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Experimental Procedures

General considerations

All preparations were performed under an inert atmosphere of dinitrogen by means of Standard Schlenk-line or glovebox (GS-Systemtechnik and MBraun) techniques. Traces of oxygen and moisture were removed from the inert gas by passing it over a BASF R 3-11 (CuO/MgSiO₃) catalyst, through concentrated sulfuric acid, over coarsely granulated silica gel, and finally P₄O₁₀. *n*-Hexane was freshly collected from a Solvent Purification System by M. Braun (MB SPS-800). THF and toluene were used as p.a. grade and distilled from Na/benzophenone prior to use. C₆D₆ was dried by distillation from Na/benzophenone. Indium(I) iodide was purchased from Onyxmet, while potassium bis(trimethylsilyl)amide (KHMDs) was purchased from Sigma Aldrich and Oxygen from Linde. These starting materials were used as delivered. Sulfur was sublimated before use. The ligand precursor **1** was prepared according to published procedures.^[1]

Characterization

The NMR spectra were recorded with a Bruker Avance 400 and a Bruker Fourier 300 spectrometer (T = 300 K) with δ referenced to external tetramethylsilane (¹H and ¹³C). ¹H and ¹³C NMR spectra were calibrated by using the solvent residual peak (C₆D₅H: δ (¹H) = 7.16) and the solvent peak (C₆D₆: δ (¹³C) = 128.06), respectively. Elemental analysis were performed with a Vario MICRO cube (Elementar Analysensysteme GmbH); the presence of residual solvent molecules was verified by ¹H NMR spectroscopy.

Synthetic procedures

IV: THF (15 mL) was added to a mixture of InI (0.97 g, 4.00 mmol), KHMDs (0.80 g, 4.00 mmol), and **1** (1.09 g, 2.00 mmol) at -78 °C. Warming to room temperature and stirring in the absence of light for 22 h produced a dark brown suspension. The volatiles were removed, and the grey residue was extracted with *n*-hexane (20 mL). The volatiles were removed in vacuum, yielding a red solid, which was redissolved in toluene (10 mL). Oxygen was bubbled through the toluene solution and the mixture was afterwards stirred for one day. Yellow crystals (126 mg, 8 % with respect to **1**) suitable for X-Ray diffraction analysis were obtained from a concentrated toluene solution at room temperature; ¹H NMR: (300 MHz, C₆D₆): δ = 0.91 [d, 12H, ³J_{HH} = 6.5 Hz, CHMe₂], 1.11 [d, 12H, ³J_{HH} = 6.8 Hz, CHMe₂], 1.33 [d, 12H, ³J_{HH} = 6.8 Hz, CHMe₂], 1.56 [d, 12H, ³J_{HH} = 6.5 Hz, CHMe₂], 1.61 [s, 12H, CMe], 1.62 [s, 12H, CMe], 3.05-3.16 [m, 8H, CHMe₂],

3.42 [br, 4H, CH₂], 4.10 [br, 4H, CH₂], 4.49 [s, 4H, CH], 7.04-7.07 [m, 6H, ArH], 7.22-7.25 ppm [m, 6H, ArH]; ATR-IR: $\tilde{\nu}$ = 3057, 2955, 2922, 2862, 1555, 1513, 1461, 1435, 1398, 1317, 1251, 1238, 1188, 1091, 1016, 1010, 934, 853, 793, 734, 658 cm⁻¹; elemental analysis calcd (found) C₇₂H₁₀₄In₄N₈O₂·0.60 C₇H₈: C 56.21 (56.44), H 6.74 (6.63), N 6.88 (7.15); m.p. decomposition above 113 °C.

Due to the poor solubility in different solvents (C₆D₆, THF-d₈, Toluene-d₈), only small signals were visible in the ¹H NMR spectrum by the measurement with 256 scans. No signals were visible in the ¹³C{¹H} NMR spectrum by the measurement with 4096 scans.

In-situ NMR experiment (IV): THF (15 mL) was added to a mixture of InI (0.97 g, 4.00 mmol), KHMDS (0.80 g, 4.00 mmol), and **1** (1.09 g, 2.00 mmol) at -78 °C. Warming to room temperature and stirring in the absence of light for 22 h produced a dark brown suspension. The volatiles were removed, and the grey residue was extracted with *n*-hexane (20 mL). The volatiles were removed in vacuum, yielding a red solid. A portion of it was dissolved in C₆D₆ and transferred to a Young NMR tube. The inert gas atmosphere (N₂) was replaced by oxygen and the tube was immediately transferred to the NMR spectrometer. The respective spectrum is shown in Figure S1.

V: THF (50 mL) was added to a mixture of InI (2.42 g, 10.0 mmol), KHMDS (1.99 g, 10.0 mmol), and **1** (2.71 g, 5.00 mmol) at -78 °C. Warming to room temperature and stirring in the absence of light for 22 h produced a dark brown suspension. The volatiles were removed, and the grey residue was extracted with *n*-hexane (50 mL). The volatiles were removed in vacuum yielding a red solid. Sulfur (0.51 g, 2.00 mmol) and toluene (20 mL) were added to the solid and the mixture was stirred for eight days. Yellow crystals (0.21 g, 0.13 mmol, 5% with respect to **1**); suitable for X-Ray diffraction analysis were obtained from a concentrated toluene solution containing five drops of THF at room temperature. ¹H NMR: (400 MHz, C₆D₆): δ = 1.17 [d, 12H, ³J_{HH} = 6.8 Hz, CHMe₂], 1.39 [d, 12H, ³J_{HH} = 6.8 Hz, CHMe₂], 1.43 [s, 12H, CMe], 1.46-1.49 [m, 24H, CHMe₂], 1.54-1.58 [m, 4H, CH₂], 1.64 [s, 12H, CMe], 3.41 [br, 4H, CH₂], 3.54 [sept, 4H, ³J_{HH} = 6.8 Hz, CHMe₂], 3.61 [sept, 4H, ³J_{HH} = 6.8 Hz, CHMe₂], 4.57 [s, 4H, γ -CH], 7.18-7.19 [m, 8H, ArH], 7.21-7.23 [m, 4H, ArH]; ¹³C{¹H} NMR: (101 MHz, C₆D₆): δ = 21.1 [CMe], 23.1 [CMe], 25.0 [CHMe₂], 25.1 [CHMe₂], 25.5 [CHMe₂], 26.6 [CHMe₂], 28.4 [CHMe₂], 28.6 [CHMe₂], 49.5 [CH₂], 97.5 [γ -CH], 123.5 [*m*-C(Dipp)], 124.9 [*m*-C(Dipp)], 126.2 [*p*-C(Dipp)], 142.9 [*o*-C(Dipp)], 144.8 [*o*-C(Dipp)], 145.5 [*ipso*-C(Dipp)], 166.7 [CN], 167.3 ppm [CN]. ATR-IR: $\tilde{\nu}$ = 3058, 2956, 2924, 2864, 1649, 1624, 1558, 1513, 1434, 1395, 1316, 1264, 1186, 1099, 1074, 1019, 999, 934, 849, 793, 757, 701, 612, 523 cm⁻¹; Despite repeated attempts, satisfactory elemental analyses could not be obtained; m.p. decomposition above 130 °C.

VI:

Route a: THF (15 mL) was added to a mixture of InI (0.48 g, 2.00 mmol), KHMDS (0.40 g, 2.00 mmol), and **1** (0.54 g, 1.00 mmol) at -78 °C. Warming to room temperature and stirring in the absence of light for 22 h produced a dark brown suspension. The filtrate was added to sulfur (0.26 g, 1.00 mmol) and the reaction mixture was stirred for 6d. The volatiles were removed, and the green residue was extracted with toluene (20 mL). Filtration and concentration of the filtrate to about a half gave rise to **VI** as yellow crystals suitable for an X-ray diffraction analysis. (0.17 g, 0.25 mmol, 25%).

Route b: THF (20 mL) was added to a mixture of KHMDS (0.20 g, 1.00 mmol), S₈ (0.13 g, 0.50 mmol), and **1** (0.27 g, 0.50 mmol) at room temperature. The solution was stirred for one day. The volatiles were removed, and the residue was extracted with toluene (10 mL). Filtration and concentration of the filtrate to about one third gave rise to yellow crystals of **VI** suitable for an X-ray diffraction analysis. (0.09 g, 0.13 mmol, 27%).

¹H NMR: (400 MHz, C₆D₆): δ = 1.13-1.15 [m, 12H, CHMe₂], 1.21 [t, 12H, CHMe₂], 2.20 [s, 6H, CMe], 2.31 [s, 6H, CMe], 2.50-2.54 [m, 2H, CH₂], 2.80-2.88 [m, 2H, CH₂], 2.91-3.07 [m, 4H, CHMe₂], 7.04-7.06 [m, 1H, ArH], 7.11-7.15 [m, 2H, ArH], 7.18-7.20 [m, 3H, ArH], 13.36 ppm [br, 2H, NH]; ¹³C{¹H} NMR: (101 MHz, C₆D₆): δ = 17.4 [CMe], 22.4 [CMe], 23.1 [CHMe₂], 23.3 [CHMe₂], 24.0 [CHMe₂], 24.7 [CHMe₂], 28.5 [CHMe₂], 28.9 [CHMe₂], 48.4 [CH₂], 96.4 [γ-CS], 123.6 [*m*-C(Dipp)], 123.7 [*m*-C(Dipp)], 124.5 [*p*-C(Dipp)], 138.2 [*o*-C(Dipp)], 138.3 [*o*-C(Dipp)], 145.5 [*ipso*-C(Dipp)], 166.5 [CN], 172.2 ppm [CN]; elemental analysis calcd (found) C₃₆H₅₂N₄S₄·0.80 C₇H₈: C 67.27 (66.99), H 7.92 (7.70), N 7.54 (7.30).

Crystallographic details

The single crystal X-ray diffraction data were recorded on a GV-50 diffractometer with Titan^{S2} detector from Rigaku Oxford Diffraction (formerly Agilent Technologies) applying Cu K α radiation ($\lambda = 1.54184 \text{ \AA}$) **IV**, **V**, and **VI**. Empirical multi-scan^[2] and analytical absorption corrections^[3] were applied to the data. Using Olex2,^[4] the structures were solved with SHELXT^[5] structure solution program using Intrinsic Phasing and least-square refinements on F^2 were carried out with SHELXL.^[6] For all single-crystals X-Ray structure determinations, the non-hydrogen atoms were refined anisotropically, while all hydrogen atoms were located in idealized calculated positions and were refined isotropically according to the riding model.

IV: Maxima in the Fourier difference maps of **IV** indicated the presence of a second species, which allowed for the refinement of a second In_4 ring (0.024(1)) without bridging oxygen atoms. In this compound, also unresolved residual electron density around a center of inversion was present, which could be assigned a disordered solvent molecule of toluene. The disorder could not be resolved completely, therefore the solvent mask of Olex2^[4] was applied and the presence of a solvent accessible void including 54 electrons was confirmed, which we assign a fully occupied toluene molecule. In the subsequent refinement a modified reflection file without the contribution of the solvent was used.

V: The data reduction was calculated as a twin structure. In this compound, unresolved residual electron density around a centre of inversion was present, which could be assigned two disordered solvent molecules of toluene and one disordered solvent molecule of tetrahydrofuran. The disorder could not be resolved completely, therefore the solvent mask of Olex2^[4] was applied and the presence of a solvent accessible void including 150 electrons was confirmed, which we assign two fully occupied toluene molecules and one fully occupied tetrahydrofuran molecule. In the subsequent refinement, a modified reflection file without the contribution of the solvent was used.

IV: The structure contains a toluene molecule.

CCDC 1934795 (**V**), 1934796 (**IV**) and 1934797 (**VI**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data for $C_{72}H_{104}In_4N_8O_2$ (IV), $C_{72}H_{104}In_4N_8S_4$ (V), and $C_{36}H_{52}N_4S_4$ (VI).

	IV	V	VI
Empirical formula	$C_{72}H_{104}In_4N_8O_{1.96}$	$C_{104}H_{144}In_4N_8OS_4$	$C_{43}H_{60}N_4S_4$
CCDC No.	1934796	1934795	1934797
Formula weight	1572.27	2109.78	761.19
Temperature/K	123.0(2)	123.0(1)	123.0(1)
Crystal system	triclinic	monoclinic	orthorhombic
Space group	P-1	C2/c	P2 ₁ 2 ₁ 2 ₁
a/Å	11.7484(2)	16.2239(1)	9.2217(2)
b/Å	12.8340(3)	24.1502(2)	18.6267(5)
c/Å	14.8693(3)	23.9945(2)	24.4822(6)
$\alpha/^\circ$	106.288(2)	90	90
$\beta/^\circ$	110.634(2)	100.9261(9)	90
$\gamma/^\circ$	98.668(2)	90	90
Volume /Å ³	1934.67(8)	9230.9(2)	4205.3(2)
Z	1	4	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.349	1.518	1.202
μ/mm^{-1}	9.744	9.144	2.328
F(000)	804.0	4368.0	1640.0
Crystal size/mm ³	0.166 x 0.06 x 0.056	0.148 x 0.08 x 0.06	0.26 x 0.083 x 0.077
Radiation	Cu K α (λ = 1.54184)	Cu K α (λ = 1.54184)	Cu K α (λ = 1.54184)
2 θ range for data collection/ $^\circ$	6.81 to 148.936	6.648 to 148.13	5.962 to 134.988
Index ranges	-14 $\leq h \leq 14$, -16 $\leq k \leq 15$, - 18 $\leq l \leq 18$	-18 $\leq h \leq 19$, -29 $\leq k \leq 29$, - 29 $\leq l \leq 25$	-8 $\leq h \leq 10$, -20 $\leq k \leq 22$, - 21 $\leq l \leq 29$
Reflections collected	41307	26078	12714
Independent reflections	7732 [R_{int} =0.0356, R_{sigma} =0.0236]	9159 [R_{int} =0.0398, R_{sigma} =0.0359]	7213 [R_{int} =0.0344, R_{sigma} =0.0472]
Data/restraints/parameters	7732/6/410	9159/0/409	7213/0/473
Goodness-of-fit on F^2	1.033	0.906	1.048
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0207$, $wR_2 =$ 0.0499	$R_1 = 0.0273$, $wR_2 =$ 0.0654	$R_1 = 0.0348$, $wR_2 =$ 0.0860
Final R indexes [all data]	$R_1 = 0.0232$, $wR_2 =$ 0.0510	$R_1 = 0.0350$, $wR_2 =$ 0.0671	$R_1 = 0.0389$, $wR_2 =$ 0.0884
Largest diff. peak/hole / e Å ³	1.04/-0.66	0.40/-0.87	0.64/-0.25

NMR and IR spectra

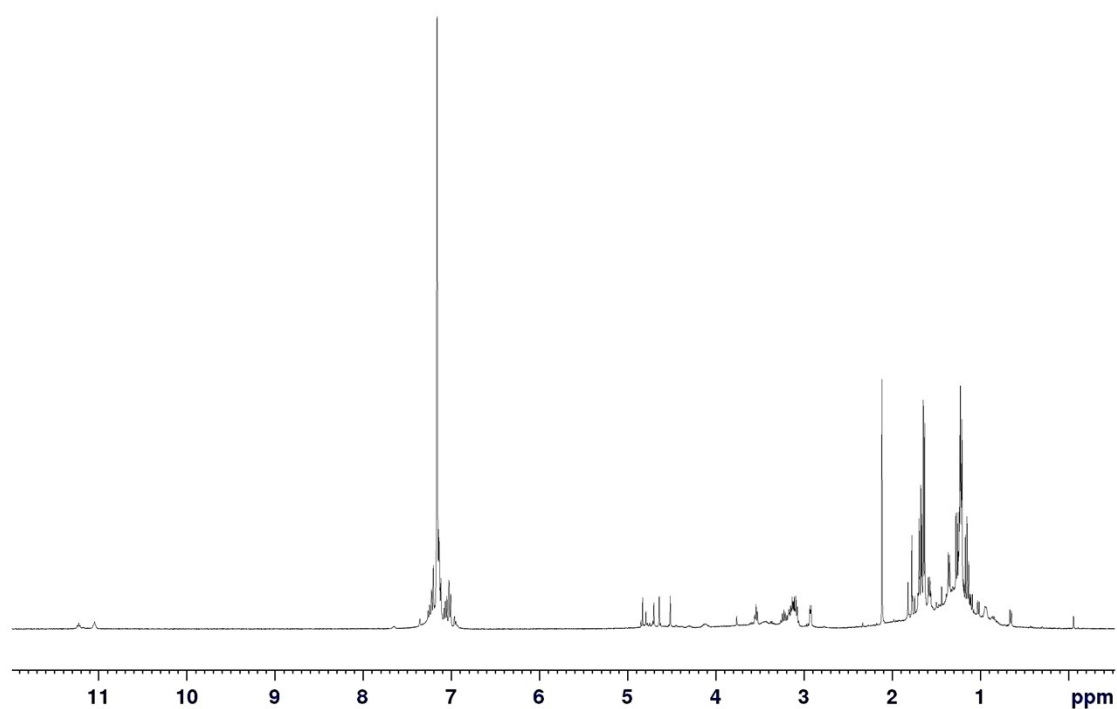


Figure S1: *In-situ* ^1H NMR spectrum (400 MHz) of the crude **IV** in C_6D_6 .

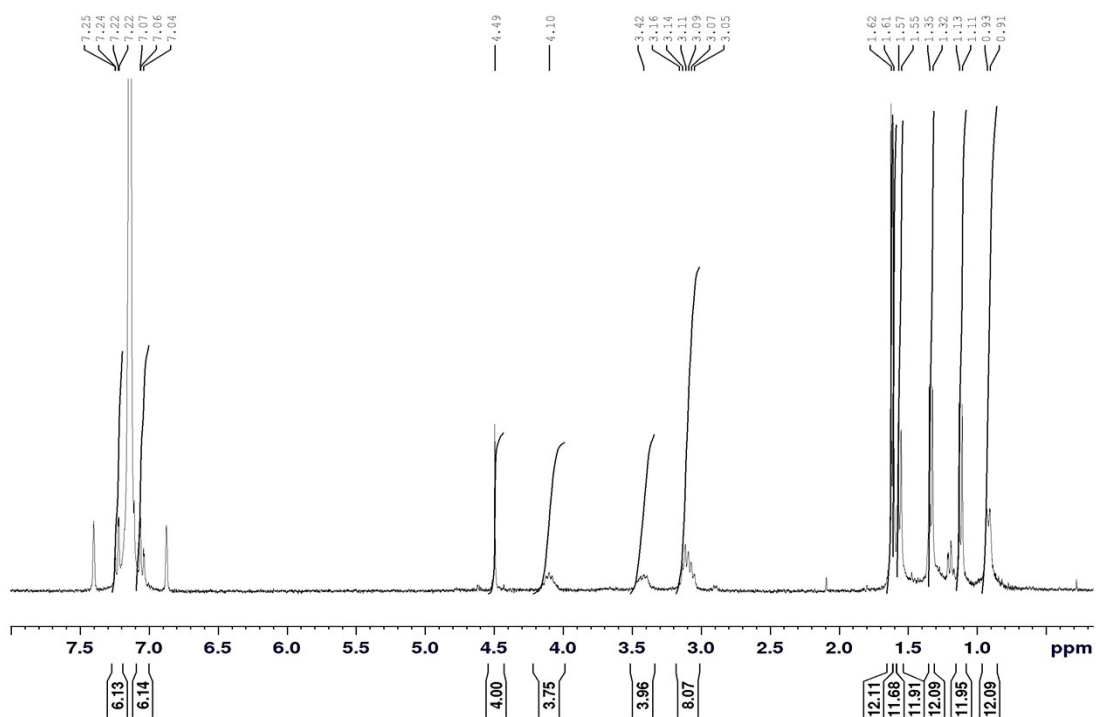


Figure S2: ^1H NMR spectrum (300 MHz) **IV** in C_6D_6 .

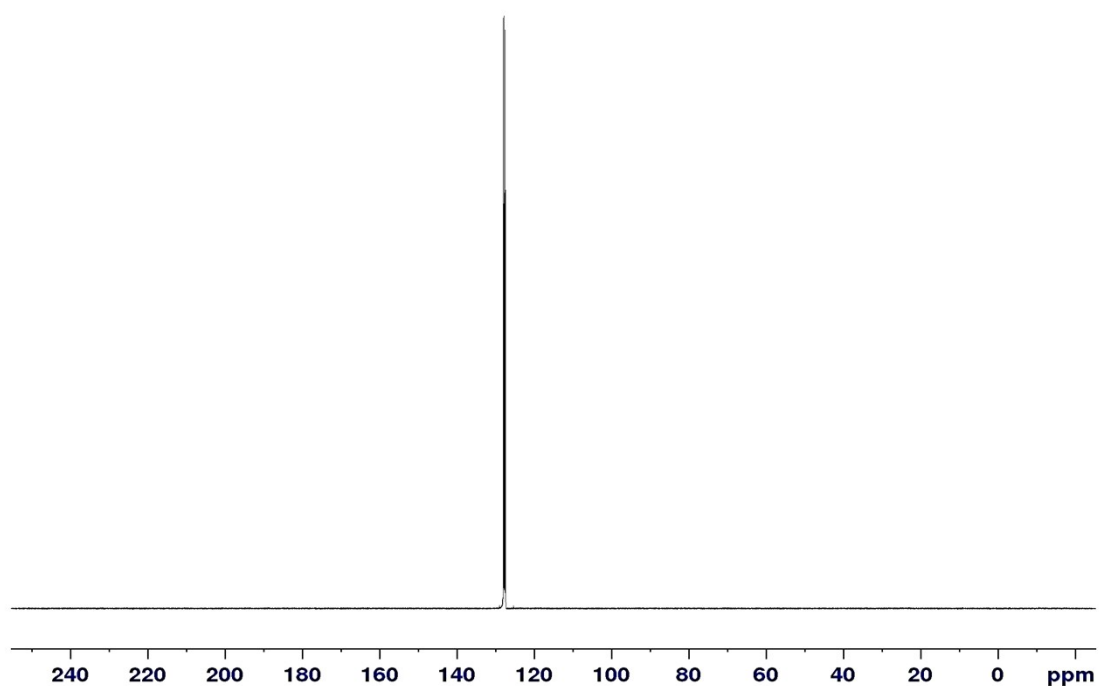


Figure S3: ^{13}C NMR spectrum (101 MHz) **IV** in C_6D_6 .

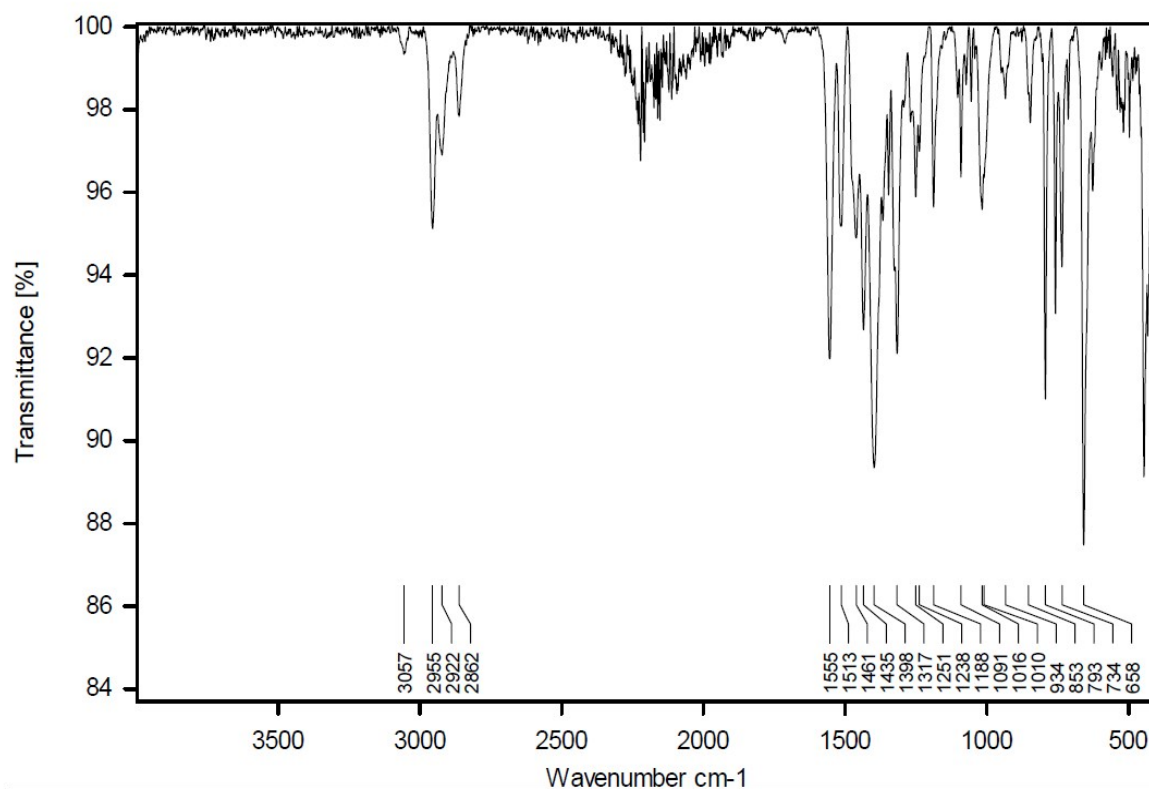


Figure S4: ATR-IR spectrum of **IV**.

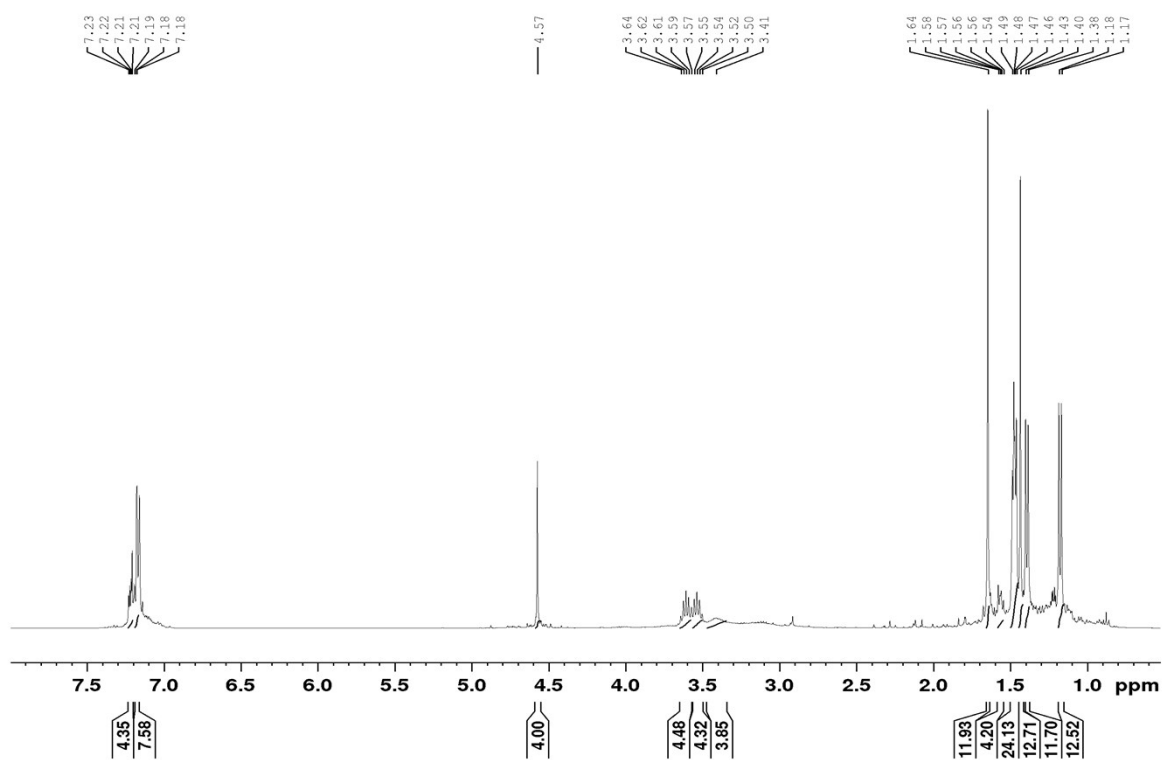


Figure S5: ¹H NMR spectrum (400 MHz) of **V** in C₆D₆.

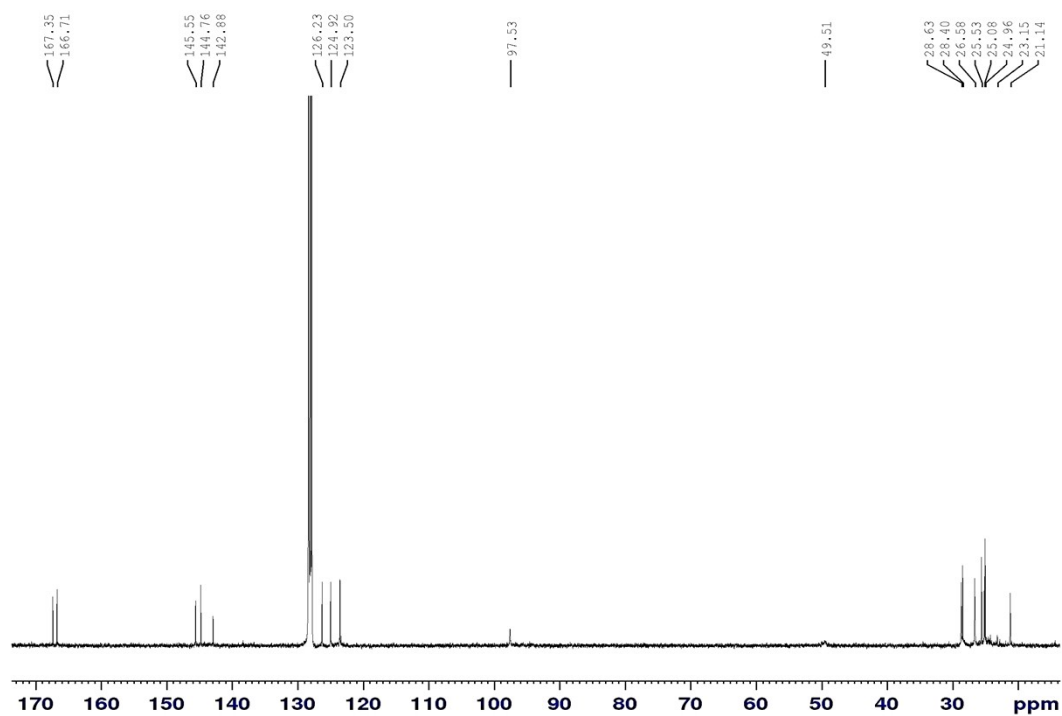


Figure S6: ¹³C NMR spectrum (101 MHz) of **V** in C₆D₆.

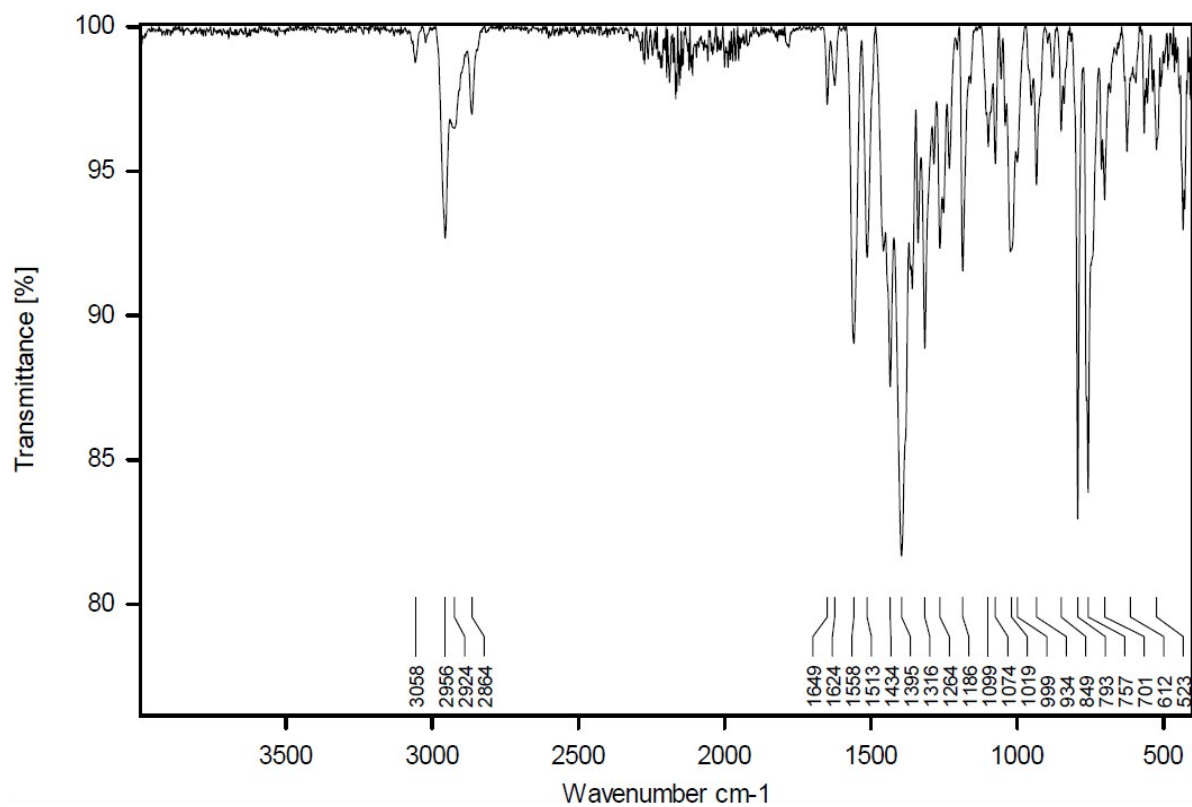


Figure S7: ATR-IR spectrum of **V**.

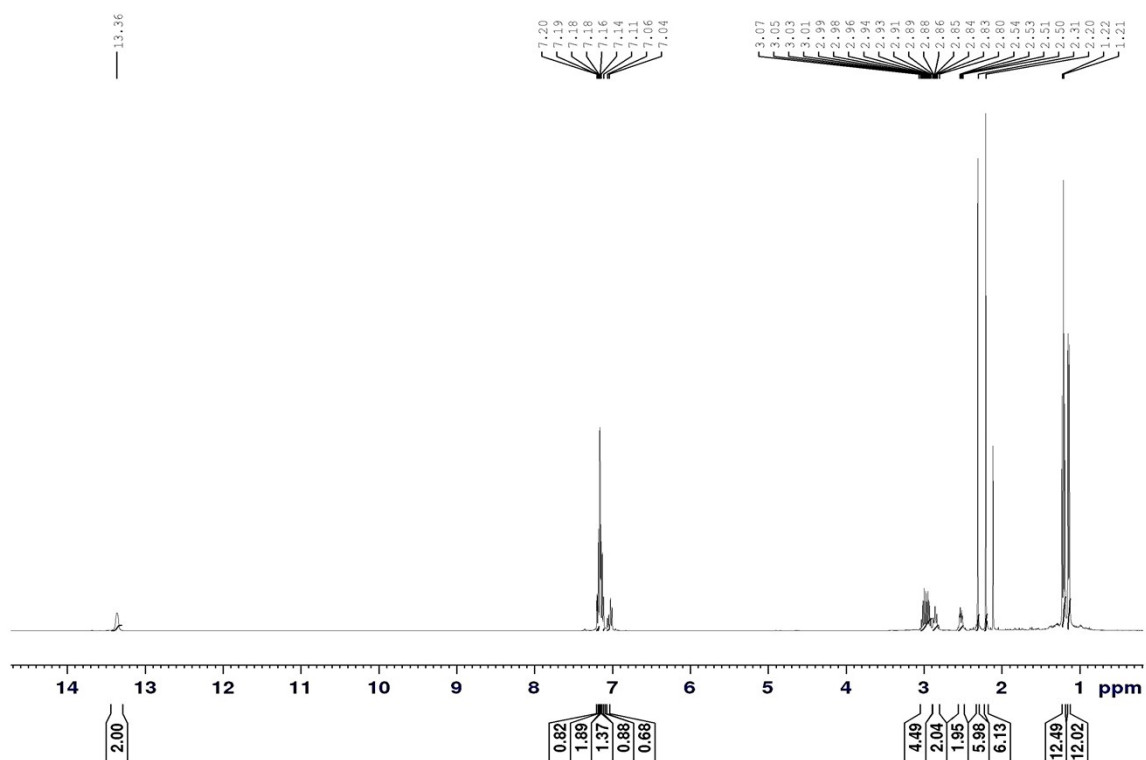


Figure S8: ^1H NMR spectrum (400 MHz) of **VI** in C_6D_6 .

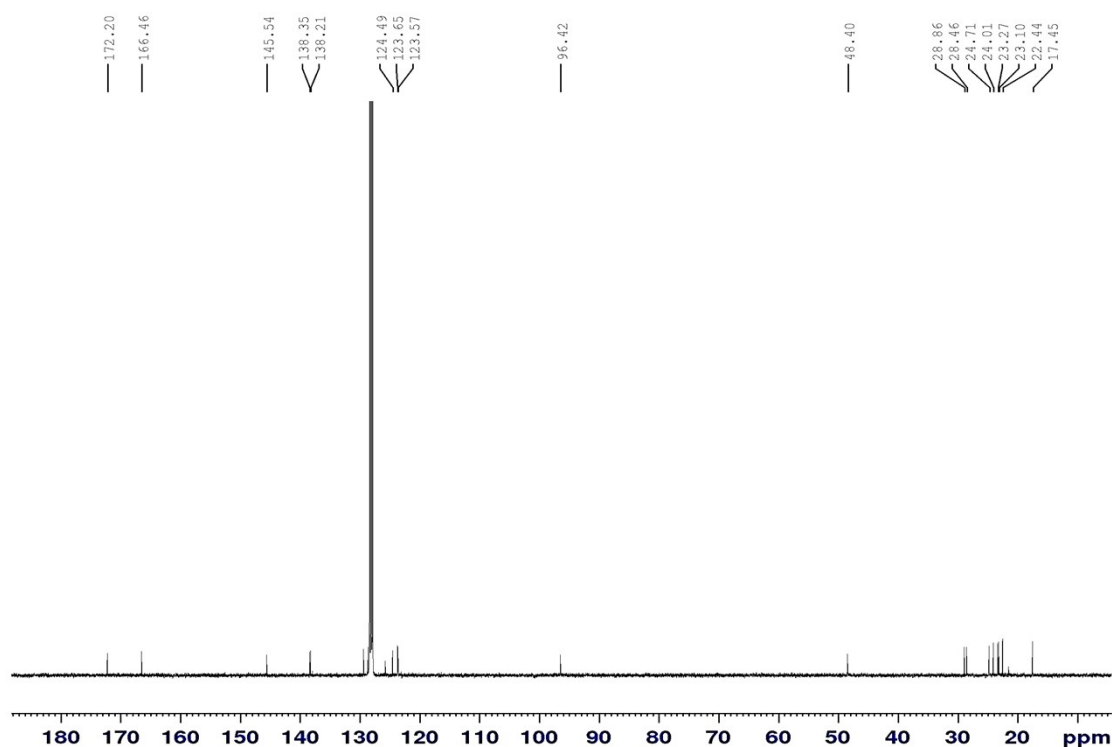


Figure S9: ^{13}C NMR spectrum (101 MHz) of **VI** in C_6D_6 .

Computational details

Calculations were performed with the Gaussian 09 program package^[7] and the M06 hybrid functional^[8] using def2-SVP basis sets^[9] for geometry optimizations and frequency calculations, and def2-TZVP basis sets^[9] for single-point calculations, in both cases in conjunction with the related quasi-relativistic pseudopotentials for indium.^[10] For **IV** and **V**, the geometry optimizations were performed using the XYZ coordinates derived from the XRD analysis as initial structures. The absence of imaginary frequencies confirmed stationary points as minima. To derive the contribution of London dispersion the D3 version of Grimme's dispersion with the original zero-damping function was used.^[11] Graphical representations of the frontier orbitals were generated using ChemCraft.^[12]

Thermal corrections obtained at the M06-GD3/def2-SVP level of theory were calculated for standard conditions, i.e. 298.15 K and 1 bar. All energies are given in kJ mol^{-1} .

The coordinates of the optimized structures are given in the following:

In_4O_2 (IV)				In_4O_4			
In	1.85058100	0.94266800	0.25104200	In	0.68265100	1.50297800	0.40028700
N	1.51462300	1.40693700	2.42170500	In	-2.78117200	0.63859700	0.38062400
N	3.66425200	2.14766700	0.36755400	O	-2.53407700	-1.33806600	0.49485400
N	2.41817100	-3.45963300	0.47057000	O	-0.98888700	0.82100900	-0.64808500
N	1.93560400	-1.63726500	2.95874700	N	0.93437300	3.76110800	0.27181800
C	2.15132700	-4.02665200	-0.80595300	N	0.09244200	1.85261200	2.47111300
C	1.94512000	2.54287900	2.94060700	N	-4.62084900	1.54829700	-0.20228000
C	4.67790000	1.89183300	-0.59441700	N	-2.81041100	1.87100000	2.15074800
C	2.49638300	2.38249900	-3.40956000	C	1.23003100	4.19056400	-1.04995700
H	3.06368100	2.13472700	-4.32540800	C	4.78649700	3.28899400	-0.98386600
H	1.61920000	2.98723300	-3.69686300	H	5.26710200	3.57542200	-1.93694100
H	2.10571300	1.44697100	-2.97730800	H	5.58718300	3.18048000	-0.22959600
C	4.53470000	2.32007100	-1.93204300	H	4.28550600	2.31608800	-1.09881000
C	3.45045500	-1.20072700	-2.65366100	C	-0.74103600	0.83929400	3.08268500

H	3.41008300	-1.40478900	-3.73830200	H	-0.76124800	-0.05057200	2.42442400
H	4.16815400	-0.37628600	-2.50040800	H	-0.33790500	0.45948600	4.04220500
H	2.45203400	-0.84412300	-2.34700800	C	0.52515200	2.88826100	3.19802200
C	2.82932000	-2.50077900	3.41279500	C	3.76822500	4.33427100	-0.53521100
C	0.64027200	0.50608100	3.14284800	C	3.41523100	4.02191900	0.46348600
H	-0.09839200	0.07150200	2.43447500	C	0.99860000	4.09142600	2.67132500
H	0.02185600	1.03099100	3.89455300	H	1.28590500	4.84497500	3.41072200
C	2.81078700	-3.52265300	-1.94888000	C	2.56721400	4.40615500	-1.46370600
C	4.79714900	4.21065400	0.96165600	C	-5.63099500	0.73065300	-0.77723300
H	5.79989500	3.75381700	1.01202300	C	1.08848600	4.53339400	1.32270100
H	4.74693900	5.03196900	1.68801300	C	-5.45338200	0.18008300	-2.05984800
C	4.70015200	4.62750900	-0.05498600	C	0.49388700	2.80321500	4.70373400
C	5.79156500	1.11155300	-0.20119200	H	0.96139200	1.87024900	5.05843900
C	3.72892400	3.18253500	1.20550000	H	1.03330900	3.64671400	5.15392200
C	3.27376800	-3.97900000	1.34287800	H	-0.53285000	2.81665100	5.10484400
C	5.92804100	0.61104300	1.22362500	C	-4.79571300	2.84884800	0.04068800
H	5.32970700	1.27501300	1.87292800	C	-2.17362400	1.32611800	3.33275900
C	3.35177600	3.14368900	-2.40126300	H	-2.19070100	2.04957000	4.16445400
C	2.69826300	3.33920700	-1.53590600	H	-2.76547700	0.45319600	3.67295700
C	4.13056300	-5.12473000	0.88728500	C	-1.27303600	4.13330700	-1.51582400
H	3.51684400	-5.94664500	0.48696700	H	-1.28446700	3.45698900	-0.63947300
H	4.76498700	-5.51303900	1.69403900	C	2.79385100	4.71804100	-2.80686400
C	4.77713000	-4.79783800	0.05509100	H	3.82275300	4.88808200	-3.14254500
C	1.43271300	3.00166800	4.27958900	C	0.16424700	4.27838300	-1.97206600
H	0.33280200	3.07927500	4.26726400	C	-6.74790400	0.38040500	0.01699800
H	1.83789200	3.98655000	4.54654400	C	-7.70275300	-0.47982300	-0.52593500
H	1.70363800	2.29212300	5.07921000	H	-8.57484400	-0.76229000	0.07204900
C	1.35939600	-0.64224500	3.84983500	C	0.44944800	4.58979300	-3.30337400
H	2.13355500	-0.19181900	4.50206900	H	-0.36886200	4.67051500	-4.02526000
H	0.62237000	-1.12331700	4.52692400	C	-5.89105500	3.56573700	-0.69312500
C	3.79030400	4.48700700	-2.97494100	H	-6.87298500	3.36465800	-0.23066900
H	4.38317600	4.36712600	-3.89850100	H	-5.73005600	4.65300700	-0.68131800
H	4.40644800	5.06022500	-2.26147400	H	-5.95717900	3.21674000	-1.73646800
H	2.91067800	5.10302100	-3.22687500	C	4.45104300	5.69579300	-0.40745700
C	1.11830600	-4.98547000	-0.93025100	H	4.90141900	5.99977100	-1.36855600
C	3.45502100	-3.53058000	2.66294000	H	3.76032200	6.49971900	-0.10841000
C	4.20169300	-4.09722400	3.22412000	H	5.26661700	5.65286200	0.33407800
C	5.33530100	-0.78829200	1.35474000	C	-4.20197300	0.44873600	-2.86330200
H	4.27072800	-0.80379300	1.06050000	H	-3.61434000	1.21077900	-2.32290400
H	5.39717900	-1.16291200	2.39133100	C	-6.43224600	-0.68552300	-2.55724700
H	5.87124600	-1.50654500	0.70546500	H	-6.30564000	-1.12129500	-3.55449400
C	3.86106200	-2.43410200	-1.85821300	H	-7.55468200	-1.00601000	-1.80632900
H	3.93931400	-2.13144100	-0.79883700	C	-8.31284100	-1.68255500	-2.21135000
C	2.90015400	3.38875200	2.32230900	C	1.36655800	6.00669300	1.18200600
H	3.09299900	4.32156400	2.85761400	H	1.39882300	6.34393000	0.13717200
C	3.27054700	-2.40251300	4.84900800	H	0.58242200	6.57118600	1.71281400
C	3.79745700	-1.44903600	5.02927200	H	2.32157100	6.26356400	1.66834000
H	3.94695200	-3.22130300	5.12379100	C	-6.84048200	0.82196300	1.46511100
C	2.40770600	-2.41997500	5.53425200	H	-6.35238500	1.80771600	1.56761200
C	5.52188600	1.95632600	-2.85481800	C	1.75528700	4.80720500	-3.72452400
H	5.42092100	2.28399800	-3.89562000	H	1.96390000	5.04868100	-4.77118300
C	6.61470900	1.18462500	-2.48415100	C	-3.22063100	3.12225300	2.03091200
H	7.37053000	0.90686100	-3.22472000	C	-4.03818700	3.58742400	0.96501100
C	2.45555600	-4.02672100	-3.20389500	H	-4.24796000	4.65932800	0.98326500
H	2.97117200	-3.65135700	-4.09537500	C	-2.18070800	3.51494600	-2.56652300
C	6.74244700	0.76540900	-1.16303000	H	-1.77477200	2.55487700	-2.92885500
H	7.60268700	0.15282200	-0.87291000	H	-3.18093600	3.32681100	-2.13730100
C	7.36080400	0.64152700	1.73771400	H	-2.33318600	4.18063300	-3.43411800
H	7.99973600	-0.10181100	1.23064800	C	-4.49299800	1.02552200	-4.24213800
H	7.38764700	0.40204900	2.81341300	H	-5.07103800	1.96291600	-4.17793200
H	7.82585600	1.63195400	1.59894400	H	-3.55234800	1.24499600	-4.77500700
C	1.45961900	-4.98653700	-3.33761900	H	-5.06801600	0.32151500	-4.86822300
C	1.19299100	-5.36955100	-4.32793800	C	-1.81603700	5.48692100	-1.06497300
C	0.79138000	-5.44575400	-2.20824200	H	-1.72908800	6.23153300	-1.87615500
C	-0.01455300	-6.17942500	-2.32031700	H	-2.87972200	5.41027900	-0.78254300
C	0.35914200	-5.52222500	0.26843900	H	-1.26451400	5.87652800	-0.19315700
H	0.64033500	-4.91327700	1.14628900	C	-6.06402100	-0.15589200	2.34534000
C	5.24261500	-2.91047700	-2.29319000	H	-5.01825300	-0.27488100	2.01290900
H	5.25327100	-3.20110900	-3.35816300	H	-6.04901800	0.17813600	3.39687900
H	5.58080400	-3.78328400	-1.71034300	C	-6.52225700	-1.15958800	2.30749600
H	5.98375900	-2.10301900	-2.16006600	C	-3.33732400	-0.80607300	-2.95098300
C	0.72700200	-6.97514800	0.55819200	H	-3.79660600	-1.57448900	-3.59878100
C	0.44838800	-7.63269300	-0.28416800	H	-2.34363500	-0.55622700	-3.36151600
H	0.19383500	-7.34008400	1.45187100	H	-3.18518100	-1.26382700	-1.95410800
H	1.80647400	-7.11034700	0.73629200	C	-8.26754500	0.98140100	1.96677700
C	-1.14515500	-5.36744700	0.08970700	H	-8.79262900	0.01345100	2.03519000
H	-1.53521500	-6.00391700	-0.72532300	H	-8.27089700	1.41617100	2.97939800
H	-1.37955300	-4.31326900	-0.12677300	H	-8.86228600	1.63997600	1.31160500
H	-1.67379600	-5.65677500	1.01474600	C	-2.85640800	4.14537200	3.07105000
In	1.26181600	-1.67088500	0.82819000	H	-1.76402300	4.17014800	3.22640300
O	-0.67221400	-2.26303800	0.74880300	H	-3.18006200	5.14771300	2.76207600
In	-1.85810500	-0.95473700	-0.26823700	H	-3.33145300	3.92619300	4.04168500
N	-1.53622800	-1.40412900	-2.44169400	In	-0.68393100	-1.50408500	-0.40044700
N	-3.67037900	-2.16471200	-0.38165000	In	2.77823200	-0.63889700	-0.38969600
N	-2.41148000	3.47079800	-0.45405000	O	2.52801100	1.33772200	-0.50463100
N	-1.96763000	1.64969800	-2.95657400	O	0.98970100	-0.82311100	0.64564900
C	-2.13617100	4.03763100	0.82133700	N	-0.93657900	-3.75950400	-0.25944100
C	-1.96861200	-2.53623900	-2.96764400	N	-0.09730200	-1.86334000	-2.47031300
C	-4.67394200	-1.91618800	0.59222500	N	4.62146000	-1.54429000	0.19127500
C	-2.46804100	-2.42890800	3.39020800	N	2.80623000	-1.87659200	-0.15641900
H	-3.02915000	-2.18863500	4.31191700	C	-1.22832000	-4.18234600	1.06530700
H	-1.58930100	-3.03650900	3.66717200	C	-4.78827500	-3.29397900	0.99257400
H	-2.08016200	-1.48968100	2.96333800	H	-5.24906300	-3.55443500	1.96271700
C	-4.51582000	-2.35005900	1.92625400	H	-5.60362000	-3.21787400	0.25033100
C	-3.34910600	1.15885100	2.70002500	H	-4.29509500	-2.31339500	1.06954100
H	-3.34933100	1.36728000	3.78472100	C	0.73355900	-0.85166700	-3.08820800
H	-4.03966400	0.31445600	2.52973100	C	0.75401900	0.04087600	-2.43341600
C	-2.33144300	0.82621800	2.42896000	H	0.32818600	-0.47687700	-4.04879900
C	-2.85380000	2.52552800	-3.40087500	C	-0.53029000	-2.90338300	-3.19085000
C	-0.67360600	-0.49272100	-3.16390100	C	-3.76709000	-4.34333900	0.56114300
H	0.06480000	-0.05441300	-2.45888900	H	-3.41711300	-4.04892700	-0.44450800
H	-0.05823900	-1.00746100	-3.92425700	C	-0.99984200	-4.10502200	-2.65677000
C	-2.74988600	3.49147100	1.97169600	H	-1.28721100	-4.86325700	-3.39134900
C	-4.81398200	-4.21758100	-0.99014700	C	-2.56307300	-4.39647000	1.48675000
H	-5.81679100	-3.76200400	-1.05223800	C	5.63251100	-0.72588600	0.76355900
H	-4.75689600	-5.04208000	-1.71245900	C	-1.08961500	-4.53841800	-1.30548600
H	-4.72838500	-4.62905800	0.02955500	C	5.45822500	-0.17558100	2.04670500
C	-5.79135500	-1.13371200	0.21383700	C	-0.50133000	-2.82628900	-4.69699000

C	-3.74474100	-3.18951100	-1.23023200	H	-0.97101100	-1.89605600	-5.05590400
C	-3.25802200	4.00830400	-1.32519500	H	-1.03976100	-3.67314700	-5.14203100
C	-5.93889100	-0.62543200	-1.20730900	H	0.52492100	-2.83975200	-5.09944200
H	-5.36128100	-1.29720800	-1.86725300	C	4.79740500	-2.84535100	-0.04816100
C	-3.33103000	-3.18013000	2.38054200	C	2.16637400	-1.33711100	-3.33913200
H	-2.68269900	-3.37162200	1.50966200	H	2.18316500	-2.06355400	-4.16818100
C	-4.06901200	5.18899700	-0.87495700	H	2.75624000	-0.46463000	-3.68381600
H	-3.41443700	6.02040900	-0.56910900	C	1.27627600	-4.12808400	1.51568400
H	-4.74976400	5.54468900	-1.65864800	H	1.28568700	-3.45147800	0.63951800
H	-4.66020500	4.92529200	0.01792800	C	-2.78368900	-4.69263900	2.83456900
C	-1.45391100	-2.98724100	-4.30840000	H	-3.81082300	-4.86012400	3.17689300
H	-0.35478800	-3.07688300	-4.28771200	C	-0.15815500	-4.26314300	1.98325300
H	-1.86843300	-3.96464600	-4.58813000	C	6.74898400	-0.37824400	-0.03246300
C	-1.70978600	-2.26687200	-5.10314800	C	7.70724000	0.47870000	0.50959600
C	-1.40703200	0.65468400	-3.85783400	H	8.57956800	0.75863100	-0.08919400
H	-2.19289700	0.20404700	-4.49602700	C	-0.43688800	-4.55995300	3.31907700
H	-0.68343800	1.13730000	-4.54815000	C	0.38480900	-4.63384200	4.03783200
C	-3.77310600	-4.52475700	2.94869800	C	5.89507600	-3.55952100	0.68495900
H	-4.37672600	-4.40597600	3.86538100	H	6.87541800	-3.36187600	0.21765100
H	-4.38042100	-5.09872400	2.22823600	H	5.73263700	-4.64665900	0.67874500
C	-2.89617600	-5.13980600	3.21225500	H	5.96580700	-3.20606100	1.72645000
C	-1.15006400	5.04533900	0.93965400	C	-4.44520700	-5.71015000	0.46309900
C	-3.45864200	3.56236600	-2.64332000	H	-4.90533300	-5.98878100	1.42720000
H	-4.19814600	4.14358300	-3.19892600	H	-3.74730900	-6.51903900	0.19509200
C	-5.32088700	0.76259800	-1.34045500	H	-5.25294700	-5.69084200	-0.28804900
H	-4.25472000	0.75533000	-1.05177200	C	4.20921500	-0.44550500	2.85352800
H	-5.38113800	1.14123300	-2.37576200	H	3.62257800	-1.21019400	2.31588800
C	-5.83817800	1.49000600	-0.68693500	C	6.43966200	0.68814900	2.54249300
C	-3.77122500	2.37524400	1.88479400	H	6.31548900	1.12437500	3.53984500
C	-3.83075900	2.05886200	0.82809500	C	7.56215700	1.00522900	1.79023100
C	-2.92361300	-3.38570300	-2.35489700	H	8.32275100	1.67957400	2.19435300
H	-3.11813000	-4.31463100	-2.89654400	C	-1.38259800	-6.00656100	-1.14943500
C	-3.30532900	2.43784000	-4.83436900	H	-1.28024200	-6.35322800	-0.11165500
H	-3.83561900	1.48689500	-5.01757700	H	-0.70026000	-6.58785100	-1.78941000
H	-3.98077900	3.26043000	-5.09993800	H	-2.40663300	-6.22688300	-1.49297700
H	-2.44662800	2.45689800	-5.52486100	C	6.83837800	-0.82081900	-1.48053200
C	-5.49195700	-1.98739300	2.86150600	H	6.35092100	-1.80711300	-1.58092100
H	-5.37932400	-2.31797900	3.90019600	C	-1.74122500	-4.77050900	3.74870600
C	-6.58841700	-1.21423100	2.50553600	H	-1.94537900	-4.99944600	4.79905400
C	-7.33560700	-0.93838200	3.25551500	C	3.21826900	-3.12704400	-2.03366800
H	-2.39165300	3.99415200	3.22622300	C	4.03872400	-3.26784900	-0.96832200
C	-2.86991900	3.58581000	4.12390900	H	4.25052800	-4.65938000	-0.98419500
C	-6.73175600	-0.79161200	1.18703500	C	2.19618100	-3.51616500	2.55914000
H	-7.59531600	-0.17823900	0.90882300	H	1.79854200	-2.55324200	2.92315600
C	-7.37839100	-0.62744100	-1.70258500	H	3.19448000	-3.33460700	2.12289800
H	-7.99657400	0.12676500	-1.18592100	H	2.35032800	-4.18234200	3.42604700
H	-7.41453200	-0.38473900	-2.77727300	C	4.50453900	-1.01885500	4.23291200
H	-7.86026700	-1.60932000	-1.56023600	H	5.08534700	-1.95458900	4.16943400
C	-1.44176300	5.00051500	3.35329600	H	3.56552700	-1.24028400	4.76783600
H	-1.17485900	5.38470500	4.34305100	H	5.07824200	-0.31205100	4.85699800
C	-0.82320400	5.50767500	2.21720200	C	1.80476100	-5.48588300	1.05999800
H	-0.06183500	6.28830400	2.32292300	H	1.72442000	-6.22803900	1.87416500
C	-0.43377500	5.63774300	-0.25858400	H	2.86494100	-5.41630800	0.76271200
C	-0.81779800	5.13803600	-1.16605400	H	1.23917400	-5.87497100	0.19652900
C	-5.16782400	2.83343800	2.29268100	C	6.05901000	0.15520600	-2.36029800
H	-5.19706200	3.14911000	3.35015000	H	5.01350200	0.27277300	-2.02657600
H	-5.51510100	3.68544200	1.68476000	H	6.04293700	-0.17990700	-3.41146700
H	-5.89302600	2.01022300	2.17016300	H	6.51570200	1.15965900	-2.32422200
C	-0.70749200	7.13358600	-0.39192700	C	3.34162400	0.80723100	2.94067600
H	-0.27739000	7.69638100	0.45464900	H	3.80193500	1.57898900	3.58377600
H	-0.25111200	7.53193300	-1.31333500	H	2.35004900	0.55632400	3.35579800
H	-1.78543100	7.36546600	-0.42404500	H	3.18463100	1.26105200	1.94283600
C	1.06507200	5.36249700	-0.19767500	C	8.26436000	-0.97949200	-1.98546000
H	1.53299100	5.85201900	0.67560600	H	8.78826600	-0.01108800	-2.05653700
H	1.23851000	4.27430300	-0.14301600	H	8.26563500	-1.41566500	-2.99747600
H	1.56358800	5.75314100	-1.10258800	H	8.86136800	-1.63658900	-1.33085600
In	-1.27798200	1.66867700	-0.83271100	C	2.85345300	-4.15382300	-3.06997200
O	0.66539000	2.23599300	-0.78628300	H	1.76095400	-4.18022500	-3.22385900
				H	3.17821200	-5.15484100	-2.75791900
				H	3.32735400	-3.93749000	-4.04182000

In ₄ S ₂				In ₄ S ₄ (V)			
In	-1.73202600	1.07150700	-0.01174500	In	-0.92791700	2.33220900	-0.25856600
N	-0.88364100	1.36188500	-2.08201500	S	2.58174800	0.92950900	-0.37132300
N	-3.14254100	2.70262300	-0.53285200	S	3.09418700	-1.42532200	-0.41425000
N	-3.43256900	-3.04516500	-0.32085800	S	0.95258500	1.85922600	1.19596500
C	-2.17109900	-1.49895000	-2.72885500	N	-1.33239300	4.49133200	-0.47474900
N	-3.67332800	-3.51967100	1.00278200	N	-0.54303700	2.20863100	-2.39550400
C	-0.90785000	2.54274300	-2.67879800	N	4.47754600	1.95172600	-0.04016300
C	-4.44368900	2.73122200	0.04190100	N	2.43760600	2.06410100	-2.23469200
C	-3.29456900	3.05612800	3.43349900	C	-1.39942600	5.23981700	0.73942500
H	-4.18403200	3.02911200	4.08857200	C	-4.70364100	4.06098600	1.86705800
H	-2.46140500	3.49610500	4.00642700	H	-5.09741100	4.67635200	2.69486300
C	-3.00965300	2.01820800	3.19749800	H	-5.56138800	3.55848500	1.38843400
C	-4.66309600	3.24987600	1.33668600	H	-4.05770000	3.27659900	2.29145900
C	-4.48320500	-0.30358000	2.36851500	C	0.24848000	1.09979500	-2.89160300
H	-4.79669500	-0.40755600	3.42243700	H	0.31114200	0.33255600	-2.09727700
H	-4.83165100	0.68326900	2.01867300	H	-0.24235800	0.56807200	-3.72802900
H	-3.37827800	-0.30409500	2.35891200	C	-1.12680500	3.06225600	-3.23642200
C	-3.11113400	-2.21294400	-3.32504400	C	-3.95679300	4.90870100	0.84080000
C	-0.32199500	0.20731000	-2.75334900	H	-3.73574600	4.25293500	-0.02092100
H	0.18395900	-0.43886600	-2.00873500	C	-1.68437500	4.30830700	-2.87752900
C	0.47839900	0.49420000	-3.45625100	H	-2.07356600	4.88623400	-3.71104300
C	-4.46679500	-2.75997500	1.88986600	C	-2.64146700	5.43193800	1.38704100
C	-3.57621600	4.94443900	-1.37966500	C	5.50999000	1.22643000	0.61167700
H	-4.55077600	4.73881000	-1.85533500	C	-1.64871600	5.01137300	-1.64783800
H	-3.07416300	5.73852200	-1.94809700	C	5.40091700	0.92058200	1.98244400
C	-3.80014500	5.31432600	-0.36710100	C	-1.19384500	2.71618800	-4.69993800
H	-5.51296800	2.17917200	-0.70076100	H	-1.66884500	1.73212200	-4.84547100
C	-2.74416200	3.69314700	-1.33225900	H	-1.77090500	3.46349500	-5.25871600

C	-4.22847500	-3.39796200	-1.32795300	H	-0.19069300	2.65585600	-5.15328100
C	-5.31752500	1.64128700	-2.10467100	C	4.61744500	3.21789600	-0.40810400
H	-4.33418000	1.98744500	-2.47116500	C	1.66406600	1.48249300	-3.31059600
C	-3.55829600	3.86773200	2.16965600	H	1.64092900	2.13901300	-4.19626100
H	-2.62913900	3.85211200	1.57323900	H	2.16826200	0.55011000	-3.63451100
C	-5.46850400	-4.18802500	-1.01165400	C	1.13834100	5.53350400	0.62489600
H	-5.26894200	-5.03150300	-0.33436400	H	1.08211400	4.61184800	0.01575500
H	-5.95672800	-4.56202400	-1.92069200	C	-2.65558900	6.15077400	2.58673600
H	-6.18256800	-3.53654100	-0.47836500	H	-3.60917000	6.31540000	3.09965300
C	-0.17548400	2.75277000	-3.97787400	C	-0.19955700	5.72031500	1.31063400
H	0.88113000	2.44758800	-3.90253100	C	6.56778100	0.70835400	-0.16941500
H	-0.20204400	3.80799800	-4.27787500	C	7.49319200	-0.13587100	0.44659000
H	-0.63254500	2.15902400	-4.78753600	H	8.30925800	-0.56278300	-0.14517900
C	-1.31243000	-0.64959500	-3.53566300	C	-0.27318500	6.43309400	2.50962700
H	-1.91623700	0.02860400	-4.17511900	H	0.64554600	6.82293400	2.95782800
C	-0.71011400	-1.26815300	-4.23357900	C	5.78062300	3.99725100	0.13357300
C	-3.85891300	5.32066200	2.52474600	H	6.72356100	3.65528900	-0.32549500
H	-4.74478600	5.40660900	3.17783400	H	5.67694000	5.07259900	-0.06539300
H	-4.04880400	5.93859400	1.63113500	H	5.88706500	3.83575100	1.21849300
H	-3.00832900	5.76866400	3.06525400	C	-4.85931300	6.04130100	0.35590400
C	-3.06843100	-4.72499500	1.43090800	H	-5.16039200	6.69368100	1.19390800
C	-4.04485900	-3.05792400	-2.67900300	H	-4.36943000	6.68081500	-0.39352900
C	-4.78426200	-3.49943500	-3.35090000	H	-5.78148800	5.63676600	-0.09365700
C	-5.27587800	0.11872900	-2.10079300	C	4.26236300	1.44369300	2.83377000
H	-4.41544900	-0.25664900	-1.52055900	H	3.62581400	2.08478500	2.19623000
H	-5.17868900	-0.28417900	-3.12365400	C	6.35835700	0.07845400	2.55478600
H	-6.19324400	-0.31291300	-1.65831600	H	6.28105800	-0.17218000	3.61866200
C	-5.05563500	-1.42036300	1.50155900	C	7.39216200	-0.45438300	1.79708800
H	-4.76253200	-1.21617300	0.45685600	H	8.12503100	-1.12263900	2.25861500
C	-1.64425300	3.65479700	-2.20638700	C	-2.02046300	6.46571500	-1.76945000
H	-1.45308100	4.58929300	-2.74012600	H	-1.94407600	7.01728200	-0.82301700
C	-3.26232100	-2.11433100	-4.81924800	H	-1.36829000	6.94897400	-2.51460400
H	-3.48529700	-1.07789600	-5.12623400	C	-3.05123700	6.55661500	-2.14954600
H	-4.06518800	-2.76271100	-5.19136100	C	6.67165200	0.99695700	-1.65557200
C	-2.32747500	-2.39455500	-5.33187600	H	6.09218600	1.91205000	-1.87236500
C	-5.95351600	3.18194200	1.87211600	C	-1.48929100	6.65506700	3.14385700
H	-6.13102600	3.57860700	2.87808800	H	-1.52542400	7.21744600	4.08150300
C	-7.00504100	2.61471100	1.16483100	C	2.82922200	3.33322500	-2.22638500
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C	-4.68810000	-3.24814900	3.18046400	H	3.95239000	4.94613100	-1.43029500
H	-5.30928600	-2.66494000	3.86954800	C	2.28886600	5.34504100	1.60318600
C	-6.77948200	2.11892700	-0.11466300	H	2.06461600	4.55277600	2.33656800
H	-7.60876800	1.67574300	-0.67734900	H	3.19627100	5.04267700	1.05527200
C	-6.37378800	2.15924200	-3.07348100	H	2.53227900	6.27327600	2.14896300
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H	-6.43545700	3.26017300	-3.05922900	H	3.91110400	2.72554500	4.55339700
C	-4.13293400	-4.44909800	3.60082600	H	5.38389800	1.73436600	4.68710700
H	-4.32168300	-4.82009800	4.61262000	C	1.41999000	6.69373200	-0.32590600
C	-3.32351200	-5.17017600	2.73099300	H	1.44493200	7.65253200	0.22220000
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C	-2.18470000	-5.56126900	0.52459700	H	0.65164100	6.78031700	-1.11245400
H	-1.89796600	-4.93355500	-0.33667800	C	6.03743200	-0.12772500	-2.46768800
C	-6.57944900	-1.40677900	1.55613700	H	4.98308600	-0.28544900	-2.18752900
H	-6.94753400	-1.56622400	2.58448100	H	6.07785900	0.09116300	-3.54813400
H	-7.02425400	-2.19217700	0.92201700	C	6.56742200	-1.08060900	-2.29350900
H	-6.96578300	-0.43130500	1.21286600	H	3.39204900	0.29997000	3.35213400
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C	-3.81257700	-6.50223400	-0.61239700	C	8.10248000	1.25462200	-2.11024000
H	-0.89471000	-5.99318700	1.21286500	H	8.72417200	0.34497700	-2.04923100
H	-1.08024800	-6.73046800	2.01400100	H	8.11881700	1.58193100	-3.16276000
H	-0.35830500	-5.13110700	1.64108300	H	8.59453900	2.03335700	-1.50337000
H	-0.21554200	-6.46489900	0.48341200	C	2.28996500	4.29718500	-3.24998400
In	-1.74912800	-1.66043500	-0.52510300	H	1.18698400	4.33682100	-3.19867800
S	0.25755700	-3.05868700	-0.36395500	H	2.67326900	5.31079600	-3.07509800
In	1.95439200	-1.42588000	0.33941800	H	2.56538500	4.01049000	-4.27794400
N	2.19277700	-1.93964400	2.49991000	In	0.92777700	-2.33223800	0.25856300
N	3.81059500	-2.59023800	0.01831400	In	-2.58182800	-0.92961200	0.37098900
N	3.01363900	2.97158200	0.61082700	S	-3.09433400	1.42516900	0.41400100
N	2.82872600	1.01168000	3.05089200	S	-0.95262300	-1.85950200	-1.19616600
C	2.66988200	3.70723600	-0.56034900	N	1.33240000	-4.49131600	0.47511400
C	2.68795900	-3.10500300	2.86723600	N	0.54283500	-2.20844200	2.39544900
C	4.67438500	-2.27573800	-1.06548700	N	-4.47763000	-1.95187100	0.03989400
C	2.07626200	-2.51243200	-3.47292200	N	-2.43783500	-2.06423200	2.23442200
H	2.44965200	-2.23771600	-4.47663600	C	1.39949900	-5.23996900	-0.73894400
H	1.10989900	-3.03346900	-3.58680200	C	4.70354800	-4.06060700	-1.86625500
H	1.87826300	-1.57509600	-2.92619800	H	5.09762400	-4.67592700	-2.69395000
C	4.33495900	-2.62127600	-2.39084200	H	5.56104900	-3.55779900	-1.38752600
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H	3.06451200	1.29602600	-3.76028200	C	-0.24885800	-1.09964900	2.89138700
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C	2.31915200	0.78998500	-2.22087700	H	0.24193600	-0.56769400	3.72768700
C	3.83224300	1.79857500	3.39948500	C	1.12688000	-3.06178500	3.23649000
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H	0.61107100	-0.62117800	2.87536300	H	3.73554400	-4.25275800	0.02164100
H	1.01545600	-1.62503700	4.24906800	C	1.66471000	-4.30776800	2.87778200
C	3.19299300	3.32944700	-1.81526700	H	2.07415200	-4.88543700	3.71135200
C	5.05475100	-4.66757800	0.27519100	C	2.64162600	-5.43198300	-1.38641500
H	6.06386400	-4.22366600	0.23695200	C	-5.51011500	-1.22651600	-0.61182500
H	5.09305100	-5.55767500	0.91614300	C	1.64896000	-5.01110800	1.64824100
H	4.82081100	-4.97677500	-0.75643400	C	-5.40106100	-0.92057700	-1.98257200
C	5.86922800	-1.56765100	-0.79047200	C	1.19393500	-2.71550500	4.69996100
C	4.04690700	-3.66815400	0.77241200	H	1.68667700	-1.73131000	4.84536500
C	4.07638300	3.32204300	1.33457400	H	1.77123900	-3.46259700	5.25877600
C	6.25351800	-1.20021700	0.62901100	H	0.19079700	-2.65539900	5.15336100
H	5.76215400	-1.91585700	1.31203300	C	-4.61750900	-3.21806200	0.40773400
C	3.07319500	-3.39000600	-2.72253000	C	-1.66439900	-1.48255300	3.31036700
H	2.58866800	-3.67952800	-1.77356400	H	-1.64116100	-2.13909400	4.19601300
C	5.03304600	4.33016500	0.75718800	H	-2.16874800	-0.55025900	3.63431000
H	4.51895600	5.18250900	0.28804600	C	-1.13834500	-5.53384000	-0.62489300
H	5.73689900	4.70342200	1.51259600	H	-1.08238600	-4.61215700	-0.01576300
H	5.61613300	3.84402500	-0.04537400	C	2.65599100	-6.15087600	-2.58606800
C	2.44241700	-3.63036200	4.25732600	H	3.60965800	-6.31539500	-3.09886100
H	1.36153900	-3.75142700	4.44115600	C	0.19974500	-5.72061600	-1.31028900
H	2.92298100	-4.60550900	4.40650200	C	-6.56783500	-0.70839700	0.16933900
H	2.82594800	-2.94208100	5.02808800	C	-7.49320800	0.13593200	-0.44658900

C	2.32086000	0.04079900	4.00816500	H	-8.30918000	0.56293700	0.14524300
H	3.15123900	-0.44327400	4.55758900	C	0.27360700	-6.43339500	-2.50927100
H	1.69886600	0.55266500	4.77247400	H	-0.64505000	-6.82328300	-2.95758000
C	3.35801300	-4.67012900	-3.49878400	C	-5.78067400	-3.99739700	-0.13396300
H	3.77575900	-4.46314300	-4.49917400	H	-6.72352500	-3.65566500	0.32546900
H	4.07506900	-5.31910300	-2.96909600	H	-5.67685300	-5.07278800	0.06472900
H	2.42838100	-5.24462300	-3.64384600	H	-5.88740200	-3.83565800	-1.21881700
C	1.78945200	4.80773900	-0.44376300	C	4.85944600	-6.04091600	-0.35503800
C	4.41912500	2.80374300	2.59238700	H	5.16061100	-6.69333300	-1.19298400
H	5.30472700	3.26654200	3.03379500	H	4.36961000	-6.68042700	0.39443300
C	5.72653400	0.18283500	0.98958300	H	5.78156300	-5.63623800	0.09451700
H	4.62594500	0.23403400	0.91510100	C	-4.26238600	-1.44350100	-2.83386100
H	5.99470100	0.46171900	2.02320300	H	-3.62575600	-2.08448900	-2.19629300
H	6.14776500	0.95447900	0.31732700	C	-6.35848400	-0.07838300	-2.55483800
C	4.05156300	2.09321400	-1.97752800	H	-6.28120000	0.17234000	-3.61869100
H	4.26889000	1.70837600	-0.96569300	C	-7.39223800	0.45447000	-1.79707400
C	3.46481800	-3.93706800	2.02146400	H	-8.12506500	1.12281800	-2.25853400
H	3.74681200	-4.89835700	2.45694800	C	2.02106700	-6.46534100	1.77008600
C	4.46866900	1.62681000	4.75371600	H	1.94449200	-7.01715100	0.82380800
H	4.92952500	0.62833200	4.85023600	H	1.36922600	-6.94852600	2.51558000
H	5.24810700	2.37840400	4.92972400	H	3.05197400	-6.55596900	2.14989000
H	3.72202900	1.71008300	5.55988400	C	-6.67160100	-0.99692800	1.65552000
C	5.18909000	-2.22516800	-3.42662100	H	-6.09241000	-1.91221100	1.87222500
H	4.93647600	-2.48587400	-4.46051800	C	1.48981600	-6.65530500	-3.14332500
C	6.34993800	-1.50863300	-3.17101000	H	1.52612700	-7.21768600	-4.08096200
H	7.00219000	-1.20302400	-3.99460000	C	-2.82936000	-3.33338300	2.22606100
C	2.87465200	4.10379300	-2.93419600	C	-3.75908800	-3.87742600	1.31035200
H	3.29010700	3.83010700	-3.91111300	H	-3.95237500	-4.94632800	1.42982300
C	6.68415600	-1.18823000	-1.85845400	C	-2.28860500	-5.34553400	-1.60351600
H	7.60594000	-0.63117000	-1.65933000	H	-2.06430000	-4.55315300	-2.33675100
C	7.75220200	-1.28468700	0.88557300	H	-3.19624300	-5.04342400	-1.05585400
H	8.30785100	-0.48862300	0.36053800	H	-2.53164100	-6.27378400	-2.14943100
H	7.96352600	-1.16287200	1.96038300	C	-4.75992100	-2.31270500	-3.98325300
H	8.17141200	-2.25284500	0.56426500	H	-5.36760700	-3.15935600	-3.62308900
C	2.03683000	5.20701900	-2.82936700	H	-3.91081500	-2.72555700	-4.55327800
H	1.80124200	5.80611800	-3.71484300	H	-5.38356700	-1.73438100	-4.68739000
C	1.48848200	5.53900800	-1.59600700	C	-1.42019100	-6.69408000	0.32585900
H	0.81471000	6.39863300	-1.52095200	H	-1.44486200	-7.65290100	-0.22222000
C	1.22608200	5.24553200	0.89434000	H	-2.39717600	-6.56371200	0.82301200
H	1.25738500	4.37075100	1.56688800	H	-0.65208400	-6.78056100	1.11263300
C	5.38552400	2.36817600	-2.66000400	C	-6.03684400	0.12755500	2.46749700
H	5.25158500	2.68510200	-3.70896700	H	-4.98250200	0.28487600	2.18711200
H	5.95601700	3.16119900	-2.14765600	H	-6.07713000	-0.09129400	3.54795500
H	6.00302400	1.45349900	-2.67227400	H	-6.56651100	1.08062600	2.29339300
C	2.07526300	6.35087700	1.51836300	C	-3.39223200	-0.29959300	-3.35214000
H	2.13914400	7.22537300	0.84575100	H	-3.94491000	0.32106100	-4.08036800
H	1.63150200	6.69091800	2.46908600	H	-2.48947700	-0.69495400	-3.85094900
H	3.10299800	6.01958200	1.73708100	H	-3.06483500	0.36724100	-2.53423800
C	-0.22995800	5.68387700	0.80577100	C	-8.10244700	-1.25406800	2.11040100
H	-0.34500500	6.65314600	0.28734200	H	-8.72382900	-0.34421200	2.04942400
H	-0.83739100	4.93110000	0.27741300	H	-8.11874800	-1.58131800	3.16293700
H	-0.65030500	5.80336800	1.81899100	H	-8.59487200	-2.03265800	1.50363800
In	1.74383100	1.25065200	1.09500800	C	-2.29010400	-4.29739400	3.24961000
S	-0.41569700	2.19152300	1.73617400	H	-1.18711600	-4.33692100	3.19846800
				H	-2.67328400	-5.31102900	3.07455700
				H	-2.56572400	-4.01084100	4.27755900

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