.45400942634815	-0.25079276368577
C	-2.63459137956240	2.05272686114889	0.04588685953064
C	-3.35769162537301	0.81863048513819	0.13073690878882
C	-4.75934730626908	0.92794819506924	0.36875465523060
C	-5.55769755914860	-0.19270767659420	0.49555747151976
C	-4.96045123250751	-1.47718285871752	0.41770102397499
C	-3.59951062033978	-1.67055828271643	0.19505191129532
C	-2.75379131415062	-0.50192103474223	-0.00018088283954
H	-5.19499368911412	1.93339982700428	0.45112601672136
H	-5.61072556790277	-2.34737854414978	0.55259759176435
H	-3.26130516211440	2.95400985663992	0.18064424871703
H	-2.47880606891095	4.70033932073431	-0.50333623534276
H	-1.21608208393901	6.82595167074708	-0.69003939878192
H	1.29406563017406	6.80659364127935	-0.62194210040166

H	2.50994281953721	4.65469359458533	-0.36774969934217
H	3.16473884136764	2.91163596253978	0.57696360348555
H	5.03956180864443	1.84088702597996	1.09136014865782
H	5.54103086542621	-2.40135454663512	0.57386835642961
H	-6.63590825560280	-0.09902785851170	0.67151873911228
H	6.47145782323752	-0.20585552409719	1.22963167527931
C	-2.95532745043732	-3.07160660439925	0.20553632837456
C	-2.22331433404120	-3.35777051107922	-1.13105896578221
C	-1.96243409915979	-3.14840737975092	1.39531974537587
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H	-2.58550009345799	-5.38768826815699	-0.54414968544146
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H	0.89341359107356	5.61217683331473	-0.81497069428476
H	-1.10305591477478	-6.80121060830998	0.89390931213145
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H	1.66387813177713	1.22992410628511	4.11881395857940
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H	2.62139821505528	3.93536607127854	3.09314453097105
H	1.25595719748123	4.91975876737114	3.70714964916274
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C	1.59181488422477	-2.11560307340428	2.38538659742632
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C	1.30182734471501	-3.71990917016936	-1.72968017909019
C	3.39409969586700	-4.89038002668287	-1.05403009725293
H	3.11637752732546	-3.49255517339592	1.26919180165508
H	1.62313642811916	-2.60227336830789	0.85534518226111
H	1.59925049508604	-4.38677384442259	0.94734735988661
H	1.57543818411630	-3.78294898579599	-2.79801660960956
H	0.74812228322136	-4.63853987262121	-1.46342295662358
H	0.62997874337284	-2.86208834882800	-1.59892555813675
H	2.77677720967114	-5.75999197447556	-0.76790694174147
H	3.69434264265919	-5.02859240559755	-2.10809108799208
H	4.30321157970840	-4.91184647606557	-0.42680892744333
Ga	0.23633158378731	0.43385214720070	-1.30542611953370
O	0.63336565325794	0.96803100764777	1.88058888979346
C	-0.10345156310705	1.88362024442080	2.57591168807404
C	0.46963889827608	-0.33363286449287	2.46542023461883
O	-0.08720831274154	3.06498688112525	2.36635581380863
O	-0.85556055852314	1.26443440765798	3.51888334502136
H	0.34531024014893	-1.06649042298980	1.65800029529356
H	1.37277587122005	-0.57330290105833	3.05828875585759
C	-0.78337077045499	-0.17588157193720	3.34400855633419
C	-0.73203803616075	-0.87771153096815	4.68475505723811
H	-1.68931137059596	-0.47241271520360	2.78517865652600
H	0.14759535805743	-0.55136260613505	5.26693064689833
H	-1.64315093956380	-0.66941312504724	5.27013623921264
H	-0.66645621831331	-1.96909936827617	4.52572523468769
Cl	-0.22749323376535	0.17114044109843	-3.45041161450808

[InCl(Salphen)] (2 x ^tBu) Pathway (Int1 β , TS2 and Int2 β structures included under the "[InCl(Salphen)] (2 x ^tBu) Pathway" heading)

[InCl(Salphen)] (2 x ^tBu)

H	3.47169395413868	-5.99872913888077	4.86509569437714
H	1.86573064393886	-5.23865242497503	4.96496797769976
C	2.89986625555507	-5.18858711083130	5.35038319001396
H	4.12677188102582	-4.49014491503694	3.02326296914565
H	2.87870443463126	-5.40076483213769	6.43452490602239

H	2.54290892125088	-3.66258055289651	3.10564482496450
H	9.31284442738641	-3.83618512651363	0.83435107422224
C	3.57590217394885	-3.65789278706763	3.49859524039964
C	3.57176204609593	-3.83562170066146	5.03832896270335
H	1.25959187795359	-3.87016252727769	6.55285305929402
C	9.26253489637723	-2.75785454507984	0.60309996918062
H	9.04606261174823	-3.38879336381255	3.22209509931412
H	5.54051329736621	-4.78172360183122	5.13650588224689
C	6.94751505628882	-2.71807506545998	1.53353981379258
H	8.88010385247464	-2.65826204415657	-0.42868062233976
C	5.02534897312766	-3.90599255038298	5.57199226917985
H	4.05822623620383	-2.71450637549297	3.20586782608484
C	1.63928979183080	-2.85372792909021	6.41853251088219
H	10.29474697338830	-2.36499546309857	0.63168494874327
C	2.81280524942268	-2.65766432610769	5.68796524666072
C	8.95400578724226	-2.30295441448691	3.03608660485461
C	8.34752889828271	-2.06015970655671	1.63018683331061
H	5.03184338505224	-4.01842859254882	6.67120480954355
H	-0.01822175280824	-2.01492144374404	7.55920601533608
C	0.89840928796465	-1.79685248088101	7.00066459048155
H	9.96332892786937	-1.85856688182971	3.10571931763963
H	8.32850799349343	-1.87032903669311	3.83020289212045
H	5.59873217354359	-3.00582088796727	5.31074480583067
C	3.30298823279226	-1.30426471827380	5.54141904847913
H	9.53279946876605	-0.54939951371571	-0.35948990896304
C	8.24104759241885	-0.54311082046893	1.36066686285062
O	4.38567088949067	-1.10744992847928	4.84114255810163
C	1.34110740029418	-0.49888831618245	6.84719113970673
C	8.91530190784347	0.06517728089144	0.30114232767854
O	6.76192027822452	-0.27293559292490	3.18130259870153
C	2.54566405812458	-0.21266689960716	6.13447250320533
C	7.43234163044403	0.29461052934654	2.22108707934366
H	0.77714327255414	0.33732252376673	7.27989976651721
ln	5.77136791453659	0.48698771276497	4.88402660507600
C	8.84489708530341	1.45321017196720	0.02667079931824
C	2.87813424103912	1.17616262862601	6.01471858635448
H	9.39412962662401	1.87047578249547	-0.82417674983159
C	7.37268935418823	1.72471920132918	1.95963237954339
Cl	7.23291931407604	0.37818498122991	6.76588102906949
N	3.96933553570197	1.70756626050877	5.51130413904870
C	8.08352882472620	2.26392070987671	0.84260792991841
H	2.09420722214248	1.86385553201059	6.38081495170803
N	5.93762645613543	2.47716436492666	3.83234674963421
C	6.62131964593055	2.67247454211812	2.72553206434596
C	4.20930604447952	3.08634421951653	5.41465039706334
H	8.01773891363878	3.34270752160143	0.65174524660750
C	5.25406776496105	3.49488518387516	4.51751693192244
H	6.61828444227795	3.69418104300143	2.30423458120370
C	3.52077358590496	4.06899612289796	6.15619321599594
H	2.75013161807256	3.76664181968366	6.87216462288136
C	5.56442156337168	4.86619667437602	4.40533041736550
C	3.82934791727185	5.42444648350259	6.01053584510255

H	6.39117808698367	5.18279316685346	3.76162973213635
C	4.85298187967920	5.82378765930674	5.13400241733310
H	3.28688667142230	6.17112505767409	6.60126248497661
H	5.11491955663321	6.88349759208671	5.03840014785896
H	6.51026006555488	-2.55773326222003	0.53115754846088
H	6.25909109826474	-2.30945602361537	2.28569451238815
H	7.03254258533275	-3.80823986524757	1.69688272719161

[InCl₂(Salphen)] (2 x ^tBu)

H	3.11735057310559	-6.13351972506798	5.62956773226088
H	1.69497774161242	-5.27952443317983	4.97814863400853
C	2.47572569210472	-5.24305848729111	5.75971283597975
H	4.62358862466971	-4.88033976713536	4.12580612486704
H	1.98302980150947	-5.32847961373624	6.74600019216025
H	3.23733210725259	-3.95847383278796	3.45939099233237
H	9.61337065360936	-3.51339146024555	0.28810851900792
C	4.00573721465392	-3.97079083735982	4.25317809661070
C	3.34100120821542	-3.97074634655510	5.65339229860093
H	0.61871239033438	-3.69668042755630	6.07950825711350
C	9.40580002848509	-2.44902538434841	0.07471978373545
H	9.84870307728920	-3.04098157774286	2.67634583128204
H	5.01932346095049	-4.97609377777684	6.64036025624318
C	7.36510612954535	-2.60673434177285	1.50135282141518
H	8.79171510728814	-2.40820805515315	-0.84341649059445
C	4.42546601138931	-4.04925111032793	6.75821307776444
H	4.64200350733174	-3.08737027906732	4.10975473200422
C	1.12438351880512	-2.72751338415681	6.02000612674389
H	10.37350567314684	-1.95610710397339	-0.13370414869056
C	2.50198773596264	-2.68742805143951	5.82199937512167
C	9.60789369450715	-1.97250441877773	2.51520043502411
C	8.68177320454053	-1.81861995556748	1.28194200316950
H	3.95542120132887	-4.06959858006800	7.75945964261488
H	-0.75846321670958	-1.65566389308768	6.29654472916015
C	0.32291822634274	-1.56309491377055	6.14050319778861
H	10.55771766342086	-1.42858349862084	2.35438254484624
H	9.12698151475319	-1.57632459576012	3.42113703354982
H	5.10262725653267	-3.18460022067077	6.70678971105772
C	3.16053423697824	-1.38791263131628	5.74622129454432
H	9.20215760149831	-0.23911835329481	-0.93168493025700
C	8.35409197502209	-0.33022195987154	1.04413264279371
O	4.43599916233331	-1.33198733769536	5.62456023468666
C	0.92308666403009	-0.32230906276873	6.04706046696057
C	8.67849882592114	0.31518307577066	-0.14618240903998
O	7.41046986228934	-0.13463450224778	3.20978779333766
C	2.32812185737015	-0.19134189843010	5.84173180865717
C	7.65890334736090	0.42337809178532	2.08175822498128
H	0.32088891385188	0.59357904735880	6.12585876054431
In	5.66339263837433	0.17992858228872	4.54977054973316
C	8.35330549814684	1.67097100773404	-0.40823277202039
C	2.82500498316819	1.15033561096813	5.76410140417992
H	8.63548789483701	2.12743208581540	-1.36443557988104
C	7.29663224430729	1.80922814396989	1.79532544218936

Cl	7.21030734819354	0.15410164504022	6.44586765161939
N	4.04142429761895	1.56032613992835	5.49720120908579
C	7.66971618462236	2.39453659801736	0.54968900297601
H	2.05270577606326	1.92909122441457	5.92765604929593
N	6.05435092047276	2.37076860748412	3.85991210729217
C	6.58928368849215	2.66609707897676	2.69997531433456
C	4.40920291417308	2.90318990635160	5.54971745432305
H	7.39507015988884	3.44226843445379	0.36391827222581
C	5.47259701819897	3.33143090733639	4.68450787030608
H	6.46522750190418	3.70593542964213	2.33531166772937
C	3.82974396195168	3.83865802777679	6.43433946330750
H	3.05762791501665	3.49851411878668	7.13289813203183
C	5.90461833181754	4.67425221400903	4.74581074047001
C	4.25553331136348	5.17219142444924	6.45753259390488
H	6.75242707719937	4.98645780228791	4.12640263072622
C	5.29558959590761	5.59119283287647	5.61094198616374
H	3.79662733874497	5.87778160494072	7.16102519812596
H	5.65579689358986	6.62667907168948	5.64780516876901
H	6.71735036654090	-2.53391760084141	0.60938347158131
H	6.79621477305468	-2.21220112241739	2.35372190949534
H	7.58802460249191	-3.67542015220497	1.68415477153118
Cl	4.28202451522568	-0.39398602006667	2.56772005811677

IC

In	0.27744562687921	-0.27615349468592	-1.81048692670016
O	1.76009124448119	-1.75087463079933	-1.44987758278776
N	1.79002411923933	1.20363600401940	-1.00733855768405
C	2.99352663040498	-1.67053892685154	-1.04304789442071
O	-1.52395411994156	-1.38143750297029	-1.60818103036392
N	-0.90609626114997	1.46746127588180	-1.00115592837675
C	3.76925861021540	-2.89353809759571	-0.98068213745770
C	5.08036972885381	-2.82232840015313	-0.50730841016713
C	5.68719566741829	-1.61715345790385	-0.08161480929128
C	4.96143739256360	-0.44433710519312	-0.13718288786144
C	3.61644278783781	-0.42454363573548	-0.61831372924869
C	2.98987607653637	0.86851096393518	-0.60192990064602
C	1.27902033574652	2.50847066657231	-0.96070596307019
C	2.07793826783092	3.67040491679076	-0.96093280572675
C	1.49455623063724	4.94107018837468	-0.92347870281280
C	0.09562426823201	5.07466958148285	-0.91058661848795
C	-0.71702584847341	3.93647179555055	-0.93710305022666
C	-0.14993073134559	2.64603487025859	-0.95152195251897
C	-2.09615060574318	1.34439219206251	-0.46793033487712
C	-2.95933921713787	0.19687215465132	-0.45360435302600
C	-4.20175335764759	0.38743964995836	0.22410426282706
C	-5.13211929069665	-0.62856635610291	0.31582813937332
C	-4.85345208525552	-1.87392708860919	-0.29624610875008
C	-3.66424745624964	-2.14442768062157	-0.97499124751295
C	-2.65820957336646	-1.10214020462739	-1.03783213238976
O	0.09717531828585	-0.65010465939070	0.82474105525160
C	0.94472682101168	-1.37613802610400	1.72987850268325
C	-0.41203203818720	-1.86100069007292	1.43001285379372

C	-1.57567110343800	-1.69849258279703	2.37090578011475
H	1.81273379675345	-1.86811435230343	1.27062778745213
H	1.13807534369591	-0.85908223852096	2.68286023527304
H	-0.49277501497585	-2.69044388348253	0.71371528763566
H	-1.42843302344763	-0.83070083262144	3.03651784861785
H	-1.68961494181045	-2.60695661052368	2.99050103016368
H	-2.51216112725800	-1.55328725192305	1.80613607299062
H	-4.40526170878770	1.36774980478802	0.67379171193492
H	-5.61774935447954	-2.65267806265706	-0.22824576302109
H	-2.50017324874740	2.22236994494294	0.07019647925814
H	-1.80600542869101	4.04268041283411	-0.98059726077402
H	-0.36319702497630	6.06985888052944	-0.91023753894615
H	2.13309996891667	5.83163378060394	-0.93317416989777
H	3.16708459396781	3.57527075011833	-1.01948677387606
H	3.61862246944367	1.66635529879086	-0.16465851416728
H	5.41304362576735	0.50247993680167	0.18577531840143
H	5.67911334352547	-3.73575548924944	-0.45782370127559
H	-6.08149405132811	-0.47563070853892	0.84022349249188
H	6.71990969906382	-1.62211005197798	0.28329832570705
C	-3.41848622491529	-3.50388583183822	-1.66737235177012
C	-3.21411766145486	-3.27774931977739	-3.18760888379398
C	-2.17613571179387	-4.20910962143218	-1.06742029693436
C	-4.61820037115682	-4.45759818752037	-1.49351718975765
H	-4.11221363171477	-2.81234801104636	-3.63229650264498
H	-2.34921722114624	-2.62843080451414	-3.38810683420225
H	-3.04711887335509	-4.24686608681639	-3.69291001324983
H	-2.29918529631747	-4.35835545498889	0.02119755312907
H	-2.04564321625613	-5.20388146083460	-1.53118251831371
H	-1.26252331951753	-3.62613941814478	-1.24667012308122
H	-4.40639874637452	-5.40788894600827	-2.01413012475329
H	-4.80871892137530	-4.69688683997207	-0.43158905902312
H	-5.54480763740844	-4.04242915699403	-1.92840942357710
C	3.14538253852331	-4.23110352101628	-1.43724054612004
C	1.90556113289108	-4.56336877322821	-0.56863248865391
C	2.74140662793906	-4.14100145162118	-2.93101108195778
C	4.13722028932909	-5.40352398605686	-1.29260838877537
H	2.18351541854260	-4.63066684632918	0.49941059051620
H	1.12612866830850	-3.79806369958223	-0.68334799694223
H	1.48039518494239	-5.53775871747276	-0.87122692708534
H	3.62826439567608	-3.93914450042659	-3.55831266811964
H	2.30215719613654	-5.10071721982547	-3.26036967365170
H	2.00485772122860	-3.34366523770005	-3.10606388285995
H	3.65125800014470	-6.33507349331012	-1.63171676854797
H	5.04222010852108	-5.25967480457822	-1.90943697121058
H	4.45094734315415	-5.55640667060481	-0.24413458552656
Cl	0.39013685327541	0.02614701470473	-4.19021024069984

TS1

O	-0.64704123434144	-0.13882511528029	1.68550516582127
N	0.32321152678428	2.38158856646410	0.53436079235360
C	-1.26624348199088	0.62709961901814	2.52235385010961
O	2.49080180629253	-1.35776015545172	0.04517209828614

N	2.58706023647695	1.48512028937300	-0.70555683342433
C	-2.06831101387330	0.01785379178633	3.57021372791824
C	-2.76513681532894	0.85161732934788	4.44316872588970
C	-2.72919120380936	2.26583627681174	4.36027683462064
C	-1.96916326256233	2.86253817176152	3.37378061413529
C	-1.22026899629453	2.08395159989210	2.44142304769401
C	-0.50547723683796	2.83095516681241	1.44651442712444
C	0.84782107406018	3.16119518855465	-0.49584902677924
C	0.23145008323974	4.33914658044280	-0.97354822269303
C	0.77471899510860	5.06035452593601	-2.04129230867867
C	1.93674210916896	4.59687924428619	-2.68148741290670
C	2.54828279207565	3.41621868875267	-2.24827282836974
C	2.03937743447217	2.68844083087208	-1.14951679189400
C	3.83154377925186	1.12538709105035	-0.92057140599243
C	6.58068711083025	-1.34599217974164	-0.69969678150175
C	5.91247335734376	-2.49907145248463	-0.21744984127979
C	4.54765191404133	-2.53339258987936	0.06310349988989
C	3.76855643352824	-1.32794641815104	-0.15956276307136
H	6.51128551685696	-3.40069913008423	-0.06006005862279
H	4.51231986639545	1.88038924044109	-1.35910143586925
H	3.41658539695564	3.02681989472254	-2.78966490676489
H	2.34687113868415	5.13729837338976	-3.54287434992014
H	0.27068096983137	5.96636713172702	-2.39830134272769
H	-0.70836058589273	4.67023569826516	-0.51968174172176
H	-0.68472099766145	3.92322554522337	1.48369878698400
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H	4.33204556965390	-5.84938895327300	1.16895340149737
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TS2

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C	1.17603076042700	-0.30579542609119	-1.04255786216544
H	1.14919137358493	-0.17483528677296	0.05266224547360
C	1.62502477705301	-1.73925054621110	-1.33884702817734
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H	1.82109125450988	-1.90977509907519	-2.40754901797158
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I	3.48485272963948	-2.27507228355268	-0.28884748802796
H	1.63909546151528	1.77395301352472	-1.39701310348744
H	3.08066918699251	0.71654852308547	-1.27094259641275
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O	0.12816142309261	-0.53182745348145	-3.99313018504864
C	-0.76717780063890	-0.50199744949907	-3.21466095364276
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O	-0.63407735616157	-0.62716116340421	1.48873294905239
N	-1.57278184660619	-2.26614962981373	-0.69300058618374
C	0.12735247285650	-1.64871463330554	1.77674154979107
O	-1.86602934320494	1.82651874096487	0.21053965408367
N	-3.28850938136000	-0.27501042520033	-1.33606678754990
C	0.99990413216154	-1.56685847621274	2.92795852463932

C	1.83603795336813	-2.65357004307826	3.19402048476847
C	1.83978518737038	-3.84006071028990	2.42293854307202
C	0.96539099358729	-3.95846243866290	1.36164547125073
C	0.10118175541536	-2.88114513018446	1.00107277245299
C	-0.81402347592566	-3.14115265601597	-0.07452423000278
C	-2.53396983021901	-2.55764395763729	-1.67141780229585
C	-2.64127901207566	-3.79419536707308	-2.34058865074612
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C	-3.45140490013581	-1.50047309802855	-2.00292641312518
C	-4.20554190222260	0.66462780632903	-1.27956496435160
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C	-5.29416227943360	2.76978927989589	-0.81056648628863
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H	-6.15235256911869	2.35668205444768	-1.35574293746296
H	-4.31769234127650	5.54606227778223	0.86112769997967
H	-5.18849686294241	0.44357053151499	-1.73354024232133
H	-5.09255279692752	-0.91658475001017	-3.29906103472167
H	-5.27414970821197	-3.11918617271311	-4.41850871600003
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H	-0.88411847231099	-4.20323544592242	-0.37322850959688
H	0.93218478909590	-4.88005303780014	0.76682265189994
H	2.53087606761823	-2.59749731605820	4.03577985317115
H	-6.25425219342103	4.65262734189548	-0.38152529098825
H	2.52637214504386	-4.65376205650787	2.67753988730646
C	-1.87111875927068	4.38956618569651	1.43052061117927
C	-1.60635503910401	3.48881113887677	2.66465533521154
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C	-2.16764098381097	5.81207936052814	1.94833074999987
H	-2.49463641936286	3.46034845658964	3.32153120511449
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H	-0.78099740045769	5.11846979420408	-0.33332683714208
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H	-0.28503447683858	3.48328606651102	0.19184870124301
H	-1.30003614976076	6.17756365045661	2.52500311588828
H	-2.34175551792353	6.52593229720507	1.12328523706371
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C	0.99819047287621	-0.30601155908953	3.82277445824283
C	1.44739672239523	0.93923022926111	3.01718956330969
C	-0.42342947039385	-0.08137207679170	4.39882192203875
C	1.96475780963786	-0.45271299440609	5.01587533140146
H	2.49631352465462	0.83212902637321	2.68824850956900
H	0.81293936631195	1.10524753906470	2.13548010198964
H	1.38615545445005	1.84003950039407	3.65414253133525
H	-0.74131627429876	-0.95615442039512	4.99471603537533
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H	-1.15960747907304	0.08463875425131	3.59964235588621
H	1.92310250910595	0.46254908213953	5.63181480849247
H	1.69351589435675	-1.30374270330270	5.66576316654994
H	3.01190248091442	-0.58319487029113	4.68917401514943
O	-0.31685622537450	0.32068176770696	-2.40704107018884
C	0.95854073812224	0.20093227149126	-2.24660183097241
O	1.87198875359276	0.24864633661030	-3.03672364553104
O	1.17880811840565	-0.04155261429446	-0.84109947237696
C	2.51177390386070	-0.21367304252212	-0.27815157087926
H	2.29336889312133	-0.40437947711151	0.78292663990168
C	3.12410732524699	-1.47794419146245	-0.87623942822149
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H	3.49224263751723	-1.33198913359563	-1.90032363848294
H	2.40949977431003	-2.31250299005360	-0.82969578412158
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H	2.78150024695194	1.90648959649733	0.02651020608146
H	4.28780195047657	0.94713704165370	0.12923052083784
H	3.54753488007636	1.27950148964156	-1.47254048589481

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In	-2.15199977026700	-0.32167850746975	0.67009803034015
O	-0.60982268016172	-1.17011361392938	1.95510221681655
N	-2.02347566517668	-2.41883227910768	-0.28913747208924
C	0.29875748154700	-2.04413744581234	1.69767645243675
O	-2.56588004354142	1.80950617915941	0.64589017427944
N	-3.62027409470945	-0.36851100824697	-1.10383569484938
C	1.40871041175403	-2.20062342860680	2.62794366857264
C	2.45941232171156	-3.04377924712791	2.26969561209061
C	2.47643446695480	-3.78942105628725	1.06434560376482
C	1.37626022208611	-3.74169193365133	0.22905344259074
C	0.25398045499330	-2.91469239349800	0.52821765821365
C	-0.88514927342924	-3.06432708280334	-0.33362639345508
C	-3.11339942987147	-2.73473121856078	-1.09738646467583
C	-3.43873952586235	-4.05410228998674	-1.47754691191506
C	-4.57047455907249	-4.32211191880710	-2.25683643230290
C	-5.41582557539994	-3.27107591998930	-2.64955687358093
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C	-3.97010557618303	-1.65782612349640	-1.51047890022011
C	-3.91943726726386	0.70070217532511	-1.79716731484235
C	-3.65975072361680	2.08088698799970	-1.49510350231350
C	-4.11078922226416	3.00878715312190	-2.48079008744513
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C	-3.29219076571907	4.85247401244924	-1.16043600616661
C	-2.81279009827505	4.01666889045054	-0.15436200938704
C	-2.99046446389004	2.57747006307004	-0.29665087544025
H	-4.60616440730229	2.61250663216762	-3.37767587387253
H	-3.16478998095703	5.93498648178986	-1.06307868656439
H	-4.42283442119268	0.54576647330931	-2.77181769170006
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H	-2.80711404976036	-4.87599753680565	-1.12297268750813

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H	3.32351573978521	-3.13468080287082	2.93394236114984
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H	-2.33307044659787	4.57539291657236	3.26724374986952
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H	-0.11471671594849	4.41822828057971	2.02752647939455
H	-0.60132625219600	2.94269958035992	1.13646278880781
H	-1.49368082074062	6.46673123839302	1.97784493964809
H	-1.45938791163956	6.49460324682014	0.19689357187361
H	-3.02328428539811	6.57773534459370	1.06781685940956
C	1.38884476016223	-1.44399466760982	3.97307952805121
C	1.44807795130723	0.08589381413106	3.74056027601029
C	0.09785540696803	-1.81212810996512	4.74985837245482
C	2.59342899057614	-1.82345938533039	4.85875891370066
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H	0.65803209749620	0.41685334536994	3.05253474058141
H	1.32843128556122	0.61826006580773	4.70312766479810
H	0.05024158230947	-2.90346391830023	4.92305501087095
H	0.09830204510772	-1.30994823175424	5.73598493472752
H	-0.80514128000644	-1.50512923949517	4.20159621157471
H	2.52898312336641	-1.27422801368648	5.81555344555565
H	2.60988457279646	-2.90379768663635	5.09336629342274
H	3.55466251067148	-1.55292002699292	4.38611414050653
O	-0.70226433353377	0.10156440750687	-0.94223553276092
C	0.54326829387051	0.39079787056719	-0.95067837829843
O	1.34631392225249	0.22137273494294	-1.86335315329849
O	0.94733355406948	0.96977728540403	0.26766142124912
C	2.33296186304625	1.31108838624268	0.44785666710761
H	2.36213081490603	1.64561619244593	1.49845530116287
C	3.17127439402057	0.03577348033054	0.32597033455960
C	2.78774884421078	2.46053484240755	-0.45067322609373
H	3.42141773055272	-0.22494469022994	-0.70861660077478
H	2.68728136739701	-0.80541439589240	0.83872507808088
I	5.12097865035995	0.20230366033004	1.37555693298409
H	2.12752097244382	3.33168454590410	-0.30154077917022
H	3.82053873549582	2.75457462649600	-0.19076349544411
H	2.74771943171963	2.15683833138222	-1.50779999076072
Cl	-3.79799098548735	-0.71171283684557	2.44055190061409

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In	-2.44421297967406	-0.44031540303180	0.79023980094758
O	-0.90594437180231	-1.19167700158985	2.09081630405196
N	-2.11331703206027	-2.44082701834961	-0.26882768338634
C	0.13186220510432	-1.90219244970357	1.78450313727847

O	-2.78423717668583	1.68031871966249	0.80317422814380
N	-3.70583520584148	-0.41272769068489	-1.11787967916722
C	1.30426024812165	-1.83294790933919	2.63857919002133
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C	2.49969734664513	-3.34659968848245	1.09082032377435
C	1.36763550333173	-3.49004010718437	0.31503658272359
C	0.16239379975599	-2.78978026391296	0.62858290160587
C	-0.93984328617897	-3.02577712221026	-0.25860085957670
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C	-3.37438957980563	-4.07009647473371	-1.63223156386502
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C	-3.98377549278961	-1.69250704474771	-1.60776840786243
C	-3.97068971629062	0.68543552084534	-1.77788702342377
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C	-4.08338327215876	3.02196541860735	-2.37865444892218
C	-3.84499697059538	4.36839937450126	-2.18270318152083
C	-3.18949180348161	4.78479565442156	-0.99854854183234
C	-2.78729401863989	3.90033491371432	0.00112701024254
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H	-4.56392537116041	2.67323829172534	-3.30272556341151
H	-2.98752796332209	5.85356015130894	-0.88050650157976
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H	3.36190612340495	-2.44170375214132	2.83795456293815
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C	-2.82594508334161	4.05437185466412	2.53821981867632
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H	-0.07516116280205	4.03123058685572	2.19617170329825
H	-0.71262600245873	2.60456656051788	1.33055676501714
H	-1.23232881726693	6.20337716168992	2.13771426446728
H	-1.19355308373646	6.22296289097747	0.35655358056197
H	-2.74018442760950	6.47265643298230	1.22618409991927
C	1.25363885736589	-1.02380752583040	3.95433604304775
C	0.97046069322020	0.47802136196776	3.69941129895592
C	0.13905043071739	-1.61322760022134	4.85786094609223
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H	1.80590064533049	0.94796097639257	3.15362461965517
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H	0.33336417753253	-2.68206009488403	5.06450554983110
H	0.11464926043909	-1.07660580656968	5.82538682641465
H	-0.84906986837654	-1.52114304737444	4.38232347460262
H	2.50699151818161	-0.53080034215090	5.66072664240798
H	2.83237301918248	-2.15693938638142	5.00424200875239
H	3.43006115785734	-0.70500531831160	4.14442697491291
O	-0.80977853228279	0.15013816622400	-0.73634298850010
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O	1.21196295443710	-0.10816972669437	-1.68530415791770
O	1.04499965055346	0.61167015613798	0.42610807317810
C	2.48894556979404	0.71848979465317	0.31420862137561
H	2.85702423890067	0.41110842295381	1.30325005063549
C	2.98260395590067	-0.26949648995498	-0.72717418224915
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H	3.49879685013446	0.05893147435119	-1.62670058097284
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I	5.48024279816541	-0.69807598475662	0.32143706151572
H	2.45408065961371	2.83193619654509	0.78516821605964
H	3.97300289981037	2.25667296020883	0.01292105942930
H	2.48082667488688	2.46514016173907	-0.96985127503821
Cl	-4.22768136872601	-0.97823216989727	2.36149460131939

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O	-0.88383653020751	-1.43131770813865	2.01065161099518
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O	-2.06839047558993	1.18702692830504	0.95096565869701
N	-3.19286243417642	-0.42853064470286	-1.26007869408337
C	0.84809665252353	-2.62888380343064	3.07178920437745
C	1.61397806753343	-3.79455843079060	3.11754029050290
C	1.45598327671824	-4.86351949144542	2.20346670055870
C	0.50421781046294	-4.76227385372624	1.20909629567021
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C	-0.45541567182068	4.04206142141694	3.46358604567818
C	1.21824628484228	2.21032931746555	2.94748722508008
C	1.88748748898497	4.60291125108892	2.79620476273184
H	-0.80448993249408	5.05856462948572	3.20271852602476
H	-1.30048492404272	3.34409564122895	3.36585740425865
H	-0.12771615326152	4.05320056491877	4.52068057137740
H	2.12077955598400	1.93536230173369	2.37536330915190
H	1.48655740941451	2.19757172321637	4.02065532192737
H	0.44160459067680	1.45303919472424	2.77705324915513
H	2.18682352030552	4.55045314378456	3.85874659302690
H	2.77312999371337	4.34864403411020	2.18706529407882
H	1.60232154597300	5.64929652697759	2.58197214026406
C	0.65471813307960	-3.21741329838518	3.15563917495677
C	1.29037403314311	-1.80592558547290	3.08478935520623

C	-0.44735191587895	-3.24556950571278	4.24566559999338
C	1.76266530575117	-4.19925710039671	3.58878958009416
H	2.13802979812562	-1.79421874103885	2.37833973369232
H	0.55804156558186	-1.05526470212770	2.75851241781167
H	1.67175682945736	-1.51106070751909	4.08044601908574
H	-0.89307446595702	-4.25525592882452	4.31702429348368
H	-0.01191039771402	-2.99296191432227	5.23134404521882
H	-1.24626279496851	-2.52496978813086	4.01761473257581
H	2.16913290341888	-3.88308146644549	4.56649994575316
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H	2.60269212537555	-4.21778451333128	2.87080456171255
ln	-2.24008907401568	0.05318331739342	1.01328877668906
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C	-0.41758406037501	-0.25726538486514	-1.61336646983787
O	-1.35463627139692	-0.39988858476511	-2.39020222280287
O	0.84741143426221	-0.20547225234731	-2.21385963072618
C	2.04863233878675	-0.11775657947522	-1.43119954517040
C	2.03590223993637	1.17120838524638	-0.60499680119949
C	2.30743307443854	-1.38704452935835	-0.62108048363665
H	2.83199531488412	-0.01748815270974	-2.20591776098148
H	1.61868831720092	2.01443987094778	-1.17226570602382
H	1.52937500581313	1.07219596226774	0.35965933583969
I	4.08703399958905	1.85408472430376	-0.09023828064606
H	1.52470511066648	-1.52132212938340	0.13935463766274
H	2.29972367130544	-2.26608589658939	-1.28824629415605
H	3.29066798711986	-1.33077111167656	-0.12095801332606
Cl	-3.96666328570045	0.28241406000636	2.72388147427017

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C	-0.92878164026327	-2.66504611010082	1.18652217752608
O	-1.43845322023430	1.97844020191091	1.53965908596559
N	-3.18333417557048	1.33160338848436	-0.70994279481421
C	0.12773090664648	-3.46539716151791	1.78004708650708
C	0.52722791671869	-4.63083073307618	1.12436927879888
C	-0.04775528019249	-5.07147205347582	-0.09005423145713
C	-1.06921135978249	-4.33187756433713	-0.65553230816374
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C	-2.61431536492420	-2.47911190411933	-0.75620334401316
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C	-5.20159944982000	-1.52172745184308	-1.92824740807014
C	-6.15681034584790	-0.87780760604947	-2.72654535891208
C	-6.13153563624026	0.51924657776296	-2.86505980234624
C	-5.15330533332943	1.27357069820996	-2.20289177465178
C	-4.18044792816306	0.64375853190108	-1.40559110390268
C	-2.49763521479226	2.31866071603649	-1.22674937662860
C	-1.39442010299335	3.02861935526297	-0.63744279848871
C	-0.72079943654924	3.94273961515230	-1.49899484614932
C	0.38113745748610	4.65463543100568	-1.06276067386639
C	0.81521906891132	4.50681580823490	0.27591617779444
C	0.19677751877104	3.65021435974669	1.18858014836701

C	-0.90934918531624	2.84062741922836	0.72163142937281
H	-1.08341831858096	4.05197594139030	-2.52946659007261
H	1.68492183694143	5.08678050513463	0.59490792312733
H	-2.73932056927452	2.61324314805962	-2.26525588759146
H	-5.14758456627858	2.36649946378705	-2.27991114051782
H	-6.88843568664614	1.02664678894214	-3.47520892358431
H	-6.93416866424361	-1.46785691499690	-3.22664829901484
H	-5.23513604331669	-2.60838351881176	-1.79248229340700
H	-2.91847873462343	-2.98314973638278	-1.69251988386024
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H	1.32984571352146	-5.23686744136453	1.55408403150628
H	0.91657242203510	5.33056210453815	-1.73887113697533
H	0.31617973638148	-5.98697803205994	-0.57003374622290
C	0.64428425391713	3.57478814741064	2.66590485321781
C	-0.53834110995450	4.02703280934716	3.56063860124379
C	1.08046160095636	2.14299855007878	3.06228465380778
C	1.84263883179897	4.50538573576565	2.94239532608323
H	-0.85641725081050	5.05386904645984	3.29965264084308
H	-1.40033571197771	3.35136602704520	3.44769069705273
H	-0.22914077541470	4.02406748657575	4.62309550902574
H	1.95599041637900	1.82505913408456	2.47172456456610
H	1.37025166188053	2.12763139649514	4.12985575796185
H	0.26430089021126	1.42316134077179	2.91859310343570
H	2.12163819828822	4.42943273029108	4.00874043038431
H	2.72487743497828	4.21415372443924	2.34532254016479
H	1.60410580595540	5.56543563534570	2.73679514172567
C	0.78349673785670	-3.01979585931695	3.10600481238024
C	1.47865646588203	-1.64814845948138	2.92615261177255
C	-0.29144154426250	-2.92669300465315	4.21916029546120
C	1.85644528360574	-4.02154518274764	3.58048520854500
H	2.28073956937733	-1.70485017439399	2.17013448860360
H	0.75902692882874	-0.87801942885688	2.61914545506585
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H	-0.78941882123492	-3.90413695411782	4.35950417429945
H	0.18387233543152	-2.64426400626082	5.17742321337828
H	-1.05729660972650	-2.17645383298716	3.97387178016625
H	2.29161915335601	-3.66423808548260	4.53074078318936
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H	2.68387705985070	-4.11778878548938	2.85458865095614
ln	-2.34247238860506	0.11978859385520	1.02093432399564
O	-0.40493249784199	0.01634727118119	-0.57398712003810
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O	-1.42476284826426	-0.27781147252835	-2.58536816835345
O	0.81009766084293	-0.27756052431408	-2.42429783598040
C	1.88071420392561	-0.32339685241590	-1.44915963757153
C	1.48148275331033	0.52406720109697	-0.25555087603944
C	2.19934885445792	-1.76819980882375	-1.08071278022802
H	2.73680789467960	0.14328309166004	-1.95933614024423
H	1.27808138676828	1.58728829877758	-0.38455618644608
H	1.45557378212812	0.11567123236857	0.75080105058331
I	4.06923276583413	1.35591535294051	0.43660512008752
H	1.35410790055724	-2.23176339034903	-0.54612329071610

H	2.40445817463985	-2.35339677396742	-1.99315744901867
H	3.08941488308367	-1.79389792220644	-0.42948986183667
Cl	-4.11819861024997	0.17967735685435	2.67413600516868

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O	1.51380282504412	-1.16227638880587	-1.28674166073792
N	1.65198573933538	1.79754472528964	-1.54095611515985
C	2.80411927817638	-1.05299649151021	-1.11103893934495
O	-1.55700882275625	-0.70841084992761	-0.64376981284658
N	-0.91364772257251	2.16069288800088	-0.87617075921309
C	3.57651237020588	-2.26683549851908	-0.94390565048169
C	4.94848529601684	-2.15113285688537	-0.70774019879084
C	5.62001739370430	-0.91057489711084	-0.61926523802309
C	4.89812806603062	0.25414281110765	-0.78859639215753
C	3.49586322399002	0.22462279377966	-1.05293645355853
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C	1.33703468142539	5.47433127868185	-2.19258410203220
C	-0.01039648096079	5.66406721181676	-1.84270867563675
C	-0.78300271322868	4.58080402990628	-1.40661940559488
C	-0.21237658516102	3.30001064513081	-1.29952067717668
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C	-4.21715194757257	0.48999400578768	2.31952246123838
C	-4.15355044905136	-0.84939030781187	1.86924355549043
C	-3.30597243029718	-1.27407771191400	0.84268203392010
C	-2.43004164850543	-0.29479810685545	0.23076115471714
H	-3.49179694951049	2.49624657432169	2.00525609997427
H	-4.80649901411750	-1.57834557801941	2.35652512069372
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H	-0.46732803547856	6.65606978447417	-1.93134115846014
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H	5.39705466541234	1.22992296058486	-0.73161556011043
H	5.54423427173709	-3.05905654865486	-0.58214711264824
H	-4.89156111147634	0.76238734262125	3.13830811187387
H	6.69742850021423	-0.88162529757086	-0.42435804760694
C	-3.31297617151366	-2.73637686266054	0.34373111009948
C	-3.69000855439026	-2.76127323007921	-1.15997710157674
C	-1.92734606261676	-3.39612191247419	0.54680758901385
C	-4.34909835779050	-3.59280214944565	1.10016221434108
H	-4.69341630225290	-2.32518994886038	-1.31387360285468
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H	-1.62930572585258	-3.36648640056814	1.61147264765695
H	-1.96347041601834	-4.45709681475348	0.23972730823483
H	-1.15723315898381	-2.89514097547502	-0.05429298467930
H	-4.33600543477809	-4.62030130330968	0.69680624743119

H	-4.12526390055313	-3.65923429095774	2.18041856084959
H	-5.37574512915179	-3.20349000581609	0.98082803334034
C	2.89280956330578	-3.64955336753758	-1.02977017559795
C	1.84439902406569	-3.78434530466134	0.10128218254970
C	2.21345932320246	-3.82381651680261	-2.41180685246304
C	3.90401795810948	-4.80267860173608	-0.86414639093000
H	2.32679408818734	-3.68972372652036	1.09170322085299
H	1.07052320857417	-3.01139570094619	0.01073396563716
H	1.35303679673364	-4.77338291459423	0.05337422128350
H	2.96159775839731	-3.74773328065797	-3.22133882263225
H	1.74295138392482	-4.82229169560537	-2.47591171288156
H	1.43849388189662	-3.06324953599552	-2.58388964570178
H	3.37074830465292	-5.76668072540064	-0.93709451308286
H	4.67762170039936	-4.79181106084360	-1.65256658423578
H	4.40812271614922	-4.77803058242102	0.11870111482120
In	0.00755043566839	0.26379660436719	-1.70994241156319
O	0.75916074774871	0.43362548349556	1.26621342197365
C	0.53161557115013	1.52941399526611	2.05438032823192
C	0.45609764782272	-0.76208714557281	2.00367954779353
O	0.82561513631737	2.65111961486049	1.74825409869959
O	-0.07151126618517	1.15663182601619	3.20723056725274
H	-0.04971604096691	-1.46981125444481	1.33614924148508
H	1.40302943467535	-1.20201139124517	2.36846786346859
C	-0.43747668880708	-0.25061364214061	3.14371651937953
C	-0.22945391371154	-0.91933472424369	4.48571824392393
H	-1.50164467560278	-0.28728767221912	2.84933059104261
H	0.82429408038692	-0.84222189719047	4.80629738843146
H	-0.87080376460217	-0.45892328986039	5.25562876939766
H	-0.49842918922017	-1.98820351959497	4.40795777296975
Cl	-0.61657783825054	0.06338118882012	-4.00492113231451

[InCl(Salphen)] (4 x ^tBu) Pathway

[InCl(Salphen)] (4 x ^tBu)

H	3.49125512413896	-6.05102294740115	4.94146469686448
H	1.88872529401715	-5.28111247096942	5.01851105013380
C	2.91978546916926	-5.23212947711666	5.41225221728343
H	4.17083074760914	-4.56697544470285	3.08786376521866
H	2.88721090950299	-5.43217530339002	6.49841967558711
H	2.59185333574494	-3.72768267213269	3.14758475155101
H	9.36788037538825	-3.85802761066469	0.81961703693289
C	3.62140001338232	-3.72603884774865	3.54966331483686
C	3.60200724241204	-3.88638156745003	5.09106346444840
H	1.30741723815391	-3.90310671230620	6.56752467536834
C	9.31449128939035	-2.77737802875465	0.60012949033680
H	9.10897139898549	-3.43482402861673	3.21577059793732
H	5.56600642265622	-4.84084927274815	5.21734689482845
C	7.00331815914112	-2.75225116265000	1.54125256257100
H	8.92828453667092	-2.66766674231285	-0.42921152475941
C	5.05038819614974	-3.95805963636899	5.63802674304112
H	4.11259073911792	-2.78872807846378	3.25189385857010
C	1.66551952145052	-2.88162929206219	6.44286270346974

H	10.34619083611875	-2.38309053742336	0.62836231130746
C	2.84633222069352	-2.69455387049948	5.71984807861307
C	9.01463661716585	-2.34752849808586	3.03907651037335
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H	5.04659964692162	-4.05750604034028	6.73854890833693
C	-0.40376725744189	-2.09412091701196	7.81059807843218
C	0.89707458266912	-1.83734052822396	7.02295207772278
H	10.02350660764311	-1.90195726950867	3.10873872394222
H	8.39101324176278	-1.92189522574106	3.83851443707755
H	5.62922089467522	-3.06280002132363	5.37137091285355
C	3.34586626833391	-1.35142403131415	5.56154846577528
H	9.56982608789032	-0.58963645195225	-0.31669609112179
C	8.28910163512715	-0.57225738220252	1.38676988171596
O	4.43580850914531	-1.16077263049144	4.86782597398552
C	1.37068468399116	-0.54613678453374	6.84321951022220
C	8.96210917139315	0.04314270650228	0.32944108291108
O	6.81380775954721	-0.32292511493503	3.21608090982170
C	2.57918553345570	-0.26212524427739	6.14102763885372
C	7.48178244509828	0.24961658803045	2.25508726497562
H	0.81681900503214	0.30586101598405	7.25668348043779
ln	5.81198904429188	0.43904996946496	4.90913179813050
C	8.91096168581594	1.43270362064549	0.03543725307721
C	2.90808062157990	1.12755570258356	6.01817747764917
C	9.66718933895478	2.06470022443527	-1.15095764211140
C	7.42493157950755	1.67710857795235	1.99136735407055
Cl	7.26480166719505	0.35762273421270	6.80129149267251
N	4.00302097545909	1.65919086848742	5.52336431250378
C	8.13687680869026	2.21599276209708	0.87765806159166
H	2.11868384803610	1.81506104132573	6.37307761729772
N	5.98005600699921	2.43043674381006	3.85538569259965
C	6.66978290905747	2.62613499491480	2.75240849830631
C	4.24070385787326	3.03804272917094	5.42571849390115
H	8.05893655335315	3.29688372381761	0.70667878403618
C	5.29036836538337	3.44743819929115	4.53472937534049
H	6.66748317463584	3.64752594844892	2.33005506732155
C	3.54538623821682	4.02040886525537	6.16145695901589
H	2.77133569110810	3.71690289425400	6.87328822805248
C	5.59812205283824	4.81945569469815	4.42250667791905
C	3.85160880900747	5.37637178711624	6.01570999187326
H	6.42830524030602	5.13672549479456	3.78353420251728
C	4.87988327160160	5.77664748242810	5.14497820148093
H	3.30386282243937	6.12273422255929	6.60198988084629
H	5.14004672487698	6.83682020466229	5.04933876741927
H	6.56139788864729	-2.58257393573203	0.54240516980707
H	6.31793643373458	-2.35112912940250	2.30047627982540
H	7.09033706036756	-3.84390861454324	1.69378699597164
C	-0.74744876910742	-3.59425591542894	7.89012293153673
C	-1.57499770558367	-1.36430885686875	7.10990089289926
C	-0.23927018371812	-1.55631639547338	9.25245260310487
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H	-1.68248631866446	-3.73254569149481	8.46124077406124
H	0.04376750132872	-4.16967283136366	8.40222830054693

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H	-1.16425731475808	-1.71820944968937	9.83641188887601
H	-0.02212176660895	-0.47407008480653	9.26152858231163
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H	-1.40098740923085	-0.27573682142342	7.05090349531220
H	-2.51921399605897	-1.52335276743795	7.66301767256389
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C	10.66329716668981	3.12103190026745	-0.61497616222731
C	8.64901693291450	2.74041614175096	-2.10081669977316
H	11.22302782134122	0.51455784019437	-1.33751516271325
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H	9.79947283098558	0.24481131104966	-2.38746914768744
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H	10.14837293768145	3.91916837222943	-0.05239934580570
H	11.21099547899085	3.59796706752381	-1.44884407861957
H	7.93282699018762	1.99897376194492	-2.49768948530958
H	9.16784977396272	3.21283796274399	-2.95552270793621
H	8.06971192748402	3.52627291875269	-1.58550660079470

[InCl₂(Salphen)] (4 x ^tBu)

H	3.19905650203226	-6.17764069463630	5.70695429018092
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C	2.55949319984558	-5.28487866510420	5.83063500868244
H	4.72627477334353	-4.93121451389650	4.22271708478061
H	2.05440002320443	-5.37031636193281	6.81061848914998
H	3.35549136611541	-3.99638377385280	3.54162027422838
H	9.67711692249493	-3.56098333052641	0.35595303687056
C	4.11360208654020	-4.01746492537646	4.34503134728815
C	3.43113520997859	-4.01577079984854	5.73663636847734
H	0.74075340619786	-3.74874404826422	6.12730500927034
C	9.46574257363912	-2.49690612853208	0.14524150204517
H	9.94632841876062	-3.08660307573694	2.74202304267483
H	5.09423299136939	-5.02721218211232	6.74377552370092
C	7.44599642134216	-2.65643164102723	1.60144561926687
H	8.83917514288452	-2.45720813538334	-0.76447113131643
C	4.50083610667322	-4.09925093654574	6.85505217934370
H	4.75817427820544	-3.13839928730546	4.21231299894345
C	1.21687781713609	-2.76904193229032	6.07686652482205
H	10.43013630215284	-2.00367082005231	-0.07722551751418
C	2.59762768477159	-2.72709929611897	5.89516320712838
C	9.70206742109260	-2.01866550850421	2.58238390279073
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H	8.91795607246623	0.45333245174565	-2.88901995667528
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H	5.37695424558963	-5.25527758670240	-0.09658489698259
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H	-2.86695432904387	-3.07500971350231	5.03000855680901
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C	-3.12909782461170	3.16696996084096	5.62898693735359
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C	3.10713741996280	-3.54634470635223	1.91634111238823
C	2.87376605544002	-4.43036579545663	-0.45491664154115
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H	3.81468304434901	-3.19742389373899	2.68981384519232
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H	4.37540422717595	-5.85672874485385	1.28455476385129
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I	1.29227674177141	-3.10793441312583	-4.45309204060626
H	-1.23529880005263	0.00554884393012	-3.72204597731962
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H	0.03303401731813	1.23875364837950	-3.45756345843596
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C	8.74907173591882	-1.65499265582116	0.72820473067089
H	8.47273700088390	-0.88692147799427	1.47253569992233
H	9.85322292623722	-1.68906546478685	0.65530244520858
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C	2.09567455624484	2.93171509825830	-1.03880768366332
C	3.64773076229328	1.08981362759695	-1.12529454550530
C	5.91896857807303	-1.84016221984356	-1.37798656292274
C	5.26086687952285	-2.75361222196240	-0.50826465094141
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C	3.44541340883086	-1.20860813352190	-0.02557899158553
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C	3.38073153628772	-2.94958361095380	2.56233561297506
C	2.02636904680545	-3.92413157604270	0.64737096751239
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H	4.39626000583309	-2.71848597150255	2.93228444799012
H	2.77915219715906	-2.02971526766039	2.59243628591316
H	2.92481993493367	-3.68503317188551	3.25052065471892
H	2.06126884920621	-4.32984177732555	-0.37943138861688
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H	1.34292477299242	-3.06377570764733	0.66655530789121
H	3.80516149544824	-5.53828523518687	1.88660723296927
H	4.34552865833960	-5.32543658472864	0.20305032008704
H	5.30824631164939	-4.64476835083577	1.55262237677028
C	-1.87974379308270	-1.70250947568829	3.52974694191714
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H	-0.39191588640354	-3.28154165485696	3.82502365339067

H	0.23294830282074	-1.87397853696088	2.92030231087986
H	-2.66244491275324	-3.33718284451536	4.72801616071149
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H	-0.30564847691668	0.55465546470267	-4.33300463882870
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C	6.89533961623206	-3.50637119153689	-2.98668760323469
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H	-5.16711737562979	1.17521273563833	5.41514066721289
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TS2

In	-0.93472121703065	0.04223052638984	-0.64793682861170
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C	0.91186914853282	-3.99544563840743	1.47078202211922
C	0.20516468721062	-2.84860255539128	0.98982692368788
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C	-3.19222977575670	-3.87584495833629	-3.60397275146943
C	-4.10656914897761	-2.85623373966899	-3.91930399158353
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C	-3.12711062222615	-1.42278887557050	-2.20342863177047
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H	-4.74612848351065	-0.83075156358172	-3.52092229485642
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H	0.82751628454535	-4.91487246750870	0.88301120729560
H	2.27749814279026	-2.70141958564159	4.26163608254149
C	-6.63532783515610	4.69390062164800	-0.10661236925890
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H	-0.86458937964356	5.34109396665984	-0.60742097785039
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C	2.28694932223069	0.29515459483547	-0.64666228569197
H	2.07398600493316	0.35018698122531	0.43468795977568
C	2.78076902625442	-1.11938452283922	-0.96262067842180
C	3.25286607213443	1.41379680378993	-1.02766504978669
H	3.15642072805618	-1.21804398254503	-1.99157828224007
H	1.99542427009236	-1.86209502503814	-0.76154307291422
I	4.43557657599745	-1.74880723460689	0.34752125423936
H	2.80247432999347	2.38884572491646	-0.77476315429872
H	4.20143180581264	1.30950671135283	-0.47373954136888
H	3.46577591352878	1.39329856064143	-2.10897820434526
C	-7.77790176267388	3.94628822567993	-0.81881332829699
C	-6.42626573900882	6.05411440477422	-0.81511562620650
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H	-7.36083843708938	6.64460210058779	-0.80228781555576
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Int2β

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N	-3.12132803484442	-0.05645680635020	-1.37689458477631
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C	1.95581976133404	-2.48126023655764	3.25957916266724

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C	-6.81230440640340	4.93899310028863	-0.56680922265331
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H	-3.04121587986054	3.41456375390504	3.56100371558309
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C	0.01586536641566	0.30283642340389	4.48578372608847
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H	-0.80372095992975	0.43056984575513	3.76454707235698

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H	2.20734896626908	-0.94515437234130	5.59528775922055
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O	0.03965700437341	0.95273767990727	-1.83704475743138
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O	1.99956628104496	0.47068049560323	-2.85721296829624
O	1.43047278205885	-0.42009167067883	-0.80908922009504
C	2.59306845142770	-1.29102787664539	-0.73349078230369
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C	2.47251612359165	-2.31813286526457	-1.85949772132871
C	3.90171591718510	-0.51213225689375	-0.68919434775415
H	2.77691167683445	-1.91735138850193	-2.83543109407386
H	1.44851381537231	-2.71614030718567	-1.91190287858832
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H	3.86494678751043	0.22313665364957	0.13232969181464
H	4.73760094448265	-1.20599099781614	-0.49508692250613
H	4.07979532816000	0.01667168343540	-1.63757598269127
C	-7.80053938244182	4.26149119676023	-1.53424146865823
C	-6.39596056634851	6.30213604894207	-1.17072095572534
C	-7.53239681244903	5.16842480389385	0.78426701562946
H	-5.87791159082322	6.16041514922311	-2.13591713396481
H	-5.71564694086175	6.85643318542739	-0.50126217216497
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H	-7.83881979138826	4.20641331409462	1.23244307258712
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H	-6.88424542291911	5.68748860122973	1.51153307612791
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C	2.53878953617212	-6.14637992239288	2.13989994726199
C	2.52551378905333	-5.23560999850960	4.47428901033354
C	4.25932226455427	-4.45149763503068	2.80571332214190
H	4.45937534090171	-4.18866691330405	1.75230806227204
H	4.94160171618840	-5.27157822787554	3.09584750406687
H	4.50826922230702	-3.57450854377399	3.42858691100297
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H	3.21723930616800	-6.95461283439683	2.46526746545608
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Int2 α

In	-2.24344210912597	-0.36211121055910	0.79289481455509
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C	2.38580426101605	-3.05274070786714	2.29370520399070
C	2.40658790374352	-3.80898531105317	1.08560825860239

C	1.26213587323315	-3.76814361537373	0.30608963418946
C	0.13463743706370	-2.96042934083041	0.64133875965425
C	-1.01843769079776	-3.12042758774292	-0.19895912009037
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C	-3.60045744550566	-4.08905282266954	-1.31544788051059
C	-4.73428311873653	-4.34120826383647	-2.09738242378926
C	-5.55251166675645	-3.27620961534059	-2.50963309167428
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C	-4.07573306240150	-1.68162443571488	-1.38475767074251
C	-3.96135855832802	0.67069463775106	-1.70648975854204
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C	-4.09283623652388	2.97166281280198	-2.42341486086384
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C	-2.83188030220668	3.97744126197004	-0.09048048364882
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H	-2.98851264334461	-4.91976604844711	-0.94698920068798
H	-0.91023616485135	-3.89331819858806	-0.98588141871506
H	1.18628746011456	-4.36568876222839	-0.60844153941523
H	3.26396834122038	-3.11521915155923	2.94089289793830
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C	3.66628190995255	-4.61162475769393	0.71618259128590
C	-2.13755375512807	4.55110546073001	1.16280395798430
C	-2.92441582691896	4.15299316194503	2.43771981048594
C	-0.68465466512299	4.01783751696667	1.23764346642921
C	-2.06598773021392	6.09181211361646	1.12771010458129
H	-3.95418207598760	4.55433815013570	2.39499268043258
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H	-0.10740876547969	4.36647480402567	0.36182856154596
H	-0.18531060504071	4.39914792861622	2.14877140600689
H	-0.65036901361135	2.91977862517544	1.25082703268818
H	-1.56259631709348	6.45420330773116	2.04207974363552
H	-1.48605953932848	6.46199258746869	0.26260937990988
H	-3.07015911522125	6.55323247589950	1.09467891529534
C	1.35177855324587	-1.48447309436264	4.04270009189973
C	1.36922956846687	0.04880003982895	3.82464955698370
C	0.09608993324756	-1.88740224859943	4.85883142501252
C	2.59469712524188	-1.84623562293385	4.88129053972095
H	2.33375778345662	0.36106759133451	3.38924149451746
H	0.55792525786050	0.36743636342319	3.15611393325612
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C	3.14560811188023	0.07956100792054	0.49293899053793
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H	2.48793074562960	-6.00299594686879	4.50125615092799
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N	-3.26315825933851	-0.20229816017984	-1.18524618299911
C	1.19067723399987	-1.44489051988896	3.11411658157258
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C	-0.58821045984647	-0.22115315221292	-1.46991379886217
O	-1.52549738802888	-0.33539547334490	-2.25156157956619
O	0.67877004434681	-0.16913963367955	-2.07153583487763
C	1.88203342017402	-0.17535914556812	-1.28828779023401
C	1.92173741191542	1.05953939276888	-0.38486305862493
C	2.08910065760702	-1.50407121535789	-0.56391102637210
H	2.66930560660833	-0.05670788180457	-2.05671128243775
H	1.54744105034404	1.95224814649025	-0.90393236520793
H	1.40553853340992	0.92980611814631	0.57107337751279
I	3.99979819296471	1.61388306119352	0.17786050234848
H	1.30316702745640	-1.66057602350686	0.18874227449221
H	2.04369126432200	-2.33501628419618	-1.28841159827649
H	3.07415264382401	-1.52511360285497	-0.06496613214375
Cl	-4.13468792937268	0.31675724126402	2.89077605930914
C	-0.16214696442937	-6.43925177216514	-2.24222392604065
C	0.51161670145321	-7.42168426112743	-0.04143835620549
C	2.02616083942091	-5.78127524947069	-1.22579191669052
H	-0.53226385646079	-7.70155884012790	0.18878680536287
H	1.03963617379514	-7.27907891914248	0.91738195244412
H	0.99090330676713	-8.26994017589612	-0.56687238130952
H	2.07734293561842	-4.87084943192074	-1.84871647578661
H	2.52582402768137	-6.60523373280893	-1.77049613976279
H	2.60253384954403	-5.58668492689551	-0.30476526194151
H	-1.21834285164795	-6.72073005628839	-2.08241214613902
H	0.33560854265470	-7.28044143879836	-2.75856498599779
H	-0.13798887086362	-5.56759187782034	-2.91954900734088
C	0.53180016309355	5.32438127956324	-3.56037566466756
C	2.58894929152748	4.74782032117310	-2.25984765928563
C	1.22814908023099	6.79187415844377	-1.65648720942140
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H	3.09371530616063	4.71540449332089	-1.27948379569560
H	3.20999399560324	5.35703812582961	-2.94443394946405
H	0.21419117351362	7.22149699329293	-1.56372433146798
H	1.80727131675147	7.41747075569765	-2.36235579855794
H	1.71541298338418	6.86450770996429	-0.66885711416107
H	0.47793650489023	4.30362712044647	-3.97775869406474
H	1.14577804296814	5.93553248143223	-4.24700660116817
H	-0.48871766823044	5.74779756161778	-3.55444107415703

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N	-3.40617107577802	-1.33681120843362	-0.27314719404979
C	-1.07793297613242	-2.61479113365350	1.31619820041339
O	-1.59776406111477	2.00330528490399	1.69425695516389
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C	0.46460231750805	-4.50209760879639	1.14700534398343
C	-0.07822254048896	-4.93826839947373	-0.09222165731079
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C	-1.68210530882166	-3.07204842553931	0.07818168360147
C	-2.78057317461131	-2.43545587037233	-0.60144115522093
C	-4.39717217899580	-0.75847474076263	-1.07429747881409

C	-5.40847440666475	-1.49218873641838	-1.71899731465794
C	-6.36396026198789	-0.84390189968399	-2.51415642718707
C	-6.32434260027002	0.55148333849639	-2.66470545721092
C	-5.33160414067665	1.30077333640269	-2.01799214670713
C	-4.35970627839389	0.66648653309538	-1.22335509306893
C	-2.63930583572899	2.30746336105867	-1.08177922046355
C	-1.51454147172117	2.99596281412158	-0.50995601395321
C	-0.79472404787259	3.84141121009234	-1.40657372509218
C	0.35232804125686	4.51911686630374	-1.02334999719221
C	0.74397093407888	4.39967575570927	0.33961401750473
C	0.08314108168931	3.62254202077322	1.28791269395102
C	-1.04505361131504	2.82925541617736	0.85240578342814
H	-1.16772772161662	3.90621296198738	-2.43380660260345
H	1.63776004148431	4.94084919292479	0.65495481242184
H	-2.87737005897151	2.58585083864765	-2.12564732569883
H	-5.31255501211064	2.39279230874983	-2.10588228680008
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H	-7.15200169601327	-1.42929330488331	-3.00292812499255
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H	-3.08181617281361	-2.92318329666297	-1.54703295574605
H	-1.62251971750328	-4.49576091276957	-1.53653463154092
H	1.30340708641547	-5.07032158192085	1.55535448875303
C	1.21002643917833	5.36145116992646	-1.98337488105316
C	0.55293925509513	-6.14204474719263	-0.81300655954033
C	0.52594354907581	3.60196119886341	2.76804983449805
C	-0.65083090471269	4.10987722465366	3.63966383351160
C	0.93625414887321	2.17823630535157	3.21723574407727
C	1.73761481102503	4.52427468474816	3.01225762610214
H	-0.93666176429759	5.13790223105463	3.34796777356799
H	-1.53148975302581	3.45741237382276	3.53657187931076
H	-0.35141954454687	4.12722418643589	4.70480788253457
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H	1.22268258075335	2.19342275826710	4.28576699276801
H	0.10728093800903	1.46917060829163	3.09336398129343
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H	2.62106276149081	4.19142747592958	2.43937193410871
H	1.51808817023799	5.57637273344549	2.75202704938778
C	0.67253803282309	-2.98412895766436	3.19861583573687
C	1.29126361643157	-1.56959600456649	3.08108732171088
C	-0.39048160113173	-3.00647386376009	4.32605367234005
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H	2.06692538217899	-1.54040718607134	2.29624868789633
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H	1.76763579305424	-1.27978480755453	4.03558379065538
H	-0.81502014403195	-4.02163243454690	4.43698428436514
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H	-1.21046299042753	-2.30530979151457	4.11254508310336
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O	0.62709840179092	-0.30150930491339	-2.30473321597575
C	1.71703350748017	-0.28437302957557	-1.35249780488558
C	1.32172743496276	0.59775251025184	-0.18332327744764
C	2.08729296158804	-1.70357202980498	-0.93682177707217
H	2.54874829458485	0.18683918702234	-1.89848268462297
H	1.06948431394664	1.64315606524549	-0.35836040120002
H	1.31380671777959	0.23067627371345	0.83897595364719
I	3.86668193142824	1.53408599188412	0.43350969169349
H	1.26770298006020	-2.17106088931278	-0.36773100842578
H	2.29209468831811	-2.31799126251722	-1.82985626090549
H	2.99041087826950	-1.67784477965213	-0.30341227487636
Cl	-4.28563405344679	0.23281545803001	2.86204953738168
C	-0.16511513193784	-6.46464812705436	-2.13681403160527
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H	2.10835703320240	-4.92939075046189	-1.77651608811597
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H	2.61208455069766	-5.61685401395679	-0.21316033441437
H	-1.22750629813466	-6.71883023498918	-1.97204250820349
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C	1.30148170997905	6.81437294963585	-1.45777416490032
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H	1.76009454429774	6.85589092927323	-0.45482397663494
H	2.58681598867842	3.71274953032522	-2.44477310646934
H	3.11342319581052	4.69503296704495	-1.07160713824901
H	3.27458149241059	5.34447295388037	-2.73174212891526
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H	1.26314284985619	6.00530918610141	-4.06514489955973
H	-0.39196396719485	5.84650241247375	-3.41636705178072
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H	1.00801130991461	-7.23099500991290	1.05274279453861
H	0.93744630095800	-8.26635452820766	-0.39929390147856

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O	1.45930157417124	-1.16909856607995	-1.39679859136268
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O	-1.63721812311633	-0.71871138418422	-0.85096166317047
N	-0.97917074905291	2.14696819944798	-1.05504870951137
C	3.52705002196722	-2.25026324269981	-0.99959936269001
C	4.88878200129404	-2.11838886947417	-0.73321578901925
C	5.58172387628490	-0.88126351719100	-0.62941791477413
C	4.83140539398035	0.26450880335843	-0.83023330823083
C	3.43404236936799	0.22573995695339	-1.12842622560437
C	2.82801690969801	1.51310425198526	-1.31499144698477
C	1.10421516910321	3.09664861870791	-1.79751286777642

C	1.86495323922156	4.19395736606925	-2.24144686374805
C	1.28320898715311	5.46384350443026	-2.34196657197651
C	-0.07078753147491	5.65038742225406	-2.01671310282309
C	-0.84766572272558	4.56572195324349	-1.59105125775252
C	-0.27475204408826	3.28736067137503	-1.47063796530925
C	-1.87421600960726	2.17709753822642	-0.10163538348555
C	-2.59805085531500	1.07540097921198	0.46979993187374
C	-3.44748039247570	1.41848118520756	1.56524293275795
C	-4.20226512228877	0.47469818567457	2.24201286609400
C	-4.14452532834304	-0.85884981992428	1.74908388380483
C	-3.34356966004068	-1.28151373393174	0.68903715786427
C	-2.48260297245732	-0.30721003644288	0.05207316454807
H	-3.46459606714872	2.46937059262200	1.86900590322870
H	-4.77052806049161	-1.60283840501561	2.24608219112110
H	-2.07019611002865	3.15639333473955	0.37112461289608
H	-1.91239788169479	4.69906681426189	-1.37163809293996
H	-0.52931484318269	6.64059882073659	-2.11681986234679
H	1.88447413217656	6.30860709291327	-2.69669209881634
H	2.91032569261793	4.04262257473076	-2.53054270546540
H	3.49470105081516	2.37089964225550	-1.11035275008383
H	5.29797041584469	1.25305517153195	-0.77371391946913
H	5.47128331944192	-3.03100624346406	-0.59121698848488
C	-5.07057397940742	0.79356865923489	3.47125179393317
C	7.08797657397435	-0.87828710149935	-0.31320962170576
C	-3.37762735170923	-2.74271539944980	0.18870036224148
C	-3.79335247981377	-2.76151218086662	-1.30456867138597
C	-1.99210570698673	-3.41266731559261	0.35555689725186
C	-4.40100090123463	-3.59164025463214	0.97045166075808
H	-4.79543156203648	-2.31380158554644	-1.43201395674225
H	-3.07927215249808	-2.20414962414648	-1.92871662123288
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H	-1.67465189817264	-3.40035922698997	1.41499873436703
H	-2.03920351240887	-4.46906380508692	0.03425041318398
H	-1.22982187342559	-2.90627497857044	-0.25134771156937
H	-4.41040359809536	-4.61755289218172	0.56304039245083
H	-4.14810078089654	-3.66543950005047	2.04378565005609
H	-5.42622260920916	-3.19031448171003	0.88213628820801
C	2.86476756463361	-3.64300154881520	-1.09237721007547
C	1.79104407070301	-3.78331398185793	0.01375450510693
C	2.22124955386349	-3.83295037248974	-2.48927611723772
C	3.88610752616932	-4.78204804722974	-0.89517522816014
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H	1.01252923727308	-3.01826952590021	-0.10048568674723
H	1.31096302797627	-4.77762181954543	-0.03989195488061
H	2.98811986879377	-3.75223610007909	-3.28066100505478
H	1.76334355558399	-4.83690423706158	-2.55965082234664
H	1.44252928030511	-3.08163386544175	-2.68404638000830
H	3.36717339665740	-5.75333078305087	-0.97427420536162
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H	4.36648381322564	-4.74466049482226	0.09913722139101
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C	0.35613088200552	-0.77510342833765	1.86491663760455
O	0.71258845727358	2.64121268375711	1.62733124456761
O	-0.17487786172956	1.13552780366441	3.08083768878717
H	-0.14948420804916	-1.47735835900397	1.19131338333999
H	1.30226951839538	-1.21919870391030	2.22653362496830
C	-0.53818340788004	-0.27204005507334	3.00798952675624
C	-0.33158997510575	-0.94908560716311	4.34569814325674
H	-1.60137018530830	-0.30602043753333	2.71283097986991
H	0.72130257202768	-0.87348493309703	4.66928538203859
H	-0.97516966216289	-0.49452786922292	5.11724181602264
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Cl	-0.56748080749055	0.02265524310544	-4.18510072433885
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C	7.32515861235321	-1.57291631561078	1.04943906719024
H	7.68796153123083	-1.16741921697237	-2.40640295093025
H	7.50595312836310	-2.69382120284910	-1.50104168345948
H	8.93075203316908	-1.66006865690786	-1.21422584439464
H	6.79197897367544	-1.04085662563695	1.85752480683668
H	8.40293293505282	-1.58586010253981	1.29578578592115
H	6.97091046741869	-2.61835440210547	1.04240581831834
H	7.54259211932814	1.08818811135745	-1.19282649085593
H	8.73742345927715	0.51167521106147	-0.00315090985268
H	7.16733033134772	1.14276045140966	0.55687908681534
C	-5.00957063129080	2.28498563344935	3.84953164448913
C	-4.56114516985146	-0.03528550917422	4.67568327272174
C	-6.54364070140057	0.42417483017034	3.17451838851920
H	-6.92474960723406	0.99943164977018	2.31213411166108
H	-7.18174095384936	0.64769737771486	4.04911214487573
H	-6.66004918099975	-0.64864590510113	2.94218835184367
H	-3.51435031668151	0.22710671945653	4.91333705240960
H	-4.60080039484482	-1.12001925112735	4.47362246719166
H	-5.17681116442153	0.16165126750789	5.57249749807946
H	-3.98025231561320	2.60277881741133	4.09312757581974
H	-5.63708315664025	2.47269818045450	4.73849928533378
H	-5.38669781552275	2.92706176349242	3.03390105756725

[InBr(Salphen)] (4 x ^tBu) Pathway (β Pathway structures included under the “[InCl(Salphen)] (4 x ^tBu) Pathway” heading)

[InBr(Salphen)] (4 x ^tBu)

H	3.50976521851523	-6.06072721026710	4.99000849361096
H	1.90327534765700	-5.29778010099718	5.05321896862142
C	2.93275310683459	-5.23951733628619	5.44987199913090
H	4.18657214969963	-4.59600697585075	3.12285455992186
H	2.89741082527176	-5.42791453406727	6.53803704650793
H	2.60550862082736	-3.75988517006640	3.16789362325406
H	9.36390250547854	-3.85363184427234	0.80363468579287
C	3.63374182856309	-3.75110664032878	3.57323889081958
C	3.60956092906566	-3.89402731014151	5.11623583607444
H	1.31266867809336	-3.90761967795426	6.58911635040538

C	9.31219086070258	-2.77247233310428	0.58625642508447
H	9.06622128629235	-3.43945049673925	3.19566439460526
H	5.57887529508063	-4.83564775514558	5.25885717213406
C	6.98670034870173	-2.75301496257111	1.49062246911036
H	8.94154318583263	-2.66070015688778	-0.44855612474736
C	5.05598788818564	-3.95263000357448	5.66999549801785
H	4.12344797572493	-2.81598681404765	3.26655767591067
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H	10.34269767232771	-2.37663985512293	0.63127107380321
C	2.84651786921328	-2.69950633938700	5.73084889989014
C	8.97418954420147	-2.35157373292724	3.02135488137714
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H	5.04772880185998	-4.04327942026148	6.77125918577487
C	-0.40469765359233	-2.09543055125942	7.81711840187341
C	0.89418212505297	-1.83960322165571	7.02653390945440
H	9.98172291506408	-1.90596934890924	3.10808207723855
H	8.33906214094022	-1.92924208469469	3.81339202236342
H	5.63143541743308	-3.05632213642047	5.39942669507044
C	3.33870827223232	-1.35522498984596	5.55895005838204
H	9.57463660274997	-0.58377908645879	-0.32380501864463
C	8.27267596796119	-0.57090871905057	1.36408030441681
O	4.42415836905333	-1.16432612085471	4.85832367099504
C	1.36292495628287	-0.54781747440691	6.83840626173699
C	8.95920236273054	0.04712740861033	0.31681347512978
O	6.77014085585015	-0.32531486690107	3.17291836783712
C	2.56991435087818	-0.26484018820541	6.13327784850632
C	7.45526697581555	0.24904679425458	2.22468173264718
H	0.80678942319443	0.30476534306809	7.24747351140014
ln	5.80353298490054	0.43563397810576	4.88965424459941
C	8.91253236769584	1.43753747874859	0.02724593488070
C	2.89660550115149	1.12478596968770	6.00402848230502
C	9.68924183132212	2.07347327496330	-1.14320433097416
C	7.40623771757730	1.67794919892701	1.96729364134976
Br	7.36112091350010	0.37171360500737	6.88041731832793
N	3.99022938896791	1.65567644627966	5.50586275940101
C	8.13083448357399	2.21983778371920	0.86342384024615
H	2.10729286282708	1.81278727134587	6.35830456294952
N	5.95665908700351	2.42846624962049	3.82803111672848
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C	4.22792098029543	3.03440585147866	5.40943038333655
H	8.05872040213826	3.30170609152808	0.69665078030256
C	5.27226344923533	3.44495399191585	4.51291442341452
H	6.64980721706156	3.64876281598690	2.30736871630392
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C	5.58100676152828	4.81698379641785	4.40275584211611
C	3.84585520873346	5.37131946832029	6.00928325349129
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H	5.12962148447394	6.83301443696443	5.03852732572098
H	6.56071637945103	-2.58052538772586	0.48535256411042

H	6.28846240539333	-2.35522556798579	2.23985197557267
H	7.07268632472272	-3.84507312504445	1.64089960840448
C	-0.75184225483785	-3.59468427730592	7.89747964329081
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C	-0.23775095703664	-1.55793031212267	9.25868957346762
H	-0.90854526603471	-4.03420269076994	6.89652610415593
H	-1.68604783618808	-3.73052849035937	8.47044774950023
H	0.03850161723737	-4.17239690882784	8.40839108143029
H	0.60107236038663	-2.06286232469057	9.77010671807184
H	-1.15709209953009	-1.73138271397688	9.84814330982961
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H	-1.71150624500709	-1.72766624465464	6.08968246416568
H	-1.40938116990284	-0.27303564314815	7.07746674873975
H	-2.52223779839267	-1.53277914022532	7.67444719294421
C	10.45835326691517	1.02463986902191	-1.96978991583244
C	10.70924201198397	3.09333290268239	-0.58205643390514
C	8.69782499064437	2.79849286325016	-2.08442805704599
H	11.21299838004844	0.49462881195330	-1.36236535811468
H	10.99052551063096	1.52166267356460	-2.80002505841274
H	9.78032432503177	0.27272710932476	-2.41084582447611
H	11.42570272862357	2.59760417219601	0.09696258528471
H	10.20954239104555	3.89766689548045	-0.01434951470583
H	11.28056895377753	3.56504420984656	-1.40294005479946
H	7.95560735171616	2.08995781713522	-2.49357155364835
H	9.23545324637320	3.26318291576513	-2.93158041194272
H	8.14631434229431	3.59818056769129	-1.56004386348297

[InBr₂(Salphen)] (4 x 'Bu)

H	3.15079671475338	-6.19095263990707	5.77465219569215
H	1.72654282257780	-5.33627286630560	5.12877965543130
C	2.51923621917861	-5.29252376124627	5.89782929402430
H	4.62957832029101	-4.99155468527580	4.22058374743945
H	2.04039091449619	-5.35619194097086	6.89243391134922
H	3.25790303902369	-4.04232419562111	3.56275296810103
H	9.77483719136258	-3.52096119842445	0.33950884420314
C	4.03739539701318	-4.06474943216972	4.34533526603202
C	3.39474091087807	-4.03044105166657	5.75523638233296
H	0.72061008506432	-3.74562282792639	6.22343540133062
C	9.55333328377869	-2.45776437161408	0.13520411011706
H	9.94964261002164	-3.07663445566334	2.74121527816731
H	5.08213776500974	-5.03122585432181	6.73212842989903
C	7.48827421635827	-2.67037314023100	1.51632850813921
H	8.95771369320907	-2.41605560780078	-0.79497143516765
C	4.49524647851409	-4.09933873486365	6.84458679847314
H	4.69626051314425	-3.20092537530675	4.18252120168085
C	1.19814557713241	-2.76832271597279	6.14687723855931
H	10.51667763138776	-1.94670117283326	-0.04763355245906
C	2.57213922457970	-2.73465425044298	5.91718004380558
C	9.69781206598285	-2.00998348458738	2.58530182681357
C	8.79418682237538	-1.85543710015864	1.33555088906632
H	4.04012166642328	-4.10169908547142	7.85284493622255
C	-1.14514454169183	-1.69371947615018	6.53067194607674

C	0.37514663620436	-1.61603001458329	6.27920403300346
H	10.64310986260958	-1.45200508135716	2.44838533722178
H	9.19541153200687	-1.62971720757617	3.48652910248812
H	5.17748921872816	-3.24018017269827	6.77115499484855
C	3.23600788851850	-1.44726961645723	5.80649273209790
H	9.34075293134477	-0.27437915652348	-0.82030125223278
C	8.44959742489495	-0.36762992997855	1.11345339881048
O	4.51006554412350	-1.40055342807279	5.63630366677862
C	1.00891276219781	-0.38650888687977	6.16319029217615
C	8.79939863922236	0.29289256081958	-0.06255485245428
O	7.43444117910897	-0.22336098963445	3.24951679740906
C	2.40619849995483	-0.25430786136691	5.92578120355932
C	7.72488153925579	0.36016105339649	2.14064417643077
H	0.42793549561196	0.54156393160409	6.25002001511925
ln	5.69980874119908	0.13116575336809	4.57433351661971
C	8.49031089939836	1.65188668933059	-0.34578241953740
C	2.89200545554394	1.09314625914897	5.84176793210485
C	8.89319340140263	2.34786356548834	-1.66238882702116
C	7.38544860659548	1.75049298692488	1.86182240179936
Br	7.34897179549221	0.15390923162305	6.60826987046824
N	4.09878122750189	1.51032300849739	5.54903343175883
C	7.78729813077353	2.34299814013718	0.63149194845945
H	2.11855635997242	1.86562358148086	6.02646200186537
N	6.11330054441261	2.32112429807149	3.90557021965462
C	6.67218936639651	2.61483947786621	2.75780765394733
C	4.46811076599346	2.85302086727634	5.59802725930702
H	7.51252237317933	3.39430256704597	0.47117165706734
C	5.53088151865893	3.28075117926381	4.73116514701244
H	6.57034617166800	3.65770705832945	2.39571866679157
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C	5.96508733709583	4.62288109198067	4.79423488012540
C	4.31940958678180	5.12115310176416	6.50865075344074
H	6.81348182997021	4.93496696684416	4.17577071805398
C	5.35881608140266	5.53955433019103	5.66082329026367
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H	5.72095330116968	6.57425173663772	5.69882473318036
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H	6.90380219160389	-2.31133905338486	2.37444151591991
H	7.72718048488783	-3.73985897791579	1.67222360858524
Br	4.16797143062731	-0.36704265306070	2.45304969475318
C	9.66471298416973	1.40265520707637	-2.60266631057976
C	9.80000459533124	3.56003548206602	-1.34537377191013
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H	6.96364662346593	1.97355950895184	-2.63534136194818
H	7.88088697474620	3.34345496485694	-3.34353474618224
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H	9.93634219527756	1.93437526327120	-3.53317852342973
H	9.05829055487556	0.52340388767266	-2.88303797111723
H	10.71707252828368	3.23193676237760	-0.82383330989019
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H	-2.57097229821944	-1.01029988842562	8.06132911855538
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Br	0.47080092800847	0.11102142422121	-4.49707964982978
C	-7.27881717971258	-1.70164699777216	1.12944730752306
C	-7.18986083693952	0.71928383383175	0.50039311607669
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H	-7.48537580402882	0.49654513311025	-0.54035192672031
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H	-8.10785845971432	0.89979827116870	1.08981452480346
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H	7.80642404218349	-3.46008122707188	-0.51921553716682

TS1

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C	-2.05747445107476	-0.00823456101898	3.53639443217612
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C	-2.70595289001207	2.26245927050349	4.33984316920341
C	-1.97456135851651	2.82225366939314	3.30639024438403
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C	-0.56393651732557	2.77357158667331	1.34375062195254
C	0.78130310467363	3.09732085399268	-0.60616409775070
C	0.16717529285712	4.27335477937154	-1.09030677168215
C	0.72173270006322	4.99622279623733	-2.15156497276612
C	1.89380802769198	4.53753810987290	-2.77680823492121
C	2.50423100874319	3.35859971884822	-2.33648135165436
C	1.98177419777565	2.62842049212380	-1.24612669347541
C	3.78614364781785	1.08863623232668	-0.95133746973668
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C	5.86802585208769	-2.48333930436259	-0.11419625492998
C	4.48851094969864	-2.55219790443125	0.05138398658445
C	3.70277853518106	-1.36348848796530	-0.21706120188544
H	6.45314267709279	-3.38253567323107	0.09248659341833
H	4.47711832438222	1.85759096433287	-1.34820070398686
H	3.38163649141686	2.97090614739221	-2.86457881636103
H	2.31340536629895	5.08065603321010	-3.63190818453021
H	0.21974106174055	5.90111363261780	-2.51423948598068
H	-0.77830587848835	4.60186473449459	-0.64626134521758
H	-0.73859027882185	3.86662294561742	1.37961114422280
H	-1.91775640687632	3.90946712367451	3.18692789012855
H	-3.28178968908085	0.38970731627095	5.23987900726404
C	8.11189608221814	-1.38795175735006	-0.67593835399222
C	-3.48166925904846	3.08357288545096	5.38503490031364
C	3.79427986411671	-3.85177946541078	0.50938524292149
C	3.01926563806426	-3.59895493433507	1.82753986485820
C	2.83401165591775	-4.34833572091007	-0.59998693466344
C	4.81175631209957	-4.97910487027531	0.78184478278343
H	3.70043413277673	-3.24077770906978	2.62042389730131
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H	5.52639616114311	-4.71181989673294	1.58214926971164
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H	-3.76117017531593	-1.83261184663719	2.30065382747696
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H	-2.76814297684534	-3.29570073154543	2.57656687853795
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C	-0.24932978717100	-1.73648453379186	-2.00474473624505
C	0.14320229880973	0.15767848210476	-3.72412821594195
H	1.64704353012722	-0.78819566524002	-2.42743047239621
H	0.20087618503551	-2.49810097069237	-1.36832951858899
H	-1.30104730472319	-1.82494517693519	-2.28176583385167
I	0.15924755039521	-3.82703209595772	-4.15623998571357
H	-0.94993774916771	0.31050251200801	-3.73121593948394
H	0.42618444821280	-0.40462189678810	-4.63130972960101
H	0.64026546295176	1.14498761860263	-3.72685919295372
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C	4.40957968534605	-0.16307153625199	-0.63782328905891
C	5.83050600920635	-0.18931977387083	-0.78901683696741
H	6.31119284592983	0.73952310417743	-1.11386129248352
C	8.70756162426281	-0.04489637587910	-1.13806763157276
C	8.48579821675071	-2.46939369427752	-1.71828261572489
C	8.74013620161707	-1.75055474863592	0.69169157423218
H	8.48529914380985	-0.99013579642010	1.45140530008023
H	9.84250016493616	-1.80798419632069	0.61237539447313
H	8.37874148119059	-2.72604862272362	1.06047258071748
H	8.31306618497179	0.25722394451067	-2.12458183315662
H	9.80579475302741	-0.12989968063313	-1.22813551723161
H	8.49168415067274	0.76446486075745	-0.41811210133599
C	-3.36105189308945	4.59883051785503	5.13721556921317
C	-2.92312888862852	2.77744137103014	6.79601758837218
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H	-5.13506551180205	1.62904136070097	5.54146094643331
H	-1.85286366485892	3.04388474738010	6.85701647035129
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H	-2.31096948054250	4.93700808266154	5.18869285113776
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H	8.11415090595067	-3.46570212873513	-1.42264481034862
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Int1α

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O	2.42732012322093	-1.50470491258360	-0.20669734364373
N	2.48071541939357	1.36071731727650	-0.82280620109163
C	-2.10838000312570	0.06201194123678	3.58157191251506
C	-2.65003929504997	0.93152873144198	4.52098591705087
C	-2.52102530829685	2.35073042251152	4.48084463121825
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C	-0.49489167025669	2.77343499451880	1.38943935269851
C	0.75945632035756	3.05052028731298	-0.61387183935300
C	0.15500233423838	4.23551184370913	-1.08841534063264
C	0.70376727290872	4.95010006303357	-2.15957478351669
C	1.85925093742917	4.47412903139318	-2.80204307510471
C	2.46028487753250	3.28681221367841	-2.36827600589283
C	1.94351182127336	2.56562578215351	-1.26962557622882
C	3.74991645717190	1.05518114287414	-0.93940920833322
C	6.60399957715540	-1.27512379963638	-0.45314649041752
C	5.91617227371067	-2.45460952755343	-0.04493970147458
C	4.53564773058752	-2.56605617219124	0.07385674333911
C	3.71137982577852	-1.40983336026536	-0.24619268784869
H	6.52509978307099	-3.32996649505681	0.19489445446849
H	4.43463580051752	1.85238110548051	-1.29232647046573
H	3.32457149709106	2.88373793479126	-2.90689092128584
H	2.27291431070135	5.00991953033164	-3.66504219487471
H	0.20872241161596	5.86162871881082	-2.51617600728595
H	-0.77925573598785	4.57443381615461	-0.62805011262344
H	-0.57586138379738	3.87722761892356	1.45788384771503
H	-1.65359756385464	3.96273661103977	3.33375958270337
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C	8.14008504929673	-1.29275961414525	-0.55167547845618
C	-3.17141571731622	3.19925313122531	5.58860326690784
C	3.87365957574029	-3.87757084479422	0.54659237836580
C	3.05395591296043	-3.61588848204252	1.83494924368065
C	2.95469073504954	-4.43274746565892	-0.56878564376482
C	4.91692434853956	-4.96606687202421	0.87351037594348
H	3.70518687875740	-3.23206615900075	2.64026631455544
H	2.26552542539217	-2.87039160911415	1.66570779696180
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H	3.53181960500870	-4.63923785653598	-1.48803329449817
H	2.47908488860978	-5.37603020486934	-0.23936996263999
H	2.16643964874075	-3.71000172466301	-0.81730641348747
H	4.39589562394988	-5.87956991045712	1.21258172987434

H	5.52386999528112	-5.23942505642198	-0.00907124650045
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C	-2.26838974490278	-1.46758642473556	3.70677414154110
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C	-3.08836692874561	-1.86272618511871	4.95213217421565
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H	-0.34606723632882	-1.75026036611288	4.73214301909817
H	-0.98028698139467	-3.22577957459027	3.93516064211005
H	-0.24196005447349	-1.91241258301612	2.96500046049120
H	-3.17527326176862	-2.96336765158019	4.99803677595378
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H	-4.11326662523241	-1.44886378002919	4.92359367906769
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C	0.44068678313728	-0.68762908681529	-2.50743806710295
C	0.19641535320946	-2.19089911898322	-2.65747006834856
C	-0.15561366056685	0.15904333762636	-3.63779668285887
H	1.54237294159538	-0.52693378881295	-2.49273854994573
H	0.62337149785863	-2.73807292740118	-1.80724326117547
H	-0.86959921094714	-2.43299840470126	-2.79198237614907
I	1.21716538014870	-3.14356071175987	-4.42668871822187
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H	0.27763291172015	-0.10145317970749	-4.62064621083808
H	0.03869750220214	1.22664009645414	-3.43234645405823
Br	2.30557589781911	0.27967404084711	2.67921950474935
C	4.40015255493617	-0.18450270378438	-0.62916187032857
C	5.82398364876643	-0.16609678519959	-0.73192750107788
H	6.28506138122315	0.77931225299652	-1.03822975208626
C	8.70577040628590	0.06492472807586	-1.00841571374773
C	8.57836915291935	-2.36831833928003	-1.57464379437007
C	8.74327271117021	-1.62560069788424	0.83439352295046
H	8.16192258592865	-2.14712027164739	-2.57375131116836
H	8.22826397764438	-3.37348812720042	-1.28211601950418
H	9.68166454841600	-2.40576031496606	-1.65759143628068
H	8.44400633989550	-0.86790985981199	1.58043823542872
H	9.84900521776724	-1.64998918009434	0.78589952450744
H	8.40094276373494	-2.60877849878302	1.20121676879154
H	8.32595259473295	0.34786602443132	-2.00631118374750
H	9.80838789875829	0.01468582383364	-1.07006983368990
H	8.44532792059539	0.87156333134870	-0.30038272897030
C	-2.92724242164156	4.70583063060497	5.38184155405496
C	-2.57896323318935	2.79858510068237	6.96118895747161
C	-4.69946175087244	2.95381818411686	5.59796436386279
H	-5.14479712899430	3.23879502749756	4.62779616183196
H	-5.18883072848334	3.54814848149323	6.39354500189558
H	-4.93897656516483	1.89106003785175	5.77630422184075
H	-1.84951391568162	4.94672234803879	5.39108187316753
H	-3.40802733511211	5.28267314244539	6.19313387120789
H	-3.34914689616976	5.05791856354155	4.42362476103629

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H	-2.75424588774237	1.73180785297685	7.18400065711717
H	-3.03679028544162	3.39285345777029	7.77534821600969

Int2a

In	-2.23150168485857	-0.36036336420231	0.77905869413932
O	-0.72759583563458	-1.23496160282015	2.09266909636026
N	-2.15155092871811	-2.47077522595388	-0.14960618971649
C	0.19184477573808	-2.09116570751199	1.80310767896985
O	-2.57773000703476	1.78149156693798	0.72014402565605
N	-3.68486725659546	-0.39548502093845	-1.00757931745685
C	1.33494754820260	-2.23221954865186	2.69129317917461
C	2.38634514253599	-3.05139007011759	2.29137487530423
C	2.40857313880380	-3.80647686159560	1.08285146252873
C	1.26289721987644	-3.76881401784146	0.30501128454169
C	0.13412331659448	-2.96355685805772	0.64165747903569
C	-1.01814706791685	-3.12461494223323	-0.19977702464913
C	-3.24637700025031	-2.77366302561857	-0.95533555043148
C	-3.60385744457064	-4.09029178889342	-1.31392118492912
C	-4.73894836620224	-4.34134137150691	-2.09426591775989
C	-5.55347429558655	-3.27491096904095	-2.51021556743531
C	-5.22662763729962	-1.96152746160046	-2.15109771596746
C	-4.07052768736044	-1.68122461259809	-1.39256690811964
C	-3.95936245117122	0.67229820237160	-1.71376409796263
C	-3.67361693548532	2.04959389705409	-1.42353787182987
C	-4.10777634070706	2.97371713205173	-2.42315311488908
C	-3.93670722945871	4.34240622216108	-2.30388918321781
C	-3.29474228637072	4.80454265063659	-1.11891454548165
C	-2.83038306987413	3.98107947334063	-0.10006393374080
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H	-4.59609925591282	2.54870297625106	-3.30680616815682
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H	-4.46577153774236	0.51707275519247	-2.68683377709560
H	-5.88724701653611	-1.13662593363771	-2.43900858157766
H	-6.46206329017524	-3.46871620788273	-3.09320566565744
H	-5.00492747887797	-5.37349411456129	-2.35281165022744
H	-2.99521742096868	-4.92163081146708	-0.94146839557214
H	-0.91017678394743	-3.89948103378353	-0.98475160841269
H	1.18744422303968	-4.36618241770993	-0.60961422612142
H	3.26514304899974	-3.11252121420964	2.93786568025505
C	-4.39336499422886	5.36086170727906	-3.36241175418028
C	3.66783401844261	-4.60903849882539	0.71446450248067
C	-2.12748377344019	4.55698722107464	1.14750680941872
C	-2.89720989107617	4.14921855777697	2.42979573132207
C	-0.66900732417398	4.03686116662285	1.20496466133614
C	-2.06960430573174	6.09843254549845	1.11616618237586
H	-3.93099919793733	4.54101007341190	2.39849568265701
H	-2.94393033297660	3.05658361829670	2.54026873541665
H	-2.39737557085505	4.57513907898933	3.32053686903261
H	-0.10389417601304	4.39473789513191	0.32487627989121
H	-0.16389176534217	4.41909491471961	2.11251664126993
H	-0.62387440298664	2.93906066478728	1.21353158498071

H	-1.55982358436607	6.46228138865613	2.02638169150667
H	-1.50183751808312	6.47624956341302	0.24631600663862
H	-3.07798061995498	6.55124897792586	1.09512742393821
C	1.35140311665768	-1.48956397315182	4.04456540374163
C	1.36473587290746	0.04436245813864	3.83157683133443
C	0.09901108692120	-1.89882120347092	4.86220542692102
C	2.59703383278522	-1.85036054793498	4.87967610204777
H	2.32753470788698	0.36041175966874	3.39518130629468
H	0.55126265305863	0.36389764579283	3.16617440529887
H	1.25295413203376	0.55974833461755	4.80418985527172
H	0.08272119253849	-2.99318511535329	5.02145379827040
H	0.12182751600904	-1.40943222921823	5.85441555376350
H	-0.82892475108163	-1.60554792201525	4.34913351773207
H	2.55700387979550	-1.31306125776751	5.84445315502184
H	2.64755968601616	-2.93243985907706	5.10077784589338
H	3.53328432147111	-1.55205738730914	4.37464116634442
O	-0.73249948381936	-0.02160592772243	-0.81293419632154
C	0.51306250246392	0.26419908657977	-0.80472358221758
O	1.34041416638051	0.04499669190676	-1.68519726097165
O	0.88917229432926	0.90672991154232	0.39083321116523
C	2.25779040134020	1.31492280302598	0.55620473989688
H	2.26811678198441	1.70380809074247	1.58873266639168
C	3.16011569848041	0.07877306711372	0.50036399106238
C	2.66413880053922	2.43531674756164	-0.40072325573935
H	3.43383338548294	-0.21837479971362	-0.51822441881133
H	2.71938187064632	-0.76306047645790	1.05010914155064
I	5.09174922266631	0.41216202752502	1.54986774908884
H	1.96709975431528	3.28367923097758	-0.29755023032422
H	3.68310014025686	2.78622043589225	-0.15787036443171
H	2.63965456382675	2.07466181339617	-1.44046694227895
Br	-4.03847298342743	-0.69201435123296	2.63351495307746
C	3.49594408476106	-5.37729698374211	-0.60945127518122
C	3.98242222380572	-5.63263673522219	1.83201822399960
C	4.85908665890723	-3.63374263722639	0.55538191227990
H	4.66149119805260	-2.90676222246134	-0.25180271048678
H	5.78703232503228	-4.18425605946082	0.30808437531380
H	5.04391118907321	-3.05423600948440	1.47562623920439
H	3.14226264446074	-6.33868051065150	1.96230153313096
H	4.15808255270878	-5.13659628508808	2.80226687225538
H	4.89062314376671	-6.21481954065191	1.58462372995117
H	2.67280231572017	-6.11231994624633	-0.55233139107611
H	4.42292553729199	-5.93028662469157	-0.84755853027036
H	3.28807780548733	-4.69281977057108	-1.45055131264683
C	-5.06123152814099	4.68074728023591	-4.57222642424028
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H	-2.42574421769643	5.47943603419217	-4.32967035275662
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N	-2.18088944067241	-2.50403690214125	-0.12708552653929
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O	-2.71510365067500	1.66539435084328	0.86882916762043
N	-3.69787057895892	-0.43642140861746	-1.00973934304981
C	1.36488546741447	-1.98631169885508	2.63999887686910
C	2.44511703376389	-2.76465991862753	2.23103597147541
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C	1.26387161618882	-3.68719254241594	0.36954027482303
C	0.11225891040688	-2.91178433095536	0.70331327246739
C	-1.02912476756942	-3.12945411305471	-0.13757532365512
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C	-3.54423981175295	-4.11860073919228	-1.40896170345457
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C	-4.03882607248917	-1.71532279791019	-1.45782247743456
C	-3.90166425286729	0.65230901087455	-1.70747021262199
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C	-3.94510684657369	2.97430694463300	-2.36209502367836
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H	-4.35802386446438	2.58280620732859	-3.29795128215467
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H	-4.85744369295338	-5.38864995631759	-2.57055473574780
H	-2.94836735979532	-4.95251562738691	-1.02219736178203
H	-0.88547314545268	-3.91023782897040	-0.90985548512275
H	1.18026945576397	-4.34364840742170	-0.50248660529044
H	3.36313295351193	-2.71075983843574	2.81893881364814
C	-4.09114055134799	5.39080356696203	-3.25781049987684
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C	-2.30783030471032	4.42794339815571	1.43357188593440
C	-3.21757462338847	3.98932330529855	2.60980906955214
C	-0.86774066917359	3.89738760984775	1.64291205210897
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H	-4.24160275314960	4.38410477246714	2.47319509163637
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H	-0.20565986341434	4.25355915548054	0.83298699366002
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H	-0.83290912269332	2.80021581162601	1.64685151116435

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H	-1.57956896061621	6.36874802114652	0.66424095589260
H	-3.24107499654038	6.42923315328639	1.33217016787625
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C	0.24007967443664	-1.58586658599679	4.85955498659789
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H	0.29634015003463	-1.03834739844079	5.81929430591715
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H	2.45667377586694	1.74451301925852	1.33966979159685
C	2.95554131086657	0.15046343359947	-0.02575786508400
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H	3.60420260607740	2.83106536840148	-0.59417622173941
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C	-2.80377681272789	6.16577238083117	-3.63017747950009
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C	4.79657556073397	-3.34771907406394	0.25406232971738
H	4.44672904631513	-2.78204349614411	-0.62757880730030
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C	0.80941168011709	-2.62447699652304	3.08266583879685
C	1.58977061756639	-3.77754713849624	3.10524027195121
C	1.45205343839872	-4.86992319267080	2.20285999247450
C	0.46909826720105	-4.75510104733508	1.23567703539305
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C	-4.69604096992391	-2.85314615408599	-3.69010500681333
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C	-2.60522752984312	2.14886222488067	0.33037276206313
H	-3.59391293758081	2.99631956009950	-2.87212664772910
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H	-3.52851675973686	0.83550610435893	-2.77211190802607
H	-4.85999865607480	-0.71756409657911	-3.40105626119467
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H	0.31910372637643	-5.54825142501207	0.49630185755803
H	2.37143194839007	-3.85195814710340	3.86435298502289
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H	2.70916184268312	1.83606903640842	-1.23174043322908
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H	3.34170403099735	1.92528189811741	1.17152356597318
H	1.67561979238488	2.39964178586793	1.62117930497204
Br	-4.78832931117128	-1.25523962561514	2.31769363950088
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C	-2.05758603540703	6.55769978510903	-2.15332260228383
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H	-1.21657823640147	5.98261654953457	-2.58174929862050
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H	-2.18203346862185	7.48165376780453	-2.74766530580866
H	-2.90715313590326	4.81278716518286	-4.12668671961369
H	-3.83596778659260	6.33262181661448	-4.20728479161210
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H	-5.45518547434698	5.96814397119061	-1.56610608396248
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C	2.20816708380699	-6.71679300627847	3.73731469020929
C	3.85481703812140	-5.62147203980213	2.16226267216199
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H	2.77807659517689	-8.01565604657173	1.40420715726531
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H	4.00557127811739	-5.16657287520266	1.16698573831290
H	4.54629992336030	-6.47876690160631	2.26045148021456
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H	1.16633712551277	-7.05340956903018	3.88365003063317

H	2.44691262578851	-6.00076574178597	4.54279482125641
H	2.87511701360319	-7.59059998432946	3.85696620220673

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C	-0.05129816395349	-3.51602923887371	1.86451659690399
C	0.43081141031204	-4.57816947759639	1.10419682942291
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H	3.35627500000541	-5.75898348041809	-0.96771284175666
H	4.66947785452619	-4.77335602827485	-1.65649851253444
H	4.35624693686090	-4.75274859678739	0.10724284593321
ln	-0.04235007168632	0.24885611662664	-1.87770612455001
O	0.67617827291304	0.44724823608331	1.16024276145045
C	0.41911287661006	1.53213684056589	1.95239827519659
C	0.37941181254835	-0.75953487888154	1.88124786189842
O	0.69090660599257	2.66209492991596	1.65562706015604
O	-0.18456280082768	1.14022842613375	3.09984074585631
H	-0.11350301810812	-1.46403967762232	1.20052145822591
H	1.32772128147501	-1.19515072365026	2.24768633410342
C	-0.52859556871613	-0.27144558990216	3.02026811368034
C	-0.32184639041560	-0.95002916760042	4.35733337386458
H	-1.58946639610849	-0.31927178386218	2.71875743618664
H	0.72777750661902	-0.86148461058658	4.68821846441753
H	-0.97654680920764	-0.50650404583364	5.12595827205449
H	-0.57600971554420	-2.02154227354802	4.26747341905792
Br	-0.60506947837609	-0.00096870035408	-4.33025968435272
C	7.65969891585832	0.53559449120962	-0.23413931244884
C	7.84058239787026	-1.66305157140044	-1.41864570337919
C	7.32128733602332	-1.58424516947116	1.05434159328405
H	6.78999219205428	-1.04946196169124	1.86189248129549
H	8.39896641393861	-1.59997949465881	1.30103787233981
H	6.96416950089314	-2.62871814012382	1.04968709984247
H	7.68458044718506	-1.18577613796265	-2.40251788667780
H	7.49910500881836	-2.71002688638385	-1.49467162897192
H	8.92634115001097	-1.67943665172260	-1.21027545684729
H	7.54526480071710	1.07281034576891	-1.19239248518802
H	8.73868508823682	0.49531729787502	-0.00234162821621
H	7.17075603674171	1.13132221531071	0.55711217851369
C	-4.99580500095905	2.31378671138774	3.85138822089665
C	-4.54984343809789	-0.00230494807841	4.68820671991511
C	-6.53550350211794	0.45101971852302	3.19097423888448
H	-6.92093431288698	1.02536507294435	2.32983132765840
H	-7.16997087059819	0.67568290618419	4.06789613208505
H	-6.65355625961259	-0.62195650834460	2.96031325157607
H	-3.50111559193892	0.25687479852658	4.92032043416793
H	-4.59603460828901	-1.08807837818533	4.49328299997668
H	-5.16023148148609	0.20339858820991	5.58674515754199
H	-3.96539448369386	2.62850842269648	4.09429182362960
H	-5.62278055534135	2.50869954839811	4.73923680198584

H -5.36978884889850 2.95442182639473 3.03318218754524

[InI(Salphen)] (4 x ^tBu) Pathway (β Pathway structures included under the “[InI(Salphen)] (4 x ^tBu) Pathway” heading)

[InI(Salphen)] (4 x ^tBu)

H	3.55995756269109	-6.07906837280496	5.10119133861849
H	1.94056496234111	-5.34265880929552	5.14864600937048
C	2.97035985721263	-5.25478676836535	5.53909612800611
H	4.19912470753766	-4.66389819653262	3.19004702679103
H	2.94243795066142	-5.41185112014030	6.63242035581776
H	2.61035540824047	-3.84200260963853	3.21559965987288
H	9.28875805310209	-3.85519656196982	0.72582036790023
C	3.63979464394772	-3.81094744681649	3.61677942570720
C	3.62249661655731	-3.90823733062441	5.16321128474688
H	1.33732376565973	-3.91792951773291	6.65432075701391
C	9.26329690582895	-2.76946603837041	0.52739214275415
H	8.90397755551495	-3.48414350506497	3.10756342869566
H	5.61227820994085	-4.80511596523599	5.32114114984638
C	6.90310840973032	-2.72447522759757	1.33556734850976
H	8.93637703419795	-2.63248463345025	-0.51902062269970
C	5.07106707643220	-3.92492184698021	5.71424543532523
H	4.11901554999771	-2.88070234400007	3.28042713264065
C	1.67507115777339	-2.89479628569419	6.49210075299206
H	10.29733702811834	-2.39179298005221	0.62103861937823
C	2.84374158166524	-2.70971826469440	5.74897295796432
C	8.83319367878297	-2.39153120256263	2.95442455594047
C	8.30470843025927	-2.09221219329620	1.52833149325883
H	5.06714335973822	-3.99127210478768	6.81722586427837
C	-0.39059250679843	-2.10110526849373	7.86012038725669
C	0.89627393755972	-1.84613660963959	7.04973561356474
H	9.84158931394305	-1.96155091190197	3.09375033565344
H	8.17109609735745	-1.97913936754730	3.72918655644154
H	5.62756785283678	-3.02292436541429	5.42333558721968
C	3.31246421572991	-1.36307686804787	5.53604749645957
H	9.58623657510481	-0.57017402843119	-0.33824808337738
C	8.23011310801667	-0.56521159619358	1.30692632072003
O	4.37798703754630	-1.17037881337169	4.80635219793083
C	1.34833043522634	-0.55299024814846	6.83173923536886
C	8.96124645851241	0.05966095890287	0.29414260142851
O	6.66634073034144	-0.32363659626635	3.06645423373015
C	2.54267862692886	-0.27070648838367	6.10530220574660
C	7.40000712002828	0.25370727072092	2.15610461818817
H	0.78965741254535	0.30102119812166	7.23435594351690
In	5.76482506550159	0.42701970670687	4.82610990376551
C	8.94842178348446	1.45564597016210	0.02982690246856
C	2.86238659671439	1.11872541102126	5.96008172101377
C	9.77427640000485	2.09917216256557	-1.10228783920724
C	7.38812351207138	1.68802390112093	1.92711630857622
I	7.46285525125325	0.34154282215728	6.95804389764081
N	3.94941194685142	1.64948625965432	5.44703480578518
C	8.15510705335720	2.23688617359065	0.85630457545764

H	2.07639310090642	1.80673384032267	6.32154926807165
N	5.91503327295041	2.42940737256151	3.77134597479699
C	6.62719453249767	2.63531734965762	2.68519755913451
C	4.18838800389305	3.02829915597639	5.35671850608166
H	8.10804148742945	3.32287945292329	0.70849542165317
C	5.23327068258143	3.44295212205005	4.46261382558342
H	6.64987476618338	3.66362938628390	2.28065848809855
C	3.50187123730374	4.00600710188474	6.10741248441765
H	2.73277090925230	3.69829201786065	6.82270882807592
C	5.54476033265141	4.81534901209612	4.36212414463146
C	3.81124074939434	5.36213478707578	5.97266217909177
H	6.37088186519352	5.13724417318546	3.72033172072953
C	4.83476803432723	5.76763286631647	5.09857227650680
H	3.27028931101114	6.10446479525582	6.57028731218050
H	5.09762555607541	6.82787441305141	5.01132411052382
H	6.52743720200317	-2.53147248891321	0.31414243473791
H	6.17930498247198	-2.32118898005136	2.05724291500131
H	6.96112750688188	-3.81968245489384	1.47606614260078
C	-0.71454639516750	-3.60278604665716	7.98150593751804
C	-1.58156397595387	-1.40332546631578	7.16055320712447
C	-0.21755206082836	-1.52543740485645	9.28612065441726
H	-0.87577325436792	-4.06949872542872	6.99368329301849
H	-1.64034398304319	-3.73786189324909	8.56814125409942
H	0.08994957190592	-4.15592394043489	8.49751528164667
H	0.63364905073827	-2.00539367677828	9.80109460282329
H	-1.12844024684115	-1.69747479011033	9.88895941160959
H	-0.02873675677370	-0.43799971295553	9.26607596967667
H	-1.71867095373680	-1.79529644338787	6.13691445931846
H	-1.42874182110934	-0.31254307868404	7.08578020177169
H	-2.51756755614380	-1.57328023543979	7.72419161372157
C	10.54005116277595	1.05096613055014	-1.93286602162765
C	10.80305325855949	3.07798187327955	-0.48662209627130
C	8.82930059160535	2.87207815731188	-2.05304848030421
H	11.26574722513459	0.48907513204508	-1.31886491920152
H	11.10561763273831	1.55365699991076	-2.73720374992279
H	9.85618601069335	0.32591118975711	-2.40856218238977
H	11.48648160067473	2.54660227893026	0.19942339355555
H	10.30737814524892	3.88038260693670	0.08731793554147
H	11.40969744106595	3.55501492827692	-1.27863689640406
H	8.07982866208992	2.19322852701038	-2.49764601199894
H	9.40272670331650	3.33989109594385	-2.87456617317983
H	8.28567288436099	3.67544722452483	-1.52606241453841

[InI₂(Salphen)] (4 x ^tBu)

H	3.13084794730156	-6.19740481062692	5.82522879361395
H	1.70276872551299	-5.35085415779299	5.17729676004768
C	2.50201339697369	-5.29590340908924	5.93878100128439
H	4.59041105134908	-5.03450008412026	4.23753728537526
H	2.03182011044060	-5.34217612288777	6.93839081392483
H	3.22412031149853	-4.08016440439490	3.57615554521823
H	9.82773494341084	-3.49903525224971	0.33789455631896
C	4.00918018119031	-4.09968412252230	4.35307859652534

C	3.37909466691397	-4.03834008972853	5.76744889676466
H	0.71007506977875	-3.74411982731800	6.25164161090809
C	9.59562169941435	-2.43818092648554	0.13362316262189
H	9.96853698551300	-3.05967694539938	2.74287184279287
H	5.07345748718834	-5.02541195953318	6.74553626924844
C	7.51844452700538	-2.68062635168031	1.48987927706382
H	9.01017463289017	-2.40150295286949	-0.80315833370084
C	4.48867340749027	-4.09122235426134	6.84838107064345
H	4.67742786774560	-3.24652867772066	4.17302004942467
C	1.18834066204597	-2.76823110871439	6.16398711566612
H	10.55472284332647	-1.91509216269936	-0.03667909813443
C	2.56009379270113	-2.73849294603279	5.91874567414199
C	9.70679659965075	-1.99560245509909	2.58643539047566
C	8.81552906047632	-1.84853595415657	1.32699560449708
H	4.04249463235349	-4.07694159632259	7.86043347507918
C	-1.14891601259164	-1.68993396141148	6.56315824334570
C	0.36889935326173	-1.61431815607627	6.29960035641256
H	10.64725975512266	-1.42692072785202	2.46149307135687
H	9.19138740223139	-1.62380101954353	3.48389137001928
H	5.17252611781649	-3.23501823361645	6.75658763917911
C	3.22184486581416	-1.45321359493114	5.78914272550717
H	9.36739995589407	-0.25872729894035	-0.81988245287538
C	8.45901522548118	-0.36301354921758	1.10549506262943
O	4.49470787857890	-1.41145526982515	5.59078639780599
C	1.00406147773221	-0.38647385451398	6.17682744896832
C	8.81786121467461	0.30382701647141	-0.06470476215671
O	7.40747923517637	-0.23784275547610	3.22461448811603
C	2.39895508907006	-0.25801811198758	5.92348781636759
C	7.71963189518843	0.35808277943986	2.12497473025823
H	0.42660515914663	0.54291245292489	6.27030021832809
In	5.67194422249615	0.12809348239728	4.53651489782846
C	8.50903943459721	1.66301419970902	-0.34474094229245
C	2.88539853445969	1.08982135725867	5.84208945557793
C	8.91787280351210	2.36192377934885	-1.65731275618472
C	7.39060071724928	1.75193376235634	1.85578808331085
I	7.45541625220370	0.15899317222732	6.75760723451201
N	4.08805200789039	1.50789281768345	5.53476249568373
C	7.80216876853822	2.35077964835313	0.63177313626503
H	2.11580144876782	1.86135155042090	6.04379866363587
N	6.10660573842374	2.32011034367684	3.89291208991008
C	6.67880230502471	2.61715245465278	2.75280868738412
C	4.46452430304563	2.84863204639258	5.59058648375319
H	7.53110358746223	3.40348203251779	0.47566592835522
C	5.52821097843600	3.27670445879862	4.72531270238810
H	6.59120929731984	3.66350227415652	2.39825806300492
C	3.89687605905079	3.78024886347829	6.48684064343267
H	3.12744194101013	3.43996156626725	7.18797022641819
C	5.97149990942881	4.61521088701207	4.79878549100526
C	4.33257690405661	5.10950061478151	6.52047218196574
H	6.82158476491854	4.92676167969516	4.18254642048246
C	5.37286007284641	5.52832587332301	5.67387066296874
H	3.88288935463106	5.81167563790048	7.23304751828623

H	5.74208206103363	6.56009655690817	5.72012882018630
H	6.88595167669414	-2.59481479366336	0.58832872783147
H	6.92343012441929	-2.33774324660162	2.34748734817743
H	7.76970501418157	-3.74820554934881	1.63871388004428
I	3.97840040673242	-0.33960133025345	2.22428306926016
C	-1.64955428145613	-3.14371771506289	6.66374226441816
C	-1.90460564269034	-0.99864125377198	5.40299128202840
C	-1.47444020115575	-0.97436560815637	7.89607833487036
H	-1.68522972037439	-1.50110302623709	4.44416865325402
H	-1.60690793482398	0.05907889811976	5.29978656497626
H	-2.99871843677360	-1.02802908080024	5.57138750743509
H	-0.94571498204484	-1.45979885815308	8.73598974534809
H	-2.56152096707721	-1.00311155669507	8.10501929706876
H	-1.16383947321430	0.08456598745518	7.87223243222017
H	-1.46442164758175	-3.70336458473660	5.72997169214894
H	-2.73896319272254	-3.15417745745916	6.85157920201266
H	-1.16052655884993	-3.68736879840720	7.49143291499738
C	9.69293785937625	1.42117826910608	-2.59984899339173
C	9.82475698483718	3.57306599411697	-1.33282128117100
C	7.64722456855317	2.84597443645935	-2.39620737694405
H	6.99102820554887	1.99113645784961	-2.63832498787766
H	7.91144572055238	3.36293703225694	-3.33921840230388
H	7.06288479595655	3.54909000665019	-1.77789511820507
H	10.73978905348833	3.24269369327527	-0.80916071939980
H	9.30987495521107	4.30016646096150	-0.68111378416371
H	10.12414568796987	4.10187095975902	-2.25855310285711
H	10.62630977300421	1.05627412845875	-2.13566503964375
H	9.96635642545517	1.95894510887056	-3.52628912785317
H	9.08809110561215	0.54332932295252	-2.88794888322264

IC

In	0.27936838179992	-0.28258084454166	-1.97561600465229
O	1.73040482343858	-1.77290983641869	-1.55332330616268
N	1.77935725735270	1.18248389483407	-1.10385306704755
C	2.95767992718375	-1.69741921911248	-1.12000981987912
O	-1.52700580384042	-1.38617687683574	-1.79566981950557
N	-0.90968577854377	1.45386997071857	-1.14167737351821
C	3.73128335032575	-2.91405159852673	-1.03662488896424
C	5.03360768085776	-2.84607534649523	-0.53587207983609
C	5.66422172053864	-1.65561961660339	-0.09050356758859
C	4.91562425174975	-0.49057230775916	-0.17347584017450
C	3.58305824249089	-0.46040220700973	-0.68128974061487
C	2.96659186089551	0.83812376131190	-0.67150961476072
C	1.27474870237877	2.48940632164902	-1.06649307145129
C	2.07731342850884	3.64846030325330	-1.05667648147069
C	1.49615813686234	4.92077224434775	-1.03043969501242
C	0.09760100482410	5.05830056003542	-1.03832738496451
C	-0.71821091361843	3.92222665341853	-1.07532198253194
C	-0.15331980763579	2.63131060013514	-1.08045781219932
C	-2.09458221275920	1.32250790407215	-0.60053084206904
C	-2.94962893189605	0.16836290057820	-0.58677690824631
C	-4.17127397690347	0.33931136057939	0.12767397386391

C	-5.11170174102118	-0.67196746216496	0.26301423388225
C	-4.81830956745836	-1.90046491505090	-0.38407599505104
C	-3.64941258359091	-2.15746172813858	-1.10439865418009
C	-2.64898806381816	-1.11882208191362	-1.19040606530399
O	0.04126527664131	-0.66589473973816	0.71179210991245
C	0.86221630491111	-1.42402098897207	1.61357150519300
C	-0.51136575975134	-1.85821422548379	1.31258812664023
C	-1.66625716384702	-1.65981904926952	2.25870635681384
H	1.71223410543449	-1.94492583329937	1.15234976297890
H	1.07408105276488	-0.91962048884710	2.56965764260271
H	-0.62380023095786	-2.68125923365888	0.59286407660184
H	-1.48485257941058	-0.80351036372215	2.93091734947428
H	-1.81124019649580	-2.56814256653234	2.87215604930816
H	-2.59937394125069	-1.47483694933649	1.70008786846740
H	-4.35016737130322	1.31895230249690	0.58780767058713
H	-5.55483462635485	-2.70023629361623	-0.31379147352348
H	-2.49611254629574	2.19426420977892	-0.05008287481279
H	-1.80638173152243	4.02999736357561	-1.13439048831491
H	-0.35804142529716	6.05493655744401	-1.04607937464225
H	2.13688015182292	5.80985151517159	-1.03207821656727
H	3.16696499966819	3.54989218069147	-1.09851832032339
H	3.58975434630970	1.62987792541616	-0.21502715257080
H	5.34809128658959	0.46277564163939	0.15477592899744
H	5.60365273700025	-3.77315159884210	-0.48441586764192
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C	-3.42706406322820	-3.51463688199552	-1.80968539879183
C	-3.25339246637510	-3.28231328411152	-3.33250495765363
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C	-4.62744774929019	-4.46416231837987	-1.61699353528250
H	-4.15616295836870	-2.80532528132280	-3.75504768611108
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H	-3.10660566511064	-4.24982838248466	-3.84708612477527
H	-2.28742207701386	-4.39789251982093	-0.15099931735128
H	-2.04856009384591	-5.21401469321801	-1.72121946285198
H	-1.26562256151789	-3.64009619486619	-1.41520300711433
H	-4.43238356081214	-5.41056010184095	-2.15105448295023
H	-4.79535473060797	-4.71355857069768	-0.55362995620906
H	-5.56184755020403	-4.04045096456655	-2.02625607524848
C	3.12197577450834	-4.25601432942589	-1.50103072973929
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C	4.11398991751528	-5.42559025371007	-1.33442202788148
H	2.12680849877026	-4.65823216353258	0.41746622641656
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H	1.44676829710076	-5.56332758197849	-0.96620816048900
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H	9.01148133653334	-0.66354915179788	-0.04910153895625
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TS1

O	-0.71940091356485	-0.20705025186729	1.59083634963560
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C	-1.96285790591302	2.82092062479411	3.30533818774963
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C	-0.57073389490309	2.76565585834700	1.33026417668024
C	0.76709913692486	3.08210180590865	-0.62635139700235
C	0.14815049392290	4.25330458824953	-1.11588484991703
C	0.69896944367515	4.97246722966882	-2.18152406794163
C	1.87219870226544	4.51486414400946	-2.80541318253194
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C	3.77936095807131	1.08331924048720	-0.96204670605482
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H	-0.79786877195482	4.58065253198084	-0.67215686716283
H	-0.74593479781179	3.85860400762201	1.36302865640949
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C	-3.44678888587851	3.08997891974172	5.39930505879942
C	3.80579783098619	-3.85874024271840	0.49741315892978
C	3.02957223500214	-3.62264595002924	1.81770528824071
C	2.84716332773026	-4.34815173183387	-0.61653124056050
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C	0.12759145501476	0.15034714662421	-3.72249565357217
H	1.63772047128600	-0.80196228912345	-2.43768063492365
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H	-1.31205456391498	-1.83317750013509	-2.27905885631830
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I	2.59270552635872	0.59908638551310	2.96558510878621
C	4.40777517483327	-0.16402967165663	-0.63932580449347
C	5.82940012383708	-0.18262036555671	-0.78311588917533
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C	8.70811284720800	-0.02021002849297	-1.10781179681741
C	8.50749587882493	-2.44677356686164	-1.68731611520840

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H	8.32101002691175	0.27819505910805	-2.09839633387030
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O	2.43645021202882	-1.50280693819552	-0.18204725170049
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C	-2.11982733611656	0.06817621998359	3.58037459192014
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C	-2.52766625125822	2.36056846655925	4.47254998921080
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C	-1.20142241656884	2.06497041130249	2.41488370049249
C	-0.50333742359435	2.77113858304790	1.37925924159421
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C	0.14042607236523	4.22116654136124	-1.10699968789490
C	0.68505229474483	4.93191716081552	-2.18264627420193
C	1.84232445605530	4.45753700278352	-2.82308282456840
C	2.44903939333489	3.27570471973355	-2.38273337526361
C	1.93633602064687	2.55850949875264	-1.27958732733706
C	3.74920356032691	1.05550383121283	-0.94590835050442
C	6.61150141925638	-1.26360249257191	-0.45813468853582
C	5.92846553271849	-2.44724447289212	-0.05503225421119
C	4.54842798698847	-2.56385440906681	0.06646295322979
C	3.72120242054518	-1.40701891701742	-0.23995569127859
H	6.54060792250708	-3.32208023771917	0.17806605386750
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H	-1.24523787656320	0.01456183954253	-3.65914703009066
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H	0.05761854011098	1.21477520101105	-3.41163028898746
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H	6.28420472518474	0.78974105210731	-1.04201116681418
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C	8.59211134916875	-2.34399972518999	-1.58116125636399
C	8.74965937363734	-1.60912179218364	0.83119148599395
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H	8.24636057980305	-3.35188453397967	-1.29282063657807

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H	8.44222297743086	0.89078048403454	-0.29554011371233
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H	-1.49072280297971	2.97536645556941	6.96676989291371
H	-2.76399576941459	1.74644448287000	7.17607736399785
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Int2 α

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H	1.62071548104694	0.66897567510810	3.97291765815004
H	-0.49927373832787	-2.09171486259681	5.46876247504074
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H	2.33283150747781	-0.90069814175704	5.73141685117854
H	1.98219970744425	-2.64527777504559	5.66847944436729
H	3.16223715202487	-1.92212343448664	4.53091268989248
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O	-0.07597141257754	1.31805362806811	-1.63413203063197
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H	0.73775885536018	3.21780094351754	-1.81927280791491
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C	3.52694643342023	-2.25494607155509	-0.98230545900079
C	4.89259486503819	-2.12900219522813	-0.73342032758451
C	5.59296366961106	-0.89511910085179	-0.64131038910739
C	4.84554998931424	0.25392936999414	-0.83542845468464
C	3.44462306910701	0.22073123252372	-1.11613025296783
C	2.84105454698321	1.50972822235934	-1.29888066645867
C	1.11955080948281	3.09545459769389	-1.78162282510863
C	1.88044452756417	4.19031033485994	-2.23144954292672
C	1.29840080116870	5.45959157781711	-2.33772713970991
C	-0.05567468612803	5.64751686339191	-2.01329809141141
C	-0.83247161342612	4.56511121768325	-1.58166929963122
C	-0.25898584654829	3.28765890405609	-1.45517514959968
C	-1.85551196834598	2.18003455637315	-0.08203808192884
C	-2.58512992573548	1.08153113778058	0.48748111409118
C	-3.44183357410848	1.43076681695582	1.57512955149798
C	-4.20909140227340	0.49285938762049	2.24607328800581
C	-4.15232184434779	-0.84169814281834	1.75617893142542
C	-3.34028453396442	-1.27131771674764	0.70731517687153
C	-2.46805244475257	-0.30278119625183	0.07679646550589
H	-3.45615198111850	2.48245032495576	1.87591625341843
H	-4.78741592983585	-1.58177817205612	2.24740096455496
H	-2.04690416925517	3.15978416750895	0.39140710092047
H	-1.89740521774391	4.69904585546268	-1.36363132176769
H	-0.51382482788963	6.63754348884401	-2.11691301149502
H	1.89913555846684	6.30261561895583	-2.69746499705889
H	2.92585882496529	4.03770400592435	-2.51973862110676
H	3.51110508654810	2.36615274949936	-1.09881101151632

H	5.31751685076434	1.24036222846616	-0.78780976105788
H	5.47267248169035	-3.04422131136057	-0.59832483725611
C	-5.08481040056284	0.81895488614812	3.46679188065863
C	7.10193466855668	-0.89788416973091	-0.34437153302678
C	-3.36915484054369	-2.73655565642302	0.21854348971240
C	-3.75238908914002	-2.77036392616975	-1.28288391888283
C	-1.98861443577704	-3.40565599224453	0.42434051427155
C	-4.41122122845731	-3.57619916655024	0.98566045339361
H	-4.75120754533200	-2.32357217800621	-1.43648352065384
H	-3.02533788614300	-2.22001291593518	-1.89809869179550
H	-3.78802943086976	-3.81617565604333	-1.63931416403678
H	-1.69508628635166	-3.37896150271547	1.49039378393089
H	-2.02843254931322	-4.46596531364884	0.11505028918440
H	-1.21269154311196	-2.90662974964361	-0.17118008878182
H	-4.41466523368384	-4.60542210715641	0.58655722395121
H	-4.18135498505985	-3.64198699839108	2.06462676356357
H	-5.43323905814119	-3.17299108162600	0.87221253354949
C	2.85754126535815	-3.64482567382180	-1.06520691322376
C	1.79632118622214	-3.78035844422742	0.05344527491625
C	2.19730608241224	-3.83351310151333	-2.45450917120464
C	3.87657473663008	-4.78786358019833	-0.87913858447299
H	2.26547362806336	-3.67378887170836	1.04902945671534
H	1.01819354276692	-3.01386332929524	-0.05355293758665
H	1.31347706324623	-4.77371655565883	0.00711108348813
H	2.95511751717819	-3.75620269526997	-3.25489103602983
H	1.73470955645327	-4.83570752662590	-2.51884770039365
H	1.41892369280853	-3.07992684882619	-2.64170478948864
H	3.35279753109880	-5.75710653643015	-0.95102235950677
H	4.65964697609273	-4.77614462954447	-1.65814195134910
H	4.36890239573165	-4.75140392058427	0.10933496681598
ln	-0.03587352998714	0.25123812431543	-1.87618273047535
O	0.67508071835708	0.46241324887784	1.19221547649276
C	0.40550975646998	1.54405978763382	1.98359228332347
C	0.37734904523568	-0.74729903222570	1.90748032698986
O	0.67267259987787	2.67630415906136	1.69083073877890
O	-0.20482365090678	1.14722996369381	3.12613270948958
H	-0.10838941529789	-1.45190612838800	1.22161178014873
H	1.32462455769704	-1.18038529761962	2.27968156268938
C	-0.54104622697171	-0.26590600001159	3.04121422826306
C	-0.34016022771479	-0.94630380094180	4.37828895639973
H	-1.59975757519224	-0.31779368197933	2.73260327615574
H	0.70673877223853	-0.85320652130912	4.71649632300056
H	-1.00219744662697	-0.50767790463089	5.14345682029465
H	-0.58827127983472	-2.01891065041114	4.28452401521348
I	-0.62043200092673	-0.01519117066102	-4.52692384872768
C	7.68045359344996	0.52833640307517	-0.27849338359063
C	7.84175439938628	-1.67340609704501	-1.46200812416561
C	7.35255391437170	-1.58924625685295	1.01832690388078
H	6.83231186909654	-1.05153780871419	1.83110021168120
H	8.43313524098308	-1.60733017255905	1.25179270023959
H	6.99256732058259	-2.63274233075405	1.01977374732949
H	7.67488635413675	-1.19703712947851	-2.44452721551015

H	7.49647239857008	-2.71953934905765	-1.53229596675193
H	8.92987637813803	-1.69238804518876	-1.26666076232812
H	7.55538687355028	1.06416605916771	-1.23618667117114
H	8.76210127941288	0.48531914283895	-0.06003113128269
H	7.20287605529763	1.12655373484408	0.51780194648507
C	-5.01901572494287	2.31261933419305	3.83789498189757
C	-4.58028794517307	-0.00308873708074	4.67848668176184
C	-6.55807499947400	0.44824529457677	3.16937425765101
H	-6.93969687578566	1.02691935054589	2.30940954945795
H	-7.19654747695101	0.66739872169939	4.04471018666026
H	-6.67317678625603	-0.62362979427135	2.93233784515185
H	-3.53092672912589	0.24883959240615	4.91489778360407
H	-4.63148229202716	-1.08885680525651	4.48390704845561
H	-5.19509397747946	0.20690702940697	5.57294618810431
H	-3.98972720779236	2.62219233974421	4.09178587412160
H	-5.65447227650251	2.50917465207631	4.71934680546049
H	-5.38154440213593	2.95586331866464	3.01660426967151

Fluoride Ion Affinity Structures (2 x ^tBu)

Me₃Si⁺

Si	0.21419651720700	-0.07403770637091	-0.37667227112579
C	1.96865233683992	0.45995384906537	-0.19065277677034
C	-0.63713153900377	-0.93484434728113	1.01331684071137
C	-0.63711568740186	0.11457376180971	-2.00071747836779
H	2.61192420489478	-0.39712414991948	-0.48972817328370
H	2.22096418061236	0.70517715303486	0.85608064060120
H	2.22075973570517	1.30294740396992	-0.85793273998999
H	-0.42375728091167	-0.79977099572340	-2.59760789900059
H	-0.25162982987329	0.97474708266012	-2.57600564760983
H	-1.73389645515893	0.18170308948616	-1.89107007870704
H	-0.42364827299433	-2.02215981489377	0.91335964423920
H	-1.73392517374015	-0.81420213658851	0.96910037005229
H	-0.25166273617524	-0.61785318924893	1.99839956925100

Me₃SiF

Si	0.04818655918597	0.36904982732112	-0.22239455943387
C	1.92797560183798	0.43368687240372	-0.19994138976191
C	-0.61073474357926	-0.92511036044096	0.97307946873111
C	-0.61073810413449	0.09734944104475	-1.96312763222518
F	-0.50138955444026	1.84160913617917	0.29084611972347
H	2.35662629450745	-0.52947404317271	-0.53542816346535
H	2.30865127428349	0.63710029989903	0.81775299785252
H	2.30875204065930	1.22535968181694	-0.87094612781478
H	-0.27213238911084	-0.87805768349754	-2.36057373206936
H	-0.25579628281492	0.88507636506382	-2.65265800106734
H	-1.71604065432795	0.10337438653383	-1.97825919815219
H	-0.27232619873737	-1.93656481998730	0.67903437816416
H	-1.71604377790694	-0.92956000149955	0.98867227910316
H	-0.25585006542216	-0.73585910166430	2.00274356041557

[AlBr(Salphen)]

Al	-0.02391562299977	0.67138435504089	-0.51536970392949
O	1.28152579486048	-0.54556310847856	-0.09641073276283
N	1.25492741384362	2.15730658191461	0.01629362835591
C	2.57118424545718	-0.51102810345394	0.09448639910489
O	-1.30871391951697	-0.47988661408319	0.09699275043322
N	-1.32705346049817	2.20388410330966	-0.15506984382798
C	3.36162475548268	-1.71562496576366	0.03976484307196
C	4.72530390663104	-1.60370030964181	0.32632875671022
C	5.36217641911098	-0.38128449423091	0.65469903807456
C	4.62051500324502	0.78301429218017	0.67515866140135
C	3.22656632043858	0.74633849925910	0.37779463796599
C	2.52081348377836	1.98091434287064	0.34688521598660
C	0.69741095196867	3.44641961287875	-0.08988067542683
C	1.41949403846130	4.65483761486219	-0.14704304457041
C	0.74523813438885	5.87312359669724	-0.27389113046445
C	-0.65795276385405	5.89923734956523	-0.36501627432906
C	-1.38730511974481	4.70699138758081	-0.33206987705751
C	-0.72381919383206	3.47256261437171	-0.18911925887918
C	-2.63044884198811	2.04706725655401	-0.05893657952581
C	-3.32292727692975	0.80245842756088	-0.00682041529105
C	-4.74707082584793	0.83449029903948	0.00416976201536
C	-5.46609347757760	-0.34186396218661	0.09025033282187
C	-4.77177316322642	-1.57108758572482	0.19038563933086
C	-3.37674266343562	-1.67409292186131	0.20588426998833
C	-2.61815645502857	-0.45536948377613	0.09030783658943
H	-5.25596046991883	1.80421154189883	-0.06508978566754
H	-5.36960939577171	-2.48365014378868	0.26017451515388
H	-3.26640662101713	2.94528834718231	0.00013113609734
H	-2.47574726875460	4.74159214650671	-0.43700278014396
H	-1.18357499169576	6.85339413564281	-0.48328281285654
H	1.31707755733732	6.80645639629651	-0.32427697127545
H	2.51321784884714	4.64765582692532	-0.11943485171791
H	3.11453087707319	2.87025777661706	0.61359789527784
H	5.08960717038022	1.74880581271843	0.90203769226972
H	5.34704236156244	-2.50247622684864	0.29512819001213
H	-6.56141556751574	-0.33296945614250	0.08635880533831
H	6.43525870425060	-0.36815574668108	0.87411044103091
C	-2.66764678952847	-3.03447500025816	0.34828877916609
C	-1.74324239564815	-3.28010873618406	-0.87003043552329
C	-1.85917407161723	-3.03676879160998	1.66968966191460
C	-3.67012249757114	-4.20468253116805	0.41283078597613
H	-2.33035471815900	-3.27241174614808	-1.80588245414672
H	-0.95952013242380	-2.51644907221578	-0.94887476401868
H	-1.25561130597420	-4.26727308291357	-0.77978340672243
H	-2.53816607453631	-2.91729537642059	2.53353004637446
H	-1.32112417134253	-3.99452096208901	1.78687617133559
H	-1.12191677795486	-2.22154821663334	1.69094970348706
H	-3.11316290977765	-5.15224060097471	0.51756440163428
H	-4.35062764715335	-4.12483362461142	1.27952093555570
H	-4.28033326723581	-4.27880153280428	-0.50520706100285
C	2.71766844695680	-3.06342455072737	-0.33664841906100

C	1.63599397812665	-3.42411133044354	0.70827654227317
C	2.09515495900535	-2.95900512006706	-1.75218300088846
C	3.74902106629710	-4.20923407382157	-0.36357896809004
H	2.08474860521843	-3.52532472257827	1.71328657347273
H	0.85471185526338	-2.65569732714391	0.74939625212497
H	1.16098817688558	-4.38688764456171	0.44722600772201
H	2.87857406376716	-2.74882406252236	-2.50249085327484
H	1.61203634686843	-3.91583700929534	-2.02159149468661
H	1.34048942140102	-2.16269619365407	-1.81626264985385
H	3.23996184320125	-5.14747450792982	-0.64568609817092
H	4.54863966934041	-4.03106567843148	-1.10486884824490
H	4.21741471920213	-4.37131561647890	0.62398869158468
Br	-0.06650828057524	0.71866791687493	-2.85167180824156

[AlI(Salphen)]

Al	-0.02194850241274	0.67699595112451	-0.49910126933860
O	1.28339902106949	-0.54298009518498	-0.09728101994172
N	1.25780930776660	2.16243938129321	0.02043420487875
C	2.57628661875210	-0.50935167459725	0.07986082701728
O	-1.30722516722660	-0.47984892011888	0.09585484541397
N	-1.32627047673616	2.20591306749548	-0.14313738186229
C	3.36278851193299	-1.71606476773514	0.03123514340827
C	4.73153222763850	-1.60224158169616	0.29323874394874
C	5.37592315455523	-0.37673317311998	0.59314161277617
C	4.63572521947912	0.78849849535963	0.61313394826792
C	3.23661016656462	0.74982994475327	0.34128903301891
C	2.53109569826984	1.98488442706035	0.32153476533206
C	0.69690475089282	3.45200629024448	-0.06882874202805
C	1.41590290047989	4.66267232696310	-0.11324828159998
C	0.73876531151758	5.88072910995531	-0.22401767737116
C	-0.66475047845825	5.90489450472457	-0.31026341010487
C	-1.39125504723808	4.71085807903223	-0.28852963437877
C	-0.72463162926484	3.47632532274132	-0.16310931789531
C	-2.63086375389555	2.04627500172044	-0.06158158595162
C	-3.32193946972431	0.80050501781336	-0.02172573378144
C	-4.74619900378790	0.83102159392765	-0.02607576887180
C	-5.46465841934141	-0.34622854141135	0.05198375968448
C	-4.77005472645555	-1.57444376764499	0.16100972448693
C	-3.37497394162955	-1.67588229378987	0.19150416200487
C	-2.61757177833215	-0.45672273004945	0.08083309082992
H	-5.25536299141710	1.80014855733272	-0.10057726851745
H	-5.36733377275387	-2.48772420242928	0.22534036891782
H	-3.26906323334998	2.94289418807671	-0.00859303716764
H	-2.48011134064742	4.74497235682242	-0.38829603970415
H	-1.19291646410136	6.85917757387024	-0.41509101198901
H	1.30849749098099	6.81578984308859	-0.26456961561117
H	2.50959698612706	4.65888524094624	-0.08747006366344
H	3.13223738230748	2.87370974539995	0.57155842110428
H	5.10928879414416	1.75618485834201	0.82166058717652
H	5.35119897125051	-2.50248410563561	0.26460936019840
H	-6.55984487276604	-0.33863830526337	0.03564249520942
H	6.45273825675588	-0.36226224364171	0.79313446262737

C	-2.66612354295546	-3.03529608784063	0.34484711506329
C	-1.72861179514820	-3.28391201970192	-0.86264763217023
C	-1.87071135185928	-3.03268951794249	1.67411418709875
C	-3.66831088270177	-4.20606312591049	0.40307072392268
H	-2.30467853604299	-3.27849901867097	-1.80524201748484
H	-0.94423627169407	-2.52036370235598	-0.93432772242006
H	-1.24146661467513	-4.27055580419322	-0.76429570454958
H	-2.55781451383871	-2.91065620421525	2.53114806642164
H	-1.33334720590580	-3.98975857265171	1.79944430275911
H	-1.13379448225261	-2.21724436487549	1.69961551732506
H	-3.11158633546800	-5.15266064927294	0.51705851105283
H	-4.35794020611498	-4.12377965004990	1.26229759619268
H	-4.26860226582888	-4.28415475415384	-0.52112665790618
C	2.71180898407436	-3.06943154620560	-0.31236139394047
C	1.64468708100977	-3.41035306012666	0.75423343953060
C	2.06930990058309	-2.98927800186908	-1.72018690894384
C	3.74116448044380	-4.21719501460829	-0.33346080670135
H	2.10810134700771	-3.49651442190210	1.75399158923948
H	0.86488196258155	-2.64021627897877	0.79476575050038
H	1.16423143203018	-4.37615861262634	0.51550591438422
H	2.84027555596761	-2.78784622446767	-2.48541763018522
H	1.58423825443518	-3.95095169339123	-1.96768923816293
H	1.31143647786942	-2.19630589191270	-1.78431772705728
H	3.22645598693072	-5.15936569999520	-0.59099190553260
H	4.52980909524727	-4.05397072378446	-1.08975685840002
H	4.22397691674052	-4.36235097818862	0.64980654324216
I	-0.06575917138128	0.74886714412180	-3.07468974980183

[GaBr(Salphen)]

Ga	-0.02800598488296	0.68847698186586	-0.55851749923648
O	1.30793677844809	-0.60435826647286	-0.07061343977727
N	1.27983854518025	2.19322229724015	-0.01617164061474
C	2.60148068166638	-0.51913244413327	0.05485613894665
O	-1.33201834310928	-0.51838705592132	0.16267509895777
N	-1.34666322355890	2.23945492453436	-0.12905211938930
C	3.40406131092538	-1.72022023022679	0.01757352472084
C	4.77689819671954	-1.58757434902560	0.23545638583026
C	5.41609992412824	-0.34604734673104	0.47971466927644
C	4.66411861851523	0.81052887337113	0.48718596878080
C	3.25563772164202	0.75767533799839	0.25967753515998
C	2.55648967654835	1.99762918914104	0.24839696324804
C	0.69868871984527	3.47088899585054	-0.06847898356500
C	1.41201057533320	4.68670217240316	-0.09532937838460
C	0.73367133609192	5.90683487406841	-0.15628177839168
C	-0.67164564340030	5.93227544204032	-0.20585268309531
C	-1.39553783143550	4.73735389734703	-0.20000866422025
C	-0.72968527601378	3.49648948281867	-0.13054624541939
C	-2.64829312500247	2.05922079621250	-0.07721918541853
C	-3.32855042605282	0.80592546297417	-0.04994631744004
C	-4.75355665052410	0.83974473089271	-0.09955761793898
C	-5.48299017268486	-0.33039991781433	-0.03382939550465
C	-4.80150022743326	-1.56403043550760	0.10422145618595

C	-3.41033009033352	-1.67424532493086	0.17707825918352
C	-2.63639527230854	-0.45964718941986	0.08628900362399
H	-5.25487821241774	1.81102741074532	-0.19738319483243
H	-5.40777328624332	-2.47232171190151	0.15476961158230
H	-3.30020503548829	2.94828850853480	-0.04004987546024
H	-2.48728291224978	4.77276601418934	-0.26152633271182
H	-1.20322054452928	6.88859456909269	-0.26530865368794
H	1.30265484603185	6.84289287575178	-0.18200422507056
H	2.50606907268856	4.68282099443054	-0.08993821345521
H	3.17252481049886	2.88145713965580	0.48353567107679
H	5.13508382966734	1.78750168993830	0.65496233223078
H	5.40545470346036	-2.48194527681016	0.21510619159224
H	-6.57711275768864	-0.31414198360735	-0.08297630023360
H	6.49794367510489	-0.31397193380179	0.64807861129355
C	-2.71186128576375	-3.03874720090840	0.34576986898437
C	-1.75156267818271	-3.29334096401493	-0.84310001358970
C	-1.93610282407350	-3.05009434574496	1.68696331863537
C	-3.72420830774406	-4.20169235128130	0.38241653908434
H	-2.30625833116633	-3.27837525923507	-1.79846201072457
H	-0.95636759129907	-2.53888402156693	-0.89256397281067
H	-1.27805723496659	-4.28609079196192	-0.73730089603179
H	-2.63277932357217	-2.92147925025158	2.53532591148519
H	-1.41462778657815	-4.01585419477292	1.81514304071930
H	-1.18720392596829	-2.24633618129923	1.72421031394082
H	-3.17797494246157	-5.15297965750538	0.50759668033894
H	-4.43079095029425	-4.11346913341345	1.22721537103360
H	-4.30606459717133	-4.27469112867067	-0.55396302723848
C	2.75316567438866	-3.08636840844525	-0.27843362549501
C	1.70131788304847	-3.41604603954953	0.80869614595778
C	2.09149163421125	-3.04418329181262	-1.67967945606430
C	3.79077981421451	-4.22716797180766	-0.28723609850941
H	2.17598113158629	-3.46346710763253	1.80579501958762
H	0.90390220423750	-2.66291346274785	0.83483908022742
H	1.24198076280350	-4.39988963770150	0.60260520414113
H	2.85307949367911	-2.86449153342360	-2.45981702247882
H	1.60373200134838	-4.01238302097326	-1.89469493274255
H	1.33232076262723	-2.25309410805296	-1.75452915942901
H	3.28011393446212	-5.17978039035659	-0.51234639667285
H	4.56652818571442	-4.07774679086392	-1.05958547883429
H	4.29006917646887	-4.34233045618903	0.69176558864511
Br	-0.11494088668693	0.65780750539039	-2.91673567000142

[Gal(Salphen)]

Ga	-0.02656007808129	0.69093878927918	-0.55989447144994
O	1.30922627322204	-0.60319272767278	-0.07226255773727
N	1.28130282952439	2.19650387873965	-0.01323019308183
C	2.60413717637520	-0.51834882271435	0.04562292336923
O	-1.33124037464655	-0.51910590877772	0.15646534224571
N	-1.34668175362000	2.24125125728092	-0.12029767159320
C	3.40505393125214	-1.72022579660062	0.01397496538054
C	4.78023591586428	-1.58631809343453	0.21685807550589
C	5.42292679250032	-0.34318824334266	0.44189379730517

C	4.67118238057423	0.81367880660516	0.44766062163418
C	3.26034323776918	0.75950215851753	0.23610890568871
C	2.56153874902820	2.00016206796755	0.23252018197998
C	0.69846430731308	3.47399499004609	-0.05381515893613
C	1.41009214576823	4.69095211229734	-0.07168764979938
C	0.73032320631016	5.91061366462129	-0.12196022961402
C	-0.67513887191610	5.93491534320312	-0.16889888034273
C	-1.39752950537958	4.73924338068055	-0.17076689809714
C	-0.73015111845136	3.49864109924043	-0.11252193058325
C	-2.64847646103574	2.05994360792794	-0.07477208322111
C	-3.32764236914211	0.80556000528767	-0.05715225092089
C	-4.75234423342970	0.83885550781963	-0.11405325195441
C	-5.48177702699844	-0.33163663991045	-0.05415285927635
C	-4.80059002866319	-1.56499442174680	0.08740548548964
C	-3.40972874703583	-1.67470965207408	0.16754225088857
C	-2.63598183112753	-0.46010336848753	0.07899772378177
H	-5.25344875113227	1.81012298931042	-0.21286879670904
H	-5.40663842756843	-2.47360219789419	0.13463354894579
H	-3.30164626262144	2.94794841966934	-0.03774233466834
H	-2.48943153622161	4.77387335845915	-0.22933884618056
H	-1.20789961839189	6.89105183952479	-0.21973455525904
H	1.29824435443294	6.84746454061637	-0.14075027361114
H	2.50411822290570	4.68899799582731	-0.06687506817303
H	3.18221431207977	2.88321081284367	0.45755423316543
H	5.14395981425305	1.79176266168421	0.60325273230386
H	5.40772080774217	-2.48147895632928	0.19937887598858
H	-6.57557170693181	-0.31566397186366	-0.10966329499030
H	6.50650967592959	-0.31013984507377	0.59821554670126
C	-2.71225978874333	-3.03917881813647	0.34228480706392
C	-1.74655046382960	-3.29755289243542	-0.84138359606109
C	-1.94239892481168	-3.04777138803939	1.68687012558316
C	-3.72538167113166	-4.20147752816493	0.37738421182896
H	-2.29636142632325	-3.28541300317335	-1.79954497425687
H	-0.95118181255874	-2.54324187922689	-0.88927890715995
H	-1.27291483728438	-4.28967836371975	-0.73031629034311
H	-2.64261821841539	-2.91686512725430	2.53197117407743
H	-1.42205605163745	-4.01349411840611	1.81946892103166
H	-1.19317254802862	-2.24435787948515	1.72552183389726
H	-3.18020692436904	-5.15256771447139	0.50837492875516
H	-4.43625429743852	-4.11020021037628	1.21825793139870
H	-4.30244174729820	-4.27728452549236	-0.56172641450435
C	2.75200547945162	-3.09012337424153	-0.26024780282164
C	1.70941715473413	-3.40683427121886	0.83987719964174
C	2.07729371454870	-3.06583630511280	-1.65540244432472
C	3.78998175974900	-4.23052385319615	-0.26402851294799
H	2.19218605229687	-3.44154787567609	1.83361183817571
H	0.91130599278120	-2.65418916179001	0.86333568217385
H	1.24888535437529	-4.39338617831241	0.64995773488793
H	2.82937120467817	-2.89019572900319	-2.44545314630577
H	1.59068457069094	-4.03776120392672	-1.85534050564636
H	1.31377943913382	-2.27903119193000	-1.72887368972808
H	3.27736681457433	-5.18575702926805	-0.47290996098531

H	4.55866362369001	-4.09046890866833	-1.04512894742335
H	4.29800248165547	-4.33385475577390	0.71181894355498
I	-0.11758036093948	0.67937264497299	-3.13586609373705

[AlClF(Salphen)]⁻

Al	0.00786664930112	0.64418960343710	0.31659756385332
O	1.42335306407812	-0.59803076983369	0.33261014421314
N	1.33315097767152	2.20827416060105	0.10348794333761
C	2.68059158461490	-0.49474138142662	0.09844178186134
O	-1.41952089815035	-0.58370386555595	0.38010560821951
N	-1.31723984263362	2.19542768611351	0.03223096319073
C	3.48762367535182	-1.69435735476595	-0.05326738664011
C	4.86541488310430	-1.55124285319176	-0.20580817948328
C	5.51278281792086	-0.29034517744728	-0.26402109254498
C	4.74902335066787	0.86097532173560	-0.20107290549882
C	3.33625786485526	0.79847824819179	-0.03335171024827
C	2.62623416946639	2.04260706345613	-0.02474459312862
C	0.71852853356858	3.46365928940917	0.11926947799861
C	1.39054603284545	4.70302783194351	0.19476353039303
C	0.68201742218476	5.90854877573886	0.22289766884408
C	-0.72374613893687	5.89910853144650	0.19449867210427
C	-1.41181588015330	4.68303389792244	0.13418987571805
C	-0.71700597333164	3.45544396520047	0.08220629143588
C	-2.57720756673321	2.01339936820732	-0.27551443444402
C	-3.27869031902143	0.76455957228392	-0.30379526452513
C	-4.65259984755402	0.80037125530670	-0.67349855131764
C	-5.41750847755829	-0.35225874768695	-0.69426473765295
C	-4.81581748047505	-1.58628208620485	-0.33947590179870
C	-3.47613602692029	-1.70340874825837	0.02771695104128
C	-2.65713753363334	-0.50363935569132	0.04805245838254
H	-5.09664068944596	1.76956664461675	-0.94038346101538
H	-5.44466045691825	-2.48213727468272	-0.36384195048337
H	-3.18767851525765	2.89023254676828	-0.56012690087610
H	-2.50661637770291	4.68342307611207	0.15060321232478
H	-1.28417195583540	6.84110165560578	0.24012557119990
H	1.22697120822834	6.85853110303297	0.28731285379448
H	2.48365381264566	4.72534494686935	0.24906641146759
H	3.26722737427421	2.93230290130231	-0.16445199590553
H	5.22188305386752	1.84972395623633	-0.28231330786423
H	5.48917256072074	-2.44557152123196	-0.30329547020126
H	-6.47593768197975	-0.32079660569635	-0.97926253537180
H	6.60164515164784	-0.23841776020989	-0.38323101529454
C	-2.83746366983038	-3.05845074287865	0.39110313999588
C	-1.69085964563452	-3.36839542392864	-0.60280985635763
C	-2.28454385793662	-3.01032640639229	1.83867838477579
C	-3.85402282358158	-4.21509383176646	0.31558302377876
H	-2.08219175446141	-3.44507590343435	-1.63375066735650
H	-0.92744097420963	-2.57999114729644	-0.58502753690972
H	-1.20973999255530	-4.33010299769801	-0.34236440816510
H	-3.10369522262605	-2.82516101162497	2.55862531141595
H	-1.81314603937878	-3.97814517262654	2.09593811217173
H	-1.53449573706140	-2.21404331280232	1.94971245320678

H	-3.35049820829981	-5.16220317145945	0.58233546283683
H	-4.69605689956910	-4.07549191959362	1.01876239177139
H	-4.26943934784497	-4.33506869560048	-0.70185116850524
C	2.79098935966798	-3.06729073029842	-0.13068823962571
C	1.93042870159528	-3.33938997993738	1.12899249261159
C	1.90482909122116	-3.07675281392438	-1.40417856807087
C	3.80507838244394	-4.22330880381844	-0.25145304948289
H	2.55823659646749	-3.31032947085293	2.03929709830300
H	1.13122707113320	-2.59430420152692	1.23390688606997
H	1.47270939786086	-4.34460834447904	1.05965185485348
H	2.54039129478192	-3.00871686070425	-2.30647743367003
H	1.32512512446953	-4.01718472503855	-1.46097227211038
H	1.20343612960547	-2.22841346477773	-1.42497336891907
H	3.25863272782762	-5.18170271516249	-0.31873103169930
H	4.43174696835765	-4.13673752830366	-1.15774432588134
H	4.47377881655813	-4.28003929051550	0.62777987081334
Cl	0.01829173164471	0.46145420237613	-2.02965279820492
F	0.00739025458070	0.87983656441156	2.05024265726881

[AlBrF(Salphen)]:

Al	0.00406769173908	0.65816311628744	0.30780450224441
O	1.39334651179254	-0.59355196664487	0.24304792440503
N	1.32888110604213	2.20797781181854	0.10036264090711
C	2.66534210424983	-0.49620932007276	0.08455604976305
O	-1.39339006556439	-0.58557616465884	0.28748976271292
N	-1.31944552247153	2.19703804903400	0.02991099734998
C	3.47143302626997	-1.69823678048303	-0.03385767946672
C	4.85561404236783	-1.55925053520366	-0.12639358436244
C	5.51001230320842	-0.30137188269528	-0.14803298702200
C	4.74976066317006	0.85308833748323	-0.10211375727001
C	3.33138229710806	0.79412364612051	0.00615958934014
C	2.62531089344952	2.04003718995896	0.00743013953210
C	0.71656520451885	3.46584690615491	0.09504121786152
C	1.39160038072072	4.70460077391263	0.14397755865022
C	0.68549212513005	5.91140969167181	0.15456679368635
C	-0.72042032846771	5.90367323875692	0.13048522295729
C	-1.41057706830928	4.68830550134397	0.09120805582581
C	-0.71788320285046	3.45901580679040	0.06054269656518
C	-2.59086913924902	2.01759608134708	-0.23258025049314
C	-3.29280181316265	0.76962645903769	-0.25151662464928
C	-4.68390895333344	0.81032224723953	-0.54901726400779
C	-5.44598421408461	-0.34432147585922	-0.55446401776616
C	-4.82446165301922	-1.58286933293785	-0.25531158379164
C	-3.46661169394699	-1.70403489002309	0.03868877098064
C	-2.65156959832498	-0.50314765085665	0.03469132828317
H	-5.14279147516945	1.78357709751183	-0.77174412005630
H	-5.45227307882613	-2.47959946230709	-0.26194670913826
H	-3.21068159736129	2.89682003723949	-0.48378095610274
H	-2.50520139907521	4.69292136291811	0.10356758626659
H	-1.27949165264699	6.84706319946605	0.15869501176857
H	1.23256305737634	6.86125569235899	0.19784946333013
H	2.48502718625154	4.72666239260105	0.18752483791411

H	3.27115844575885	2.92888053217351	-0.10628320776526
H	5.22969624636834	1.84042762524388	-0.15043111647679
H	5.47918449675467	-2.45572986269450	-0.20101999967150
H	-6.51771031539774	-0.31061787544712	-0.78379222978589
H	6.60295141413966	-0.25361641507993	-0.22253626781423
C	-2.81117390005617	-3.06320113749809	0.35408701924445
C	-1.71455247684702	-3.36554746176983	-0.69690506707392
C	-2.19053640911728	-3.02900331779312	1.77435417382984
C	-3.83156547399716	-4.21850428442304	0.31675598566683
H	-2.15340213736169	-3.42112128660851	-1.70978682876043
H	-0.94279929510255	-2.58500228681673	-0.70114105325826
H	-1.23195010759775	-4.33592886613357	-0.47408468565142
H	-2.97557865273011	-2.85669706532747	2.53425705172767
H	-1.70246604490068	-3.99688084869771	1.99706631502314
H	-1.43986247595218	-2.23042671326596	1.86138393253309
H	-3.31684973679311	-5.16793757847681	0.55169239582425
H	-4.63916555513186	-4.08437052707814	1.06017171640135
H	-4.29449846223879	-4.32965452794520	-0.68095597087108
C	2.77684880815271	-3.07116692647375	-0.13131913463938
C	1.87524490148206	-3.33326062183204	1.10141484969638
C	1.93241758648188	-3.08973794520440	-1.43193722369152
C	3.79397499749270	-4.22791832944546	-0.21187770033477
H	2.47415439301727	-3.30762187480181	2.03097671082302
H	1.07938847985341	-2.58140524737472	1.17934173512853
H	1.40969572752218	-4.33380804749926	1.01977390038462
H	2.59251629772520	-3.00286528474051	-2.31445052762519
H	1.37313680028455	-4.04090450226917	-1.51112191888657
H	1.21449525846427	-2.25628617857157	-1.46719537664133
H	3.24931785945370	-5.18638127717972	-0.29115878792214
H	4.44909949698342	-4.14632077388659	-1.09831274413928
H	4.43387087914372	-4.28003154778116	0.68874337707199
Br	0.02850327451767	0.59064309697253	-2.31400245940032
F	0.00092954209619	0.84240218041523	2.04384252083627

[AlIF(Salphen)]⁻

Al	0.00785103630941	0.68963801711074	0.43595990655062
O	1.35873105099747	-0.55865414090045	0.22682344159116
N	1.32478086651135	2.21283053865450	0.13133081628118
C	2.64005784556772	-0.48251170218396	0.08485290341123
O	-1.35649034915377	-0.55667907388529	0.30385308646632
N	-1.30487932393260	2.19621690361227	0.05305045057814
C	3.42842357582341	-1.69199396099132	-0.03701093597898
C	4.81610750205405	-1.56740766314025	-0.11773423573498
C	5.48590686168919	-0.31886270085961	-0.12551673358919
C	4.73978191355366	0.84460765231632	-0.07582030119481
C	3.32102993143017	0.79692122574861	0.02549335831769
C	2.62092765416895	2.04418191308757	0.02316574025882
C	0.71818769417276	3.47512051450005	0.10852353213617
C	1.39373205578546	4.71257078068635	0.14809360360893
C	0.68391056774993	5.91753831858807	0.14451836222001
C	-0.72181484156029	5.90663805641655	0.11575262015982
C	-1.41080758785408	4.68997000101603	0.08613331129861

C	-0.71251554950466	3.46493526726685	0.06976499915796
C	-2.56986787608636	2.01282651886849	-0.24294746159353
C	-3.26945645990807	0.76585273810979	-0.25512597702834
C	-4.65661024472216	0.79602336479797	-0.56892431718816
C	-5.40794231600764	-0.36564853594101	-0.56954913688732
C	-4.77827451888835	-1.59419934006437	-0.25217038144998
C	-3.42078572032884	-1.70221046104701	0.05489260492667
C	-2.62039612608563	-0.49534377484596	0.04547392352907
H	-5.11921441823656	1.76325834070344	-0.80770183086085
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H	-3.17556919743299	2.88794624143248	-0.53410302559788
H	-2.50530328671287	4.69210504312346	0.09493487539023
H	-1.28227519340944	6.84928036292774	0.13306689185355
H	1.22844794576896	6.86901651733624	0.18034054954081
H	2.48683513250472	4.73731013791284	0.19432588478324
H	3.26167715879085	2.93162198268066	-0.11643967399292
H	5.22958197451898	1.82709227796556	-0.11561543801869
H	5.42891198858723	-2.47079052455335	-0.19378854805175
H	-6.47726349168531	-0.34470404696019	-0.81069760390617
H	6.57961390815396	-0.28440599178419	-0.19378051070169
C	-2.76154201637274	-3.05481261106838	0.38806131473891
C	-1.65820541000343	-3.35964197280841	-0.65372711810952
C	-2.15276877299499	-3.00324053599282	1.81257539100187
C	-3.77543998233641	-4.21613715520017	0.35519622098065
H	-2.09001077207356	-3.42435344469825	-1.66875013388094
H	-0.89071907583046	-2.57559179839860	-0.65992641049254
H	-1.17147637595771	-4.32514204408544	-0.42039458641770
H	-2.94495152362490	-2.82967557203651	2.56465681130506
H	-1.65947393290504	-3.96514816979392	2.04827192195538
H	-1.40828062971909	-2.19908352583188	1.89957886618757
H	-3.25644448530732	-5.15966110077708	0.60373909127440
H	-4.58913629255234	-4.07960293688816	1.09145189503974
H	-4.22981415361112	-4.34071349947100	-0.64469718257953
C	2.72388294757360	-3.05802572324448	-0.15084196854611
C	1.80685876091457	-3.31739643602656	1.07046858441045
C	1.89877558364780	-3.05933979281860	-1.46322906081190
C	3.73155287737446	-4.22368183468676	-0.22457024500503
H	2.39583924276731	-3.30120068507749	2.00658795545216
H	1.01626419815791	-2.56010094954615	1.14376662749033
H	1.33339484857941	-4.31301217394996	0.97986511137907
H	2.57084854278141	-2.96382020257080	-2.33522552451494
H	1.33691663152782	-4.00700297788641	-1.56127212277724
H	1.18509208194202	-2.22246333924373	-1.50077629695731
H	3.17828258873316	-5.17624197173049	-0.31242435248526
H	4.39556142026607	-4.14603136079379	-1.10455269251542
H	4.36198370663948	-4.28522009850177	0.68209139211213
I	0.04487332877798	0.74559689116806	-2.70924619291914
F	0.01279594431917	0.86612001252990	2.16015816619055

[GaClF(Salphen)]⁻

Ga	0.00865702937499	0.61634462690828	0.38393720715578
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N	1.34396808906203	2.22481274333915	0.10868854776855
C	2.75082811896515	-0.49352320631220	0.07276275831530
O	-1.54123888885182	-0.60964260142451	0.55894856067409
N	-1.33273375008815	2.21685726378053	0.08609210475729
C	3.58875090657406	-1.67069076378034	-0.11787011987301
C	4.93555419162116	-1.48804847663708	-0.42067687033464
C	5.52487553807013	-0.20958453639149	-0.59655593357342
C	4.72836743118567	0.91494482600950	-0.49562641697044
C	3.34205333923411	0.81729523019091	-0.17702652915692
C	2.61794201562950	2.05313143336197	-0.13535033628500
C	0.71994137858519	3.46933992909444	0.17218439225619
C	1.39356349566824	4.70506970558960	0.28725270145496
C	0.68750737347666	5.91022859651787	0.36216770977329
C	-0.71839576886536	5.90371238366110	0.34911746991775
C	-1.40908267177357	4.69068683629158	0.25994209765384
C	-0.71808452713970	3.46390584027497	0.15692896456061
C	-2.57286660423241	2.03030806642688	-0.28643457957051
C	-3.28571053221644	0.78816654835642	-0.33894204601345
C	-4.62340511162178	0.84815387816880	-0.82527562451811
C	-5.41050901755599	-0.28541604848563	-0.90585339770472
C	-4.86809788955886	-1.53147208142214	-0.50022599620628
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C	-2.72975726923440	-0.49118403417568	0.08728692581784
H	-5.01957553469860	1.82408568961172	-1.13875012858519
H	-5.51002764652058	-2.41420568511003	-0.58474736863048
H	-3.15562924279552	2.90773959421011	-0.62736144357080
H	-2.50356309539059	4.68642908031980	0.29792176344871
H	-1.27661440546644	6.84415561391469	0.43520530783092
H	1.23489882661074	6.85627272650274	0.45663267546616
H	2.48713808873279	4.71921577874043	0.34048389292130
H	3.23293356239832	2.94424213599727	-0.36501285067472
H	5.15370741289922	1.91447888776814	-0.66251166472435
H	5.57977666260471	-2.36374383163866	-0.54889066215356
H	-6.43914565007557	-0.23146032249890	-1.28191154985734
H	6.59234656753862	-0.12515042679429	-0.83282285246302
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C	-1.75019992201657	-3.36446573202770	-0.47917167771139
C	-2.59591607059461	-3.03206881421275	1.88905268923420
C	-4.01348360901504	-4.18441386776090	0.18758352933029
H	-2.02346018912617	-3.40005220180682	-1.54940974612566
H	-0.97277928451736	-2.60004758612838	-0.35344487403857
H	-1.32900113367937	-4.34774063929906	-0.19550654868277
H	-3.48085318409283	-2.83070424572767	2.52162458783965
H	-2.18287039239736	-4.01703038804158	2.18027244886389
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C	2.24394538379118	-3.32157665663210	1.29780948957113
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H	1.19606397128556	-2.35372417118371	-1.20815221237910
H	3.48012589729367	-5.17286506697926	-0.21846577764879
H	4.51176439334306	-4.12119497561577	-1.21864345619646
H	4.75056178410873	-4.18728718343172	0.55597258579199
Cl	-0.02658210109702	0.26304338696727	-1.96811963499342
F	0.04737014410035	0.87802934831089	2.19949822011121

[GaBrF(Salphen)]⁻

Ga	0.00518241942213	0.63154145399106	0.32691189783358
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N	1.34336310749913	2.22856596138097	0.08440747142184
C	2.73730493395169	-0.49906196282110	0.05037488543760
O	-1.50044953509422	-0.63549505672027	0.41809740719953
N	-1.33821808047761	2.22501887009267	0.07813594422461
C	3.58499116600263	-1.67621137704715	-0.07866410436379
C	4.94556980087556	-1.49395282900321	-0.31427243746465
C	5.54203422083745	-0.21632945899313	-0.46737688041768
C	4.74314061928063	0.90894761119424	-0.40118975280382
C	3.34288210843428	0.81214869428769	-0.15069988842319
C	2.62328735454334	2.05110035657954	-0.12331072780410
C	0.71982358128508	3.47528971995440	0.12499491624917
C	1.39697092602173	4.71205497191474	0.20339219957229
C	0.69552283427269	5.92010790119666	0.25982186592505
C	-0.71053009635355	5.91642303441319	0.26067379523884
C	-1.40418932370805	4.70398058800564	0.20286722183601
C	-0.71830600479517	3.47240292974270	0.12175638027020
C	-2.60071986499900	2.04202250223759	-0.21458921956594
C	-3.31731651405456	0.80158993696330	-0.24741123046841
C	-4.69317758632717	0.87993980853939	-0.61041376905864
C	-5.48839523692217	-0.24923110295014	-0.66228438936370
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H	-1.26638129327704	6.85966150808229	0.32882793317697
H	1.24616846256909	6.86661409499015	0.32521861166369
H	2.49102740294250	4.72627278476053	0.23962937391466
H	3.25018589618842	2.93954717848559	-0.32575252294984
H	5.17765977982095	1.90843620420556	-0.54154297883456
H	5.59635034936652	-2.36971790898998	-0.40125299261909
H	-6.54655696694463	-0.18058336293142	-0.94130071187567
H	6.61944976790641	-0.13243089091164	-0.65288724932968
C	-2.97327725368257	-3.06007063446599	0.29835837875758
C	-1.83401863518590	-3.35156196689670	-0.71066543715064

C	-2.42072664291258	-3.10306982266949	1.74617873866132
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H	-2.22329633309929	-3.35386988128354	-1.74496668491184
H	-1.04303451239576	-2.59277833520505	-0.64672040516215
H	-1.38910195244096	-4.34380005520921	-0.50517197587027
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H	-1.63926515048332	-2.34407529847827	1.89539570021664
H	-3.53963902769494	-5.15720197544544	0.38192385502477
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H	-4.43691224646783	-4.24287746060523	-0.85733535311689
C	2.94712103706138	-3.07933957573635	-0.01539513478631
C	2.20091936888492	-3.29535313397642	1.32598863368372
C	1.96465936161930	-3.22530450345162	-1.20572323792863
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[GaIF(Salphen)]:

Ga	0.00789004094777	0.65667890628924	0.35128452535930
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C	2.71024385785719	-0.50434295104840	0.04794895970233
O	-1.45112776202011	-0.63983425295918	0.34280347884787
N	-1.33504797556254	2.22529462593475	0.08403306816601
C	3.54784058105627	-1.68846027111485	-0.05386292143514
C	4.92206658563024	-1.51698711073134	-0.20849158996583
C	5.53990485203737	-0.24447569440057	-0.30236238667124
C	4.75179659967892	0.88926056108154	-0.25528891773562
C	3.33912236616146	0.80254335296260	-0.08364006299479
C	2.62968122587464	2.04687757974142	-0.07123549198635
C	0.72036958001372	3.47993016690612	0.10062514942464
C	1.39788622621329	4.71759747384512	0.14147244291038
C	0.69582474911587	5.92598339789216	0.17170474930488
C	-0.71007361322841	5.92148140339387	0.17783792489839
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C	-0.71674131030715	3.47605205531813	0.10023891339482
C	-2.60491757706039	2.03637114609497	-0.17531161576617
C	-3.31309123515455	0.79194624706739	-0.19806008204104
C	-4.70349429210481	0.86464818882447	-0.50238226769720
C	-5.48935881821165	-0.27131800285325	-0.54061517594838
C	-4.89396564940544	-1.53058985641465	-0.27716032874008
C	-3.54153245523634	-1.68756940080634	0.02001535632691

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H	3.26854826443470	2.93232516791098	-0.24133268687270
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C	-2.91479988467546	-3.07328146759652	0.27858769411830
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C	-2.29991283081547	-3.12081426630720	1.70110357774649
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H	-1.36730101466773	-4.34811338304584	-0.60370166176420
H	-3.08153804378718	-2.95518339214974	2.46605362872391
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C	2.07439799963358	-3.31107241329347	1.25041759443395
C	1.97788381635872	-3.20977276669087	-1.28864439453589
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H	2.57541184445753	-3.13754188856819	-2.21549191127073
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H	1.21985387408519	-2.41371799870661	-1.31435094851387
H	3.43372263197076	-5.19041944954953	-0.12264841020315
H	4.55019255645252	-4.15595399045952	-1.04747348533068
H	4.63618472147898	-4.19560700430457	0.74206676852014
I	-0.02635191179901	0.56397183476336	-2.62565579323320
F	0.04410169354542	0.80928905624105	2.17430493680197

[InClF(Salphen)]⁻

H	3.21074327518559	-6.09544265679336	5.37877199641507
H	1.75055469692087	-5.22373990456772	4.84698693647998
C	2.56212985853137	-5.22746062954817	5.59727362167358
H	4.74604264440784	-4.64634999467519	3.95746996820305
H	2.11155497792653	-5.38940998234024	6.59433318462333
H	3.22470672393366	-3.91462831719653	3.36129678219917
H	9.42410814542433	-3.60752330574861	0.35809623430113
C	4.01925512435817	-3.82861783336788	4.12527672971850
C	3.40489665528698	-3.93681224230164	5.54634993380355

H	0.68302961814077	-3.71734016815979	6.03018900626962
C	9.28184369062330	-2.53304473610408	0.14113411330893
H	9.72339250656085	-3.12801211230625	2.72427601722343
H	5.10595192874690	-4.99641123454128	6.43025146919091
C	7.23145308788870	-2.56785050104646	1.56970310127682
H	8.67578099806936	-2.45876994529937	-0.78015453135482
C	4.52254692637950	-4.07318095319697	6.61171178691620
H	4.52249019023743	-2.86426905246577	3.96605451238621
C	1.17821507262524	-2.74090822428284	6.00762853037304
H	10.27814152740719	-2.09858387214265	-0.06376329452614
C	2.55385593118523	-2.67852047431041	5.80813073630415
C	9.51480756971201	-2.05106813860921	2.57458255604600
C	8.59241472221870	-1.85754742734642	1.34398845349287
H	4.08268388271374	-4.14064554234684	7.62466447036656
H	-0.71524404848242	-1.69891968089118	6.33005443573248
C	0.36405430799692	-1.58893092439907	6.17042793479553
H	10.48047184868576	-1.53469201801851	2.41682784214048
H	9.04821894883392	-1.64690169055553	3.48370386860622
H	5.20093888731648	-3.20934738120344	6.58362700743087
C	3.20268854503475	-1.36969810580768	5.80030422483807
H	9.14775756981652	-0.31945114815382	-0.89494634171524
C	8.32894181967317	-0.35934347614382	1.09417596510261
O	4.47801632028752	-1.29212547522352	5.73445775494999
C	0.94711153136930	-0.33863805923789	6.09748182002122
C	8.64940309377550	0.25940362929287	-0.11029517151173
O	7.47914759086092	-0.08301637246243	3.29264479116405
C	2.35081092211472	-0.18609978478610	5.89409099037098
C	7.68129747492735	0.43098468125359	2.13812360382947
H	0.33248505046903	0.56806550861788	6.18852447120995
In	5.73038180576779	0.20643423228260	4.65153820160908
C	8.34766581477099	1.61840255478931	-0.38978773904571
C	2.83141509912302	1.15827380620117	5.79344670279884
H	8.62897814264724	2.05472210272665	-1.35568299035324
C	7.30979315690995	1.80777053575809	1.81884330576497
Cl	7.25267568004887	0.27550111715124	6.55363130921644
N	4.04236535197455	1.57829735437268	5.51147557576711
C	7.67658755752919	2.36609444295040	0.55847072870976
H	2.05002030708740	1.93106864484868	5.94282602609539
N	6.04479045328211	2.38480690039993	3.86472239928595
C	6.58456894065664	2.66875695660045	2.70283973413839
C	4.38459077253591	2.92900241993684	5.53479284086093
H	7.40537442948991	3.41127817269797	0.35317481966053
C	5.44307061170488	3.35585456768159	4.66278254453446
H	6.44335677531663	3.69925636389358	2.31775944546039
C	3.78599165684782	3.87471448927005	6.39575927668217
H	3.01871336596994	3.53772793188429	7.10113174095983
C	5.85074671429832	4.70748147885058	4.69375956651582
C	4.18772236060223	5.21594942195462	6.38870281033881
H	6.69567390382842	5.02044319761261	4.07082836204474
C	5.22258933569637	5.63357325735405	5.53529752672900
H	3.71460159772382	5.92935673181079	7.07474490262169
H	5.56456702291390	6.67581858699241	5.54927874713123

H	6.64678113582343	-2.57529284410422	0.63151452613290
H	6.62412817839953	-2.05706906593956	2.33001080087669
H	7.39279125530516	-3.61720676958001	1.88254729129004
F	4.69716895658170	-0.48739904198036	3.04262603251730

[InBrF(Salphen)]:

H	3.20900796169278	-6.09631284559584	5.37169316465162
H	1.73911903721053	-5.22502723338149	4.86696879657146
C	2.56364589697654	-5.22924499155093	5.60296287800242
H	4.72044993164516	-4.64150142416625	3.92667713588148
H	2.13087270345013	-5.39316226545328	6.60753218789846
H	3.18479185416843	-3.91833551210648	3.35790920255930
H	9.42585730724005	-3.60486690408051	0.34820395969058
C	3.99271432953559	-3.82737128347963	4.10722575502209
C	3.40455761386262	-3.93787200326326	5.53927961560784
H	0.69094090008117	-3.72199696968783	6.06713930328560
C	9.29099238198255	-2.52842549638473	0.13644869101434
H	9.69364796645657	-3.14435606454769	2.71937416567580
H	5.12014815742311	-4.99938149674606	6.39141421158259
C	7.21984491362510	-2.56398129288376	1.53393850352673
H	8.69849709061685	-2.44564504017451	-0.79289746492996
C	4.54087375004110	-4.07597719175503	6.58458946253998
H	4.48827936719228	-2.86080944838678	3.93704841826846
C	1.18442273312338	-2.74492735057315	6.03833283111345
H	10.29187038827676	-2.09681490543651	-0.05137981258627
C	2.55695265980749	-2.68064415562409	5.81748792658053
C	9.49182257498873	-2.06534003389782	2.57583311726975
C	8.58740831729376	-1.85817924412843	1.33416198083036
H	4.11885316323949	-4.14469600205745	7.60498465226098
H	-0.70470174642691	-1.70563401575780	6.39188105585365
C	0.37185300560839	-1.59435147071486	6.21564665531502
H	10.46179807472604	-1.55222386032118	2.43498594138980
H	9.01626356406347	-1.66634230810470	3.48249256124647
H	5.21951415434782	-3.21281372331128	6.54671257782933
C	3.20366998100948	-1.37150962995328	5.80247328297856
H	9.17827460364591	-0.30895053536210	-0.88767468931188
C	8.33389043381148	-0.35713963740017	1.09055663572227
O	4.47910317564044	-1.29417944550569	5.71871517603069
C	0.95253033651434	-0.34334665271978	6.13556377360377
C	8.67229753175999	0.26737670926980	-0.10612206200066
O	7.45874594127114	-0.09380778253701	3.27916901549956
C	2.35278184116705	-0.18880672510007	5.91082966360412
C	7.67676564242135	0.42959808737906	2.13077480523534
H	0.33856095555892	0.56258279402823	6.23747504234708
In	5.71210977267871	0.20961769730010	4.63037594507600
C	8.37973368030663	1.62910540471798	-0.38095585065864
C	2.82841227185209	1.15742078561581	5.80514908238407
H	8.67488485180565	2.07031404413297	-1.34045032366312
C	7.31559439208026	1.81000461022225	1.81640797044637
Br	7.33380812014410	0.32272495072361	6.66127994079875
N	4.03332981434674	1.58120323114029	5.50469886568493
C	7.70030189015922	2.37376536735739	0.56365795942158

H	2.04717983420923	1.92736416707674	5.96875649695345
N	6.03262307268313	2.38788700870750	3.85133330400521
C	6.58581109680957	2.67225187669058	2.69605849280140
C	4.37598204880961	2.93186508158221	5.52603432182745
H	7.43653170947374	3.42143721638641	0.36161914233457
C	5.43224150848677	3.35851724753155	4.65095791204434
H	6.45567585356455	3.70481384891536	2.31293313936272
C	3.78135616347777	3.87747369017473	6.38993445009700
H	3.01705866008215	3.54074953062085	7.09857878702987
C	5.84135923283711	4.70979985735854	4.68258306358577
C	4.18379049184557	5.21821946269986	6.38260102985417
H	6.68565370453244	5.02271436243855	4.05887691333857
C	5.21649963601454	5.63567282296405	5.52635167020160
H	3.71371294249872	5.93134342203697	7.07098053835617
H	5.55972460217196	6.67747826215421	5.54058477484126
H	6.65138440928683	-2.56498130187686	0.58573515000583
H	6.60076173057910	-2.05513214108265	2.28621147252850
H	7.37171053399674	-3.61542874554992	1.84441298102829
F	4.66880948021736	-0.47333440856673	3.02305465265275

[InIF(Salphen)]:

H	3.20616279623778	-6.10624552514417	5.39011211173439
H	1.72951360218606	-5.23961518001642	4.89743506783170
C	2.56236114873798	-5.23876777025964	5.62399522385409
H	4.69842477277660	-4.65741774244035	3.91966477593257
H	2.14131805641913	-5.39776191150676	6.63428888028354
H	3.15533053901575	-3.93861917979548	3.36542834160069
H	9.42074791257538	-3.60477313662948	0.32920937015944
C	3.97201212022938	-3.84307038634372	4.10453160553439
C	3.40115046350616	-3.94686113603355	5.54420230637910
H	0.69352541515336	-3.73287519938124	6.10154116140368
C	9.29465866102565	-2.52604686870376	0.12392035800747
H	9.65913960152708	-3.16655552997297	2.70623279473880
H	5.12590373828904	-5.00439712565343	6.38139677217603
C	7.20553894620393	-2.55962190817797	1.49426808012130
H	8.71456115511470	-2.43298490224970	-0.81224835901171
C	4.54999284773380	-4.07936080103750	6.57643173925475
H	4.46625037550511	-2.87767251048172	3.92420496957610
C	1.18507961258468	-2.75524258380721	6.06282632350391
H	10.30036494172792	-2.09902688551690	-0.04771227045366
C	2.55496342742906	-2.68939647686184	5.82614472308302
C	9.46752528590480	-2.08491043456031	2.56914900689646
C	8.58014979197139	-1.86105087745291	1.31815018657044
H	4.14051605219203	-4.14188083986924	7.60226468525976
H	-0.70162320017033	-1.71767740156168	6.43389723757676
C	0.37260541375372	-1.60546588129660	6.24469822832982
H	10.44310727383649	-1.57841044230246	2.44454850169291
H	8.98459795253249	-1.68991873383288	3.47356436059734
H	5.22903168233281	-3.21728573459213	6.52604980493294
C	3.19857486602971	-1.37929704812841	5.79830678319998
H	9.20876980794297	-0.29828739813139	-0.88374730716397
C	8.33939914685128	-0.35642238556085	1.08357578638156

O	4.47387357418985	-1.30222272294268	5.69806998957425
C	0.95018190163873	-0.35390103712931	6.15386374584603
C	8.69688622452916	0.27520804036930	-0.10405125346003
O	7.43978623250301	-0.10490092806799	3.26300359842463
C	2.34769354220329	-0.19751632723020	5.91282010289516
C	7.67534792008149	0.42712186044807	2.12081126431981
H	0.33569875255214	0.55112521105960	6.25989926590643
In	5.68883838459575	0.20633042819830	4.60089561034827
C	8.41704388248232	1.64076964036983	-0.37183291711680
C	2.81810560079477	1.15036686506642	5.80082688314875
H	8.72722104556549	2.08737063021089	-1.32402469522310
C	7.32721326084653	1.81198039252659	1.81360655105370
I	7.44384194964830	0.35135098998811	6.81059319378536
N	4.01860363309442	1.57716873204695	5.48740664503341
C	7.73119552958761	2.38293570300704	0.57017165852072
H	2.03654386589468	1.91784988696960	5.97292246603051
N	6.02205520670099	2.38630708588334	3.83609070954100
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C	4.36226834284798	2.92778977643081	5.50990057580101
H	7.47725451859282	3.43384610238986	0.37280085946032
C	5.42051344626409	3.35535552629107	4.63738388935620
H	6.47698393522210	3.71025785503775	2.31313636964294
C	3.76883552839736	3.87161018271719	6.37656931783963
H	3.00428716084857	3.53410652390579	7.08442453354974
C	5.83289399160384	4.70542716039228	4.67503249541753
C	4.17363667672572	5.21144081488739	6.37389688537823
H	6.67967914659119	5.01930147546162	4.05537232361954
C	5.20845617169201	5.62956884722115	5.52069008042879
H	3.70443805320514	5.92304978343047	7.06438850645930
H	5.55442223984986	6.67036413501816	5.53932225974581
H	6.64927408740933	-2.54936884710695	0.53889150508924
H	6.57964010280477	-2.05375018436549	2.24307990145116
H	7.34647973295078	-3.61455919651158	1.79785568186012
F	4.63572053582075	-0.46297167760295	2.99511240135141

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