

Dinuclear Indium and Thallium Diyls: Biscarbenoids or Metal Cluster?

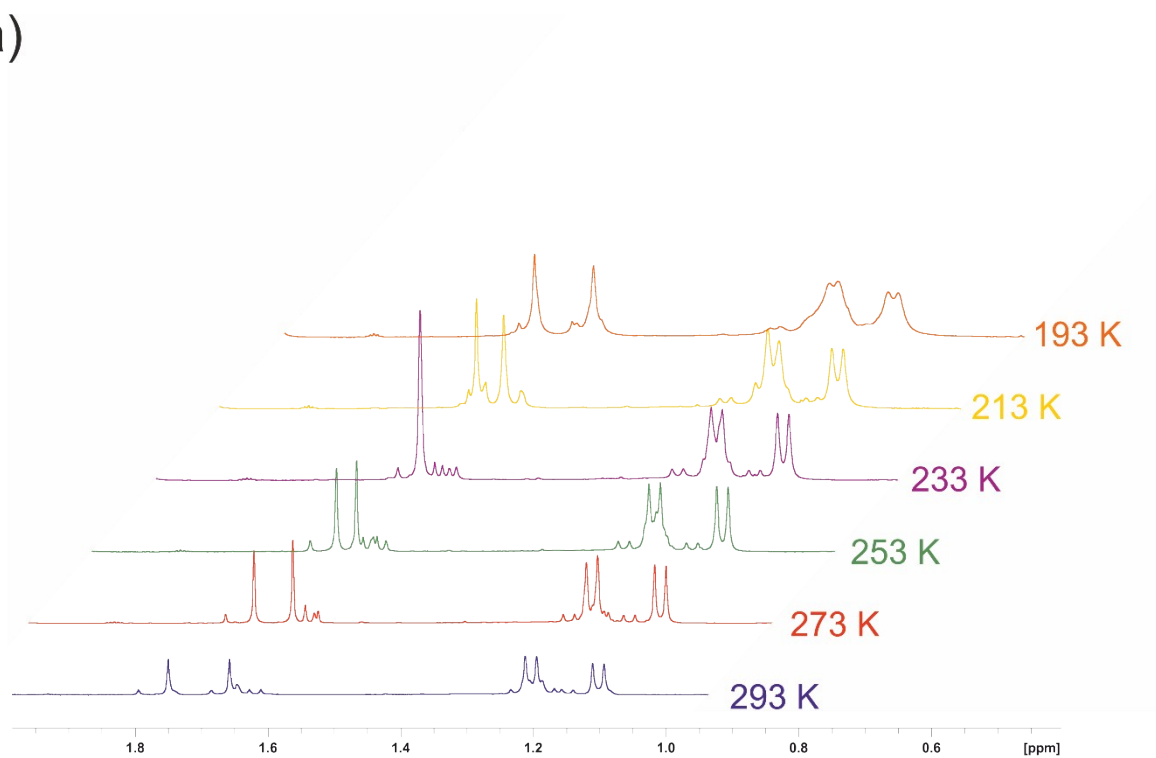
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1. Variable temperature ^1H NMR spectra

a)



b)

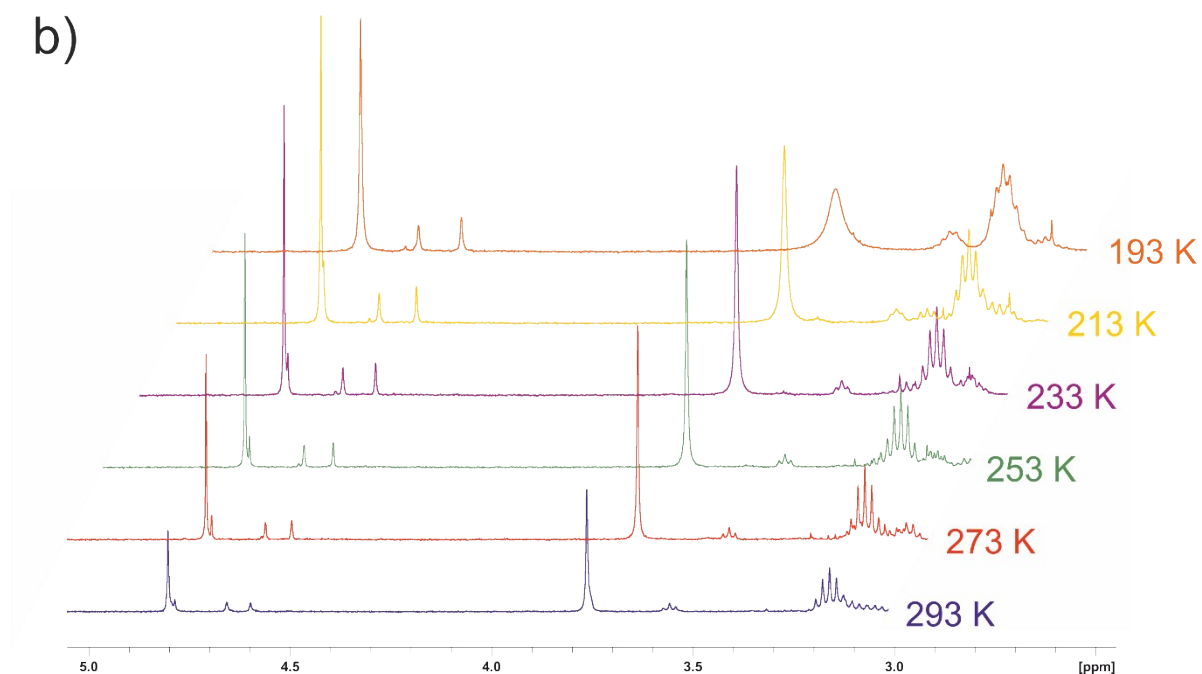


Figure S1 Excerpts (a) 0.9 – 1.9 ppm and b) 3.0 – 5.0 ppm) of the ^1H NMR spectra of a solution of **2** in toluene-d_8 at different temperatures.

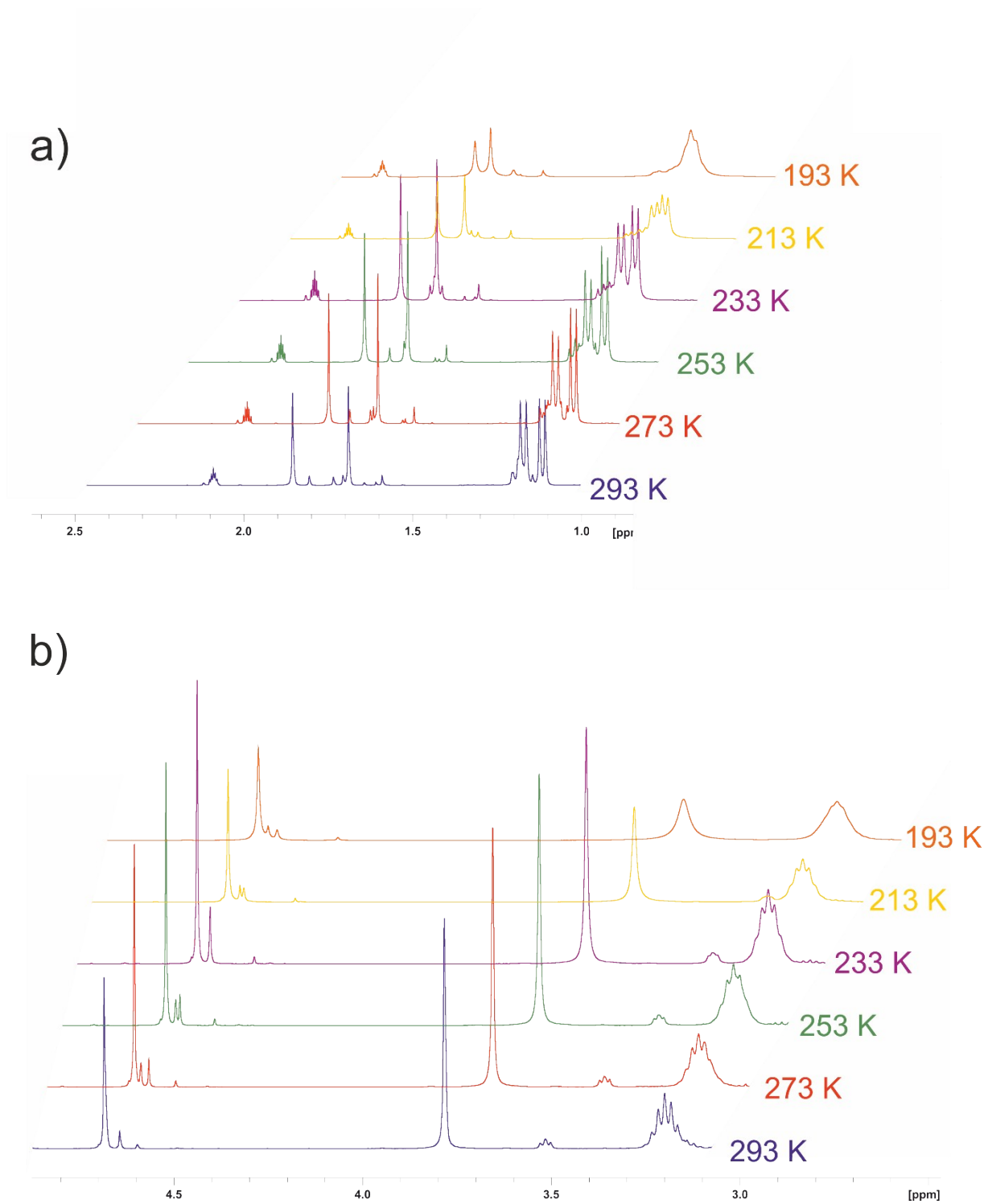


Figure S2 Excerpts (a) 1.0 – 2.5 ppm and b) 3.0 – 4.9 ppm) of the ^1H NMR spectra of a solution of **2** in toluene- d_8 at different temperatures.

2. UV-VIS experiments

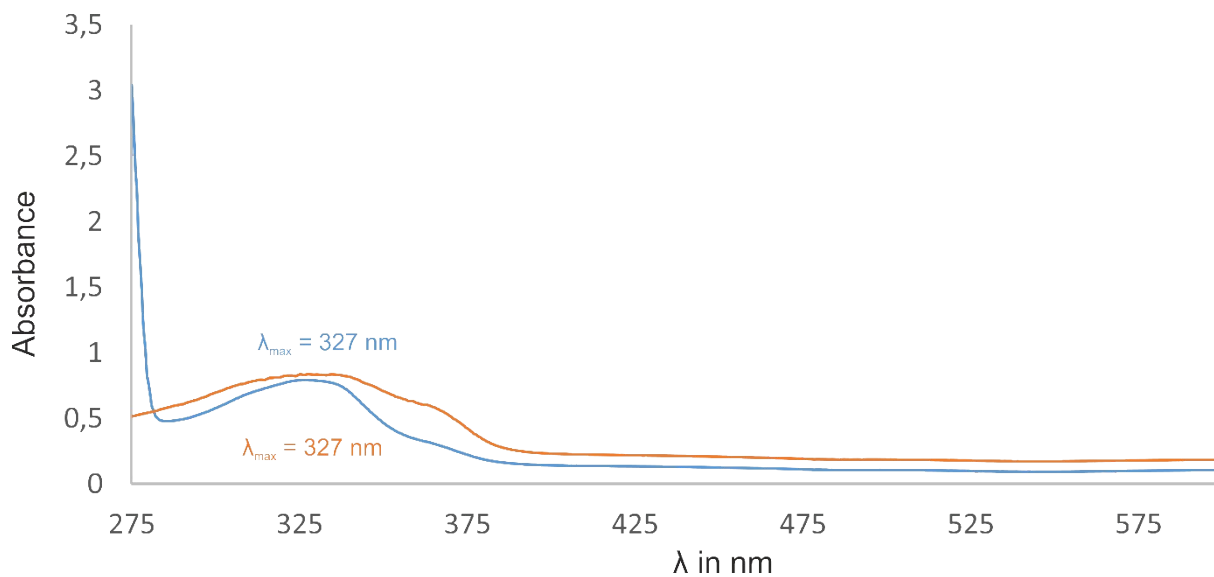


Figure S3 UV-VIS spectra of **2** as a solution in benzene (blue line) and in the solid state (orange line).

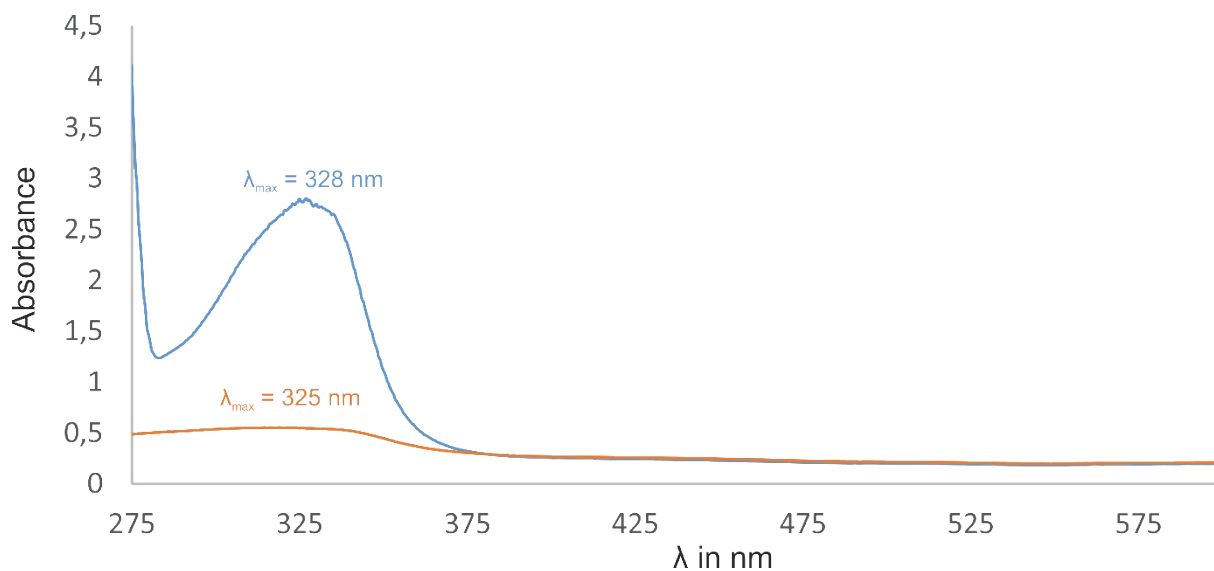


Figure S4 UV-VIS spectra of **3** as a solution in benzene (blue line) and in the solid state (orange line).

3. Natural bond orbitals

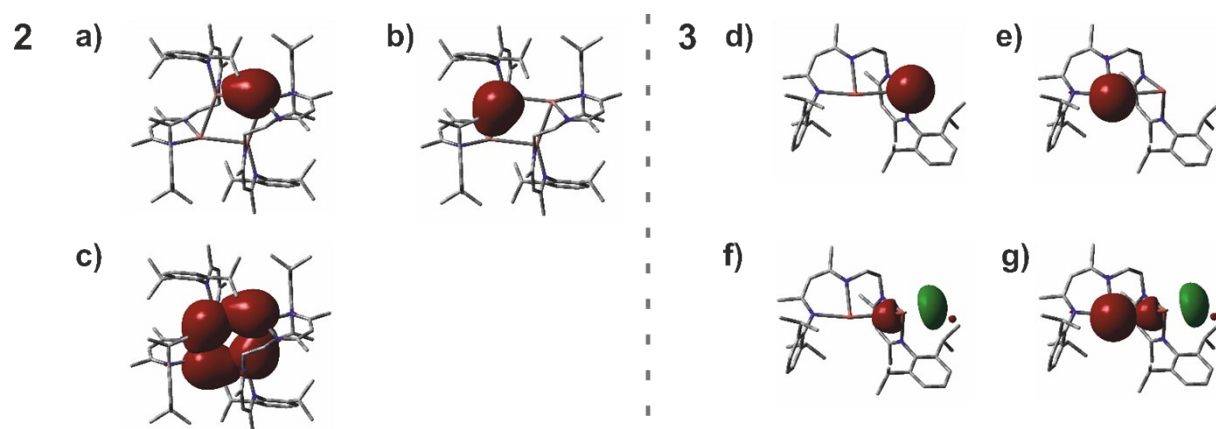


Figure S5 Calculated (B3LYP/LANL2DZ) natural bond orbitals: a) and b) show the NBOs of the respective inter- and intramolecular In-In bond and c) a combination of all four NBOs within **2**. The mostly s-type donor NBOs of **3** are shown in d) and e), while the acceptor NBO and the donor-acceptor interaction are shown in f) and g), respectively.

4. Experimental Details

General Considerations. All preparations were performed under an inert atmosphere of dinitrogen by means of both standard Schlenk line or glovebox techniques (MBraun). Traces of oxygen and moisture were successively 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. Toluene and THF were used as p.a. grade and distilled from Na/benzophenone prior to use. C₆D₆ was dried by distillation from potassium. Indium(I) iodide was purchased from Onyxmet, while thallium(I) iodide and potassium bis(trimethylsilyl)amide (KHMDS) were purchased from Sigma Aldrich. These starting materials were used as delivered. The ligand precursor **1** was prepared according to a literature procedure.^{S1}

Characterization. The NMR-spectra were recorded on a BrukerAvance 400 spectrometer (¹H: 400.13 MHz, ¹³C: 101 MHz, T = 300 K) with δ (given in ppm) referenced to external trimethylsilane. ¹H and ¹³C NMR spectra were calibrated using the solvent residual peak (δ ¹H (C₆D₅H) = 7.20) and the solvent peak (δ ¹³C (C₆D₆) = 128.0), respectively. The coupling constants *J* are given in Hertz [Hz]. Elemental analysis were performed on a Vario micro cube (Elementar Analysensysteme GmbH). The (qualitative) UV-VIS spectra were recorded on a Varian Cary 50 spectrometer in the Dual Beam mode and with a scan rate of 60.0 nm/min. The solution spectra were obtained from benzene solutions of **2** and **3**, respectively, using a Schlenk quartz cuvette. For the solid state spectra, benzene solutions of **2** and **3**, respectively, were transferred to a Schlenk quartz cuvette. By evaporation of the solvent, a thin layer of the solid compounds remained on the walls of the cuvette and was measured immediately.

2: THF (20 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 toluene (20 mL). Filtration and concentration of the filtrate to about one third gave rise to **2** as clear light yellow crystals suitable for an X-ray diffraction analysis. (371 mg, 34 %); Anal. calc. (found) for [C₃₆H₅₂N₄In₂]₂·C₇H₈: C 58.10 (57.99); H 6.91 (6.96); N 6.86 (6.74); ¹H-NMR: (400 MHz, C₆D₆): δ = 1.12 [d, 12H, ³J_{HH} = 6.9 Hz, CHMe₂], 1.23 [d, 12H, ³J_{HH} = 6.9 Hz, CHMe₂], 1.69 [s, 6H, CMe], 1.74 [s, 6H, CMe], 3.21 [sept, 4H, ³J_{HH} = 6.9

Hz, CHMe_2], 3.76 [s, 4H, CH_2], 4.84 [s, 2H, $\beta\text{-CH}$], 7.12 [s, 6H, ArH]; $^1\text{H-NMR}$: (400 MHz, ToI-d_8): δ = 1.10 [d, 12H, $^3J_{\text{HH}} = 6.8$ Hz, CHMe_2], 1.20 [d, 12H, $^3J_{\text{HH}} = 6.8$ Hz, CHMe_2], 1.66 [s, 6H, CMe], 1.75 [s, 6H, CMe], 3.16 [sept, 4H, $^3J_{\text{HH}} = 6.8$ Hz, CHMe_2], 3.76 [s, 4H, CH_2], 4.80 [s, 2H, CH], 7.08 [s, 6H, ArH]; $^{13}\text{C}\{^1\text{H}\}\text{-NMR}$: (101 MHz, C_6D_6): δ = 22.4 [CMe], 23.9 [CHMe_2], 24.60 [CMe], 26.1 [CHMe_2], 28.2 [CHMe_2], 52.8 [CH_2], 99.0 [$\beta\text{-CH}$], 123.9 [$m\text{-C(Dipp)}$], 125.6 [$p\text{-C(Dipp)}$], 142.5 [$o\text{-C(Dipp)}$], 145.5 [$i\text{-C(Dipp)}$], 163.6 [CN], 165.6 [CN].

3 was synthesized by a procedure directly analogous to **2**, employing **TII** (0.80 g, 4.00 mmol), **KHMDS** (1.33 g, 4.00 mmol), and **1** (1.09 g, 2.00 mmol) to yield **3** as clear light yellow crystals suitable for an X-ray diffraction analysis. (2.98 g, 79 %); Anal. calc. (found) for [$\text{C}_{36}\text{H}_{52}\text{N}_4\text{Ti}_2 \cdot 0.4 \text{C}_7\text{H}_8$]: C 47.24 (47.39); H 5.64 (5.42); N 5.68 (5.96); $^1\text{H-NMR}$: (400 MHz, C_6D_6): δ = 1.13 [d, 12H, $^3J_{\text{HH}} = 7.0$ Hz, CHMe_2], 1.19 [d, 12H, $^3J_{\text{HH}} = 7.0$ Hz, CHMe_2], 1.73 [s, 6H, CMe], 1.87 [s, 6H, CMe], 3.22 [br, 4H, CHMe_2], 3.78 [s, 4H, CH_2], 4.74 [s, 2H, $\beta\text{-CH}$], 7.06-7.10 [m, 2H, ArH], 7.11-7.15 [m, 2H, ArH]; $^1\text{H-NMR}$: (400 MHz, ToI-d_8): δ = 1.11 [d, 12H, $^3J_{\text{HH}} = 6.9$ Hz, CHMe_2], 1.17 [d, 12H, $^3J_{\text{HH}} = 6.9$ Hz, CHMe_2], 1.69 [s, 6H, CMe], 1.86 [s, 6H, CMe], 3.20 [sept, 4H, $^3J_{\text{HH}} = 6.9$ Hz, CHMe_2], 3.78 [s, 4H, CH_2], 4.69 [s, 2H, CH], 7.03 [d, 1H, $^3J_{\text{HH}} = 2.5$ Hz, ArH], 7.05 [s, 1H, ArH], 7.08 [s, 2H, ArH], 7.10 [s, 1H, ArH], 7.12-7.15 [m, 1H, ArH]; $^{13}\text{C}\{^1\text{H}\}\text{-NMR}$: (101 MHz, C_6D_6): δ = 21.5 [CMe], 23.2 [CMe], 23.8 [CHMe_2], 25.5 [CHMe_2], 27.8 [CHMe_2], 53.8 [CH_2], 101.6 [$\beta\text{-CH}$], 123.7 [$m\text{-C(Dipp)}$], 124.7 [$p\text{-C(Dipp)}$], 138.2 [$o\text{-C(Dipp)}$], 141.7 [$i\text{-C(Dipp)}$], 161.9 [CN], 164.4 [CN].

5. Crystallographic Details

The single crystal X-ray diffraction data were recorded on an Agilent Technologies SuperNova diffractometer with microfocus Cu K α radiation ($\lambda = 1.54184 \text{ \AA}$). Empirical multi-scan^{S2} and analytical absorption corrections^{S3} were applied to the data. The structures were solved with SHELXT^{S4} and least-square refinements on F^2 were carried out with SHELXL.^{S5} Maxima in the Fourier difference maps of **2** indicated the presence of a second species, which allowed for the refinement of a second In₄ ring (0.0781(7)) including bridging oxygen atoms according to a larger distance of the corresponding Indium atoms. In this compound, also unresolved residual electron density around a centre of inversion was present, which could be assigned a disordered solvent molecule of toluene. The disorder could not be resolved completely, therefore PLATON SQUEEZE^{S6} was applied and the presence of a solvent accessible void including 46 electrons was confirmed, which we assign a not fully occupied toluene molecule. In the subsequent refinement a modified reflection file without the contribution of the solvent was used.

CCDC 1504564 (**3**) and 1504565 (**2**) 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.

	2	3
Empirical formula	C ₃₆ H ₅₂ In ₂ N ₄ O _{0.08}	C ₃₆ H ₅₂ N ₄ Tl ₂
CCDC No.	1504565	1504564
Formula weight	771.73	949.55
Temperature/K	123.0(2)	123.3(6)
Crystal system	triclinic	triclinic
Space group	PError!	PError!
a/Å	11.49565(18)	11.1313(3)
b/Å	12.7946(2)	12.0117(3)
c/Å	14.8078(2)	14.7648(4)
α/°	106.4107(14)	66.579(3)
β/°	108.2254(14)	78.590(3)
γ/°	99.2006(15)	80.819(2)
Volume/Å ³	1909.34(6)	1768.50(10)
Z	2	2
ρ _{calc} /cm ³	1.342	1.783
μ/mm ⁻¹	9.845	17.502
F(000)	789.0	916.0
Crystal size/mm ³	0.118 × 0.074 × 0.025	0.14 × 0.111 × 0.054
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2θ range for data collection/°	6.722 to 150.89	6.598 to 148.144
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 15, -18 ≤ l ≤ 18	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -18 ≤ l ≤ 18
Reflections collected	89347	43841
Independent reflections	7726 [R _{int} = 0.0745, R _{sigma} = 0.0290]	7001 [R _{int} = 0.0767, R _{sigma} = 0.0364]
Data/restraints/parameters	7726/24/436	7001/12/412
Goodness-of-fit on F ²	1.058	1.042
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0291, wR ₂ = 0.0722	R ₁ = 0.0267, wR ₂ = 0.0645
Final R indexes [all data]	R ₁ = 0.0333, wR ₂ = 0.0750	R ₁ = 0.0314, wR ₂ = 0.0673
Largest diff. peak/hole / e Å ⁻³	0.96/-0.51	1.31/-1.42

6. Computational Details

Calculations were performed using the Gaussian 09 program package^{S7} using the B3LYP functional^{S8} and LANL2DZ basis sets^{S9} in conjunction with the related quasi-relativistic pseudopotentials for indium and thallium. When X-ray data were available, the geometry optimization were performed using the XYZ coordinates as initial structures and freezing the metal–metal distances. In a second optimization step, these restraints have been removed and the absence of imaginary frequencies confirmed stationary points as minima. The free energies (given in kJ mol⁻¹) were calculated for standard conditions, i.e., 298.15 K and 1 bar. To derive the contribution of London dispersion the D3 version of Grimme’s dispersion with the original zero-damping function was used.^{S10}

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

B3LYP-LANL2DZ

In₂^{OP}

In	3.21545200	-0.31310900	-1.06392000
In	-3.21595200	0.31537000	1.06424700
C	-5.67265200	0.17574100	-2.87113000
H	-6.47516200	0.87312500	-2.60520300
H	-6.10375400	-0.83183800	-2.82917500
H	-5.36108500	0.37616000	-3.89960100
C	0.34251100	-0.69724600	0.04341100
H	-0.29315800	-1.36599200	0.63758400
H	0.38759900	-1.12064400	-0.96962700
C	-6.18737500	-3.65087900	-1.35587900
H	-7.06662600	-4.14760300	-0.92545800
H	-5.47922800	-4.43318400	-1.66033600
H	-6.51396300	-3.11793800	-2.25812800
C	5.05666400	3.47338700	-0.91561600
H	5.90896100	3.93175400	-1.43455300
H	4.36137600	4.27572700	-0.63296900
H	4.54863600	2.81279300	-1.63038800
C	6.44062300	1.52332600	-0.05013700
C	-3.23478400	0.57806100	-2.49497600

H	-3.24900300	0.69153200	-3.57299000
C	5.52363400	2.68902800	0.34056400
H	4.62974600	2.27430400	0.81926600
C	-8.57541400	-0.77232700	0.98896600
H	-9.55173600	-1.00679900	1.40658700
N	-4.70166800	0.14477500	-0.57816200
C	6.38505100	-3.02840000	-1.59578500
H	5.65845300	-2.49406700	-2.22122200
H	6.05754600	-4.07296600	-1.50344200
H	7.34811600	-3.02194300	-2.12302800
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H	-8.02340500	-2.83857400	0.71644400
C	7.71160600	1.80163100	-0.59501300
H	8.02695200	2.83584700	-0.71371100
N	-1.72885100	0.60687100	-0.56684100
N	4.70177100	-0.14490400	0.57817900
C	-6.43857300	-1.52480800	0.05172800
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C	6.19285400	3.64920100	1.35854100
H	7.07173700	4.14578000	0.92719200
H	6.52045800	3.11562700	2.26005000
H	5.48551700	4.43169200	1.66440600
N	1.72856900	-0.60512200	0.56724000
C	-8.17152000	0.56322600	0.84521900
H	-8.84324200	1.36050000	1.15574000
C	-6.38869300	3.02873600	1.59135200
H	-7.35155600	3.02140300	2.11895700
H	-6.06277200	4.07368600	1.49775100
H	-5.66107700	2.49616800	2.21711600
C	8.57614600	0.76923600	-0.98911100
H	9.55264100	1.00298300	-1.40673200
C	6.90804600	-0.89455500	-0.30910700
C	-6.04072800	-0.16340200	-0.09526800
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C	6.04103500	0.16225400	0.09520300
C	1.95392100	-0.71306200	1.89487800
C	5.67307600	-0.17742100	2.87102200
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H	5.36217100	-0.38117900	3.89903900
H	6.10254800	0.83098700	2.83181200
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H	-0.02416900	-0.31726800	2.76284300
H	1.15753900	-0.99597500	3.89306000
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C	4.49306800	-0.30290700	1.90930300
C	8.17051400	-0.56596500	-0.84705100
H	8.84105700	-1.36372100	-1.15887800
C	3.23487200	-0.57777000	2.49510500

C	-6.90931800	0.89279200	0.30726200
C	-0.34284800	0.69922100	-0.04288700
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H	0.29282000	1.36803300	-0.63698600
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H	5.52469400	-2.42407200	0.28265200
C	7.49863300	-3.17421300	0.69195200
H	7.15634400	-4.21215800	0.80023000
H	7.58552600	-2.73867800	1.69564600
H	8.50359000	-3.19842300	0.25082300
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H	-5.52811500	2.42343500	-0.28665800
C	-0.80672900	1.02787300	-2.85816200
H	0.02430500	0.31935800	-2.76235200
H	-0.40164100	2.03203400	-2.67084700
H	-1.15756700	0.99766100	-3.89263900
C	-5.52005700	-2.68981500	-0.33746000
H	-4.62604800	-2.27442000	-0.81535700
C	-5.05373400	-3.47340700	0.91942400
H	-5.90613300	-3.93243200	1.43760900
H	-4.54702600	-2.81217600	1.63453900
H	-4.35744700	-4.27520100	0.63768300
C	-7.50316400	3.17059600	-0.69617400
H	-8.50793100	3.19430300	-0.25459000
H	-7.59010600	2.73366600	-1.69926000
H	-7.16205600	4.20877100	-0.80594700
H	3.24920700	-0.69153400	3.57308700

ln₂^{dim}

ln	-1.23165100	0.47229700	-0.62802900
ln	2.10389900	1.11439200	-1.31959000
C	3.03855900	-1.02632100	2.70106200
H	4.12168400	-0.90815000	2.83047400
H	2.87120700	-2.05148300	2.35356700
H	2.56108700	-0.90165800	3.67679700
C	-0.53520800	3.43043200	-1.21167300
H	-0.87416300	4.39178700	-1.61895800
H	-0.16022500	2.84721800	-2.06353600
C	1.56526200	-3.98030900	0.23238400
H	2.09575600	-4.87265200	-0.12606600
H	0.48797900	-4.18973000	0.19120900
H	1.84206600	-3.82744300	1.28367000
C	-1.33000500	-1.97471800	2.88519600
H	-1.43908400	-3.04497000	3.10573100
H	-0.78430000	-1.50987200	3.71733700
H	-0.71864700	-1.87707200	1.97986700
C	-3.44722500	-1.88084900	1.48345700

C	1.67227400	1.01251900	2.23088300
H	1.48182700	0.92770000	3.29496400
C	-2.71450400	-1.29877100	2.69840800
H	-2.53741700	-0.23342200	2.51345900
C	5.72438000	-2.99047400	-0.93216400
H	6.45544500	-3.71272600	-1.28824100
N	2.85212800	-0.11072700	0.39530600
C	-3.84769800	-1.46699600	-3.28327300
H	-2.77143600	-1.43596500	-3.07014300
H	-4.03580900	-0.87285300	-4.18788200
H	-4.11477800	-2.50933100	-3.50194700
C	4.35467200	-3.28463000	-0.99022900
H	4.02950000	-4.24050900	-1.39487600
C	-3.83783200	-3.23650700	1.50637200
H	-3.63005400	-3.83608100	2.38983600
N	1.22695600	2.44550600	0.29969300
N	-3.27656000	0.27494200	0.23565700
C	3.38645800	-2.36244400	-0.53777100
C	2.50028000	-0.00785700	1.69652800
C	-3.55152400	-1.41501500	3.99965100
H	-3.73484000	-2.46390500	4.26659900
H	-4.52710500	-0.92228500	3.89931100
H	-3.01866900	-0.94603800	4.83778500
N	-1.63620900	2.65663400	-0.58367600
C	6.14553100	-1.75410500	-0.41891400
H	7.20828900	-1.52511500	-0.38406000
C	6.28978900	1.41038000	-0.59317500
H	7.15023100	0.92115200	-1.06913800
H	6.61855300	2.39108900	-0.22231300
H	5.52835800	1.57283600	-1.36689400
C	-4.48518100	-3.82662400	0.41087600
H	-4.77781200	-4.87336900	0.44672300
C	-4.37647400	-1.69969700	-0.80407800
C	3.82585600	-1.11449100	-0.00916800
C	1.14024800	2.18151000	1.61888800
C	-3.72724900	-1.10786500	0.31936000
C	-2.69640900	3.30127100	-0.05326300
C	-5.46614100	0.91204400	1.23814100
H	-6.08469900	0.37730500	0.50725500
H	-6.00155700	1.81195200	1.55220700
H	-5.35691200	0.24857300	2.10327300
C	-2.77382100	4.83082000	-0.08571400
H	-1.86510200	5.29705900	0.31350300
H	-3.62326300	5.18174300	0.50556100
H	-2.90845700	5.19585300	-1.11315400
C	-4.10612700	1.26785700	0.64046700
C	-4.74571600	-3.05951300	-0.73432200
H	-5.24014600	-3.52223100	-1.58545300

C	-3.81285900	2.64877400	0.53505700
C	5.21676700	-0.80160600	0.04897900
C	0.66549200	3.69973100	-0.25687000
H	1.44439600	4.19484600	-0.85707800
H	0.36240600	4.40895700	0.52096100
C	-4.67089700	-0.91443300	-2.08864200
H	-4.36332200	0.12547500	-1.93304300
C	-6.18386500	-0.90422900	-2.43214200
H	-6.36824100	-0.28437300	-3.31981900
H	-6.78141800	-0.49999400	-1.60487200
H	-6.55434000	-1.91478800	-2.64835200
C	5.72945900	0.54731900	0.56986100
H	4.88357800	1.09369400	1.00056700
C	0.44726500	3.15741300	2.57686100
H	-0.58120300	3.37222600	2.26205100
H	0.98889500	4.11156100	2.63321300
H	0.41215000	2.73685200	3.58478600
C	1.90263500	-2.73680200	-0.63364000
H	1.30834800	-1.89820200	-0.25293700
C	1.47374300	-2.97371500	-2.10579200
H	2.02770800	-3.80940100	-2.55418600
H	1.65534900	-2.08110700	-2.71717700
H	0.40286200	-3.20999300	-2.15783800
C	6.79472200	0.38441100	1.68517400
H	7.70392600	-0.10208200	1.30866300
H	6.41471700	-0.21985000	2.51923200
H	7.08394800	1.36769200	2.08015800
H	-4.57956600	3.30976300	0.92302900

In₄

In	-1.24052200	1.41283400	-0.30969400
In	1.24532200	-1.42036300	0.31233300
In	1.62939400	1.62511300	0.89501900
In	-1.63291800	-1.61689700	-0.89758700
N	-0.52610100	1.75372300	-2.35409000
C	-1.24132400	5.77444800	2.80077800
H	-1.39800700	6.46918400	1.96641400
H	-0.20331400	5.88468500	3.14291700
H	-1.90158200	6.08443300	3.62188600
C	-0.38078800	2.94911800	-2.95033800
C	6.09501500	2.71188500	1.11380700
H	6.04393400	3.69281900	0.63237800
H	6.59424600	2.03598700	0.40910600
H	6.71830200	2.78922400	2.00874800
C	-0.86774200	4.17110100	-2.40395100
H	-0.60935700	5.05876100	-2.97019000
C	-3.67509000	-4.34148100	0.80739800
N	-2.25134200	-0.83882800	-2.90946100

C	0.07897600	-0.51605800	3.02761600
H	-0.71898600	-0.70953300	3.75501200
H	-0.35782800	0.14346800	2.26750000
C	6.24925600	0.43880400	-2.07688100
H	6.51846400	0.73422500	-3.10001300
H	6.44995300	-0.63554500	-1.97326400
H	6.91372200	0.97904100	-1.39143800
C	-1.20454300	-0.23603500	-3.78215300
H	-0.72399000	-1.03666400	-4.37052100
H	-1.64428200	0.47070200	-4.49530400
C	-3.17259100	-5.16983200	-0.38218000
H	-2.99482100	-4.48842200	-1.22122200
N	-2.12882300	3.44679300	-0.42067400
N	-3.71148800	-2.26338700	-0.55856800
C	-3.78784300	-0.55233200	-4.86119600
H	-3.73156700	0.54143400	-4.94921200
H	-4.79520700	-0.85917300	-5.15156800
H	-3.08128200	-0.97851700	-5.58440100
C	-3.95718500	-2.94535200	0.70518400
C	-3.21356400	3.75307900	0.49946500
C	5.61917400	-1.85863000	1.44420400
H	6.55726400	-1.86468900	0.87240700
H	5.85697300	-1.58508500	2.48099900
H	4.97333400	-1.07491300	1.03377300
C	-1.72224100	4.39844500	-1.29909200
C	-3.87122200	0.08068200	2.77486900
H	-4.07126900	-0.21115600	3.81537700
H	-4.07336500	1.15472900	2.67798300
H	-2.80903200	-0.08378300	2.56648600
C	4.56610800	-3.63303000	-0.04779100
C	4.58223800	1.61829600	2.75898400
H	5.49379400	1.64967400	3.34443000
C	4.92183600	-3.24261400	1.39305400
H	3.99317900	-3.15954600	1.96640000
C	0.35201900	3.07268400	-4.28876100
H	1.40897400	2.79309100	-4.18361400
H	0.31457000	4.10395900	-4.64785000
H	-0.09137900	2.43021800	-5.06000400
C	-2.23154200	5.83016700	-1.13628000
H	-1.69860800	6.50802500	-1.80850700
H	-2.10292600	6.18066700	-0.10695100
H	-3.30236200	5.89454100	-1.36308000
C	-4.02507600	4.35477700	2.72374300
H	-3.82444200	4.64367800	3.75315200
C	-1.51538800	4.30486500	2.38199300
H	-0.81039300	4.04794100	1.58359400
C	4.36148200	4.29063000	-3.16327800
H	4.52522000	4.80710100	-4.10656300

C	-2.94130100	4.12479700	1.84841900
C	-3.48231000	-1.01290700	-3.43096200
N	3.70733700	2.26985300	0.55645800
C	-4.75432600	-0.72220900	1.78556600
H	-4.52717300	-0.35697200	0.77846600
C	1.22829100	-3.36247700	-3.57171900
H	1.42221700	-2.31771700	-3.30117800
H	0.17756000	-3.45042700	-3.87942400
H	1.85702400	-3.60845600	-4.43822500
C	4.62702200	2.91785400	-3.05357000
H	4.99875500	2.37419000	-3.91955000
C	5.61330600	-3.86871500	-0.96297700
H	6.64432300	-3.77234100	-0.62914100
C	-5.79999600	4.30964700	-2.08543400
H	-6.77644200	4.40507200	-1.59236000
H	-5.98190900	4.03247700	-3.13269900
H	-5.32429200	5.29849100	-2.07456800
C	-5.35264500	4.22489700	2.29214600
H	-6.17418700	4.40615400	2.98143400
N	2.24686400	0.84310500	2.90647900
N	2.13232100	-3.45370700	0.42470900
C	-3.88814700	-4.98809300	2.04299200
H	-3.68193900	-6.05255600	2.12895600
C	4.43268300	2.22629600	-1.83789300
C	4.70670400	2.17965100	1.46705100
C	5.80934100	-4.31253500	2.08361000
H	6.78521500	-4.40508600	1.58885400
H	5.33662700	-5.30284000	2.07368900
H	5.99229900	-4.03465000	3.13050300
C	-4.71083700	-2.17452800	-1.46915900
N	0.52977700	-1.75865200	2.35614700
C	-1.82859900	-5.87338700	-0.06328200
H	-1.07501700	-5.14690300	0.26105300
H	-1.45175200	-6.39298200	-0.95499500
H	-1.94508300	-6.62038800	0.73393400
C	3.88683700	4.99352800	-2.04599100
H	3.68125700	6.05807400	-2.13249400
C	-4.43524100	-2.22110300	1.83635100
C	1.82599000	5.87868900	0.06046000
H	1.94133200	6.62508800	-0.73749300
H	1.44923100	6.39870600	0.95198100
H	1.07292400	5.15123100	-0.26289500
C	-5.61190900	3.86214900	0.96183600
H	-6.64242700	3.76573300	0.62646700
C	5.35203400	-4.23081400	-2.29307600
H	6.17254800	-4.41187300	-2.98364200
C	2.94131000	-4.13036300	-1.84590400
C	3.95415800	2.95131100	-0.70739500

C	3.47820100	1.01573900	3.42762000
C	3.21566400	-3.75994500	-0.49702000
C	-4.62875300	-2.91324600	3.05182600
H	-5.00021900	-2.37006300	3.91822500
C	0.38596500	-2.95303100	2.95483300
C	-4.56335700	3.62614600	0.04826000
C	-6.09912000	-2.70651500	-1.11532400
H	-6.04799300	-3.68668000	-0.63235200
H	-6.72232900	-2.78530000	-2.01020000
H	-6.59848700	-2.02954900	-0.41170900
C	2.23815600	-5.83570800	1.14425200
H	2.11336600	-6.18641300	0.11453700
H	1.70325200	-6.51368900	1.81481300
H	3.30823200	-5.89951200	1.37492500
C	-4.91707800	3.23683100	-1.39339200
H	-3.98739400	3.15128600	-1.96469700
C	-4.58643600	-1.61456200	-2.76183400
C	-0.34751600	-3.07489700	4.29302200
H	0.09278300	-2.42838900	5.06264500
H	-0.30679300	-4.10488100	4.65547500
H	-1.40536500	-2.79939000	4.18585300
C	1.72773500	-4.40420200	1.30526600
C	-0.07951900	0.51197800	-3.02997600
H	0.71833700	0.70538900	-3.75747800
H	0.35581700	-0.15162900	-2.27251800
C	4.02382400	-4.36005600	-2.72288600
H	3.82169300	-4.64808800	-3.75224300
C	0.87458400	-4.17551500	2.41091600
C	3.67305000	4.34755600	-0.81019000
C	1.20065600	0.23822500	3.77873500
H	0.71652400	1.03856300	4.36442800
H	1.64185700	-0.46511800	4.49418800
C	1.51457600	-4.30944600	-2.37763600
H	0.81068200	-4.05039400	-1.57897000
C	-4.36271800	-4.28597100	3.16079800
H	-4.52591200	-4.80297700	4.10388700
C	1.23854800	-5.77949700	-2.79347900
H	0.20033800	-5.88909400	-3.13518200
H	1.39448400	-6.47268600	-1.95767800
H	1.89830800	-6.09190800	-3.61407300
C	3.17086200	5.17664700	0.37899800
H	2.99440300	4.49591800	1.21887800
C	3.78495200	0.55253200	4.85680100
H	3.72875500	-0.54137700	4.94292600
H	3.07927500	0.97756200	5.58152900
H	4.79265800	0.85872000	5.14665300
C	4.75160200	0.72735800	-1.78606300
H	4.52400800	0.36272400	-0.77882700

C	-5.61846900	1.85505600	-1.44676700
H	-6.55746900	1.86329200	-0.87649200
H	-4.97561000	1.06902600	-1.03621100
H	-5.85541500	1.58313000	-2.48416300
C	3.86887500	-0.07614500	-2.77520600
H	4.06899200	0.21536100	-3.81579700
H	2.80664300	0.08793500	-2.56696500
H	4.07130900	-1.15011800	-2.67787800
C	-1.22949800	3.35632300	3.57493200
H	-0.17929100	3.44501100	3.88423800
H	-1.42205700	2.31176100	3.30270800
H	-1.85972000	3.60034300	4.44090700
C	4.22755300	6.21862900	0.83662700
H	4.44726800	6.93876200	0.03694300
H	5.17148200	5.73971100	1.12498400
H	3.85591500	6.78188300	1.70342200
C	-6.25189400	-0.43398900	2.07707500
H	-6.52077400	-0.73033800	3.10002600
H	-6.91643100	-0.97377500	1.39134400
H	-6.45274200	0.64041800	1.97442800
C	-4.22977800	-6.21055100	-0.84158500
H	-4.45086000	-6.93102600	-0.04257600
H	-3.85781200	-6.77352500	-1.70842400
H	-5.17299300	-5.73060400	-1.13052700
H	0.61779100	-5.06234800	2.97919400
H	-5.49790200	-1.64676700	-3.34739900

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C	5.61390900	-0.06748700	3.08184400
H	6.40741000	0.67796100	2.94729600
H	6.08246900	-1.05239200	2.96441800
H	5.22990600	0.01458000	4.10205400
C	-0.34179700	-0.69278600	-0.10761700
H	0.31252200	-1.30855700	-0.74076800
H	-0.39008000	-1.19979200	0.86768900
C	6.18560700	-3.81169800	1.26335500
H	7.06692500	-4.29293000	0.81924000
H	5.45351400	-4.59913500	1.48823000
H	6.49703500	-3.35560000	2.21180500
C	-5.11498600	3.43000100	1.01661400
H	-5.96934100	3.85771100	1.55778800
H	-4.40150200	4.24079700	0.81515400
H	-4.63059500	2.70498900	1.68529100
C	-6.52186200	1.58915900	-0.03794400
C	3.20562600	0.38309000	2.58699200
H	3.17777200	0.42479400	3.67060800
C	-5.56750500	2.75847300	-0.30791200
H	-4.67198800	2.35710700	-0.79422600

C	8.69579800	-0.80463100	-0.78096400
H	9.67595500	-1.02215600	-1.19885800
N	4.79801100	0.05452400	0.73952400
C	-6.52982300	-3.07451000	1.05473000
H	-5.77920700	-2.60965200	1.70856900
H	-6.22188600	-4.11157100	0.86325700
H	-7.47840700	-3.09939500	1.60732400
C	7.79829700	-1.84736000	-0.50313100
H	8.09318200	-2.87415300	-0.70964300
C	-7.79842400	1.84719100	0.50321600
H	-8.09340800	2.87398400	0.70958500
N	1.71860600	0.56030500	0.63534300
N	-4.79808000	-0.05453100	-0.73953000
C	6.52168900	-1.58926800	0.03789400
C	4.49578200	0.13070000	2.05360300
C	-6.18626300	3.81138200	-1.26390500
H	-7.06757200	4.29259200	-0.81974800
H	-6.49778300	3.35504300	-2.21220900
H	-5.45430800	4.59886700	-1.48906200
N	-1.71864600	-0.56018400	-0.63560700
C	8.31800000	0.52105100	-0.51722400
H	9.01507800	1.32769300	-0.73412800
C	6.53054200	3.07470400	-1.05383400
H	7.47926100	3.09959800	-1.60619600
H	6.22270800	4.11175800	-0.86216100
H	5.78001700	2.61012700	-1.70797500
C	-8.69575300	0.80440000	0.78137100
H	-9.67587300	1.02187600	1.19937900
C	-7.05224500	-0.82808700	-0.02428700
C	6.14402200	-0.23791100	0.30190400
C	1.93741700	0.57207000	1.96343400
C	-6.14407400	0.23780500	-0.30179000
C	-1.93756700	-0.57195700	-1.96368000
C	-5.61417400	0.06745900	-3.08178700
H	-6.40763100	-0.67802900	-2.94720900
H	-5.23024300	-0.01455600	-4.10202900
H	-6.08277100	1.05233800	-2.96429300
C	-0.77751200	-0.82383000	-2.93950100
H	0.03808000	-0.10273300	-2.80215100
H	-1.12202800	-0.74647800	-3.97351900
H	-0.35689000	-1.82949400	-2.80023600
C	-4.49596300	-0.13071300	-2.05363500
C	-8.31782700	-0.52128300	0.51781500
H	-9.01476300	-1.32797500	0.73499200
C	-3.20583700	-0.38303500	-2.58713200
C	7.05236600	0.82791600	0.02472600
C	0.34179900	0.69291300	0.10724600
H	0.39014500	1.19989600	-0.86806800

H	-0.31255500	1.30870400	0.74034400
C	-6.67813200	-2.29308200	-0.27886000
H	-5.70427600	-2.31112500	-0.78018300
C	-7.69556100	-3.00472200	-1.20860600
H	-7.36267500	-4.02865700	-1.42611900
H	-7.80644800	-2.47270400	-2.16210300
H	-8.68886800	-3.06870400	-0.74542400
C	6.67842200	2.29290400	0.27958700
H	5.70445400	2.31096400	0.78069500
C	0.77728400	0.82396200	2.93915800
H	-0.03832000	0.10289600	2.80172200
H	0.35670900	1.82964300	2.79987400
H	1.12170700	0.74658000	3.97320500
C	5.56713800	-2.75851100	0.30748200
H	4.67159600	-2.35712600	0.79373400
C	5.11473500	-3.42971200	-1.01725000
H	5.96911700	-3.85743200	-1.55837400
H	4.63055000	-2.70450000	-1.68585800
H	4.40110800	-4.24045000	-0.81606400
C	7.69573900	3.00414100	1.20976000
H	8.68916800	3.06808400	0.74683400
H	7.80631000	2.47185700	2.16314600
H	7.36296400	4.02807300	1.42745700
H	-3.17807300	-0.42474400	-3.67075000
TI	-3.34225700	-0.39545000	1.20637400
TI	3.34237300	0.39555300	-1.20650300

TI₂^{dim}

TI	-1.14787500	-0.33002100	-0.56017000
TI	2.19990600	-1.16013300	-1.18781800
N	2.76006000	0.37822600	0.64119500
N	1.06508800	-2.26474800	0.74132600
N	-3.47030100	-0.20926200	0.28682700
C	1.34860000	-0.51745400	2.44901900
N	-1.71560400	-2.71250600	-0.30593100
C	2.25503100	0.42396000	1.89041300
C	-3.98832600	-2.59411400	0.61708500
H	-4.78971500	-3.23612700	0.96705600
C	-3.91180700	1.16656000	0.32007100
C	-4.30072300	-1.20960700	0.64964700
C	-4.45992200	1.75947700	-0.85828700
C	-2.82689700	-3.29401600	0.17838600
C	5.59702000	-0.27524600	1.10806800
H	4.70569900	-0.77113400	1.50652300
C	-4.58350000	3.91697500	0.30126800
H	-4.84129900	4.97351100	0.29428900
C	-4.04417500	3.32774900	1.45505300

H	-3.88731200	3.93795200	2.34217700
C	1.92159700	2.87600700	-0.72439000
H	1.29814200	2.12087800	-0.23254000
C	6.54343700	0.01680100	2.30145400
H	6.79009000	-0.91407000	2.82989000
H	6.07913500	0.70366600	3.02066800
H	7.48619000	0.47046400	1.96829500
C	3.76838100	1.32144600	0.21133000
C	4.40178300	3.35611100	-0.98560200
H	4.12152900	4.26159600	-1.51968300
C	-5.71256200	-0.86238100	1.13366500
H	-5.67856500	-0.18507900	1.99501500
H	-6.26287900	-1.76274500	1.41956800
H	-6.27727600	-0.34574900	0.34760200
C	6.26905400	-1.26020300	0.11367200
H	7.18099300	-0.82723500	-0.31841800
H	5.59479300	-1.50734600	-0.71768800
H	6.54454000	-2.19480200	0.62123900
C	0.85683300	-1.77273700	1.97657100
C	5.14925800	1.00619100	0.39444500
C	0.55751000	-3.60477100	0.36601200
H	0.18061800	-4.17766700	1.22175500
H	1.39104100	-4.18524100	-0.06238500
C	3.39080600	2.50713900	-0.48782500
C	-3.70330000	1.95933800	1.48895500
C	-0.55877400	-3.53386100	-0.71917300
H	-0.12383700	-3.08239400	-1.62480000
H	-0.82629000	-4.56405800	-0.99399800
C	5.76031000	3.05570000	-0.80535400
H	6.52571400	3.72215900	-1.19608300
C	-2.92631600	-4.82498900	0.27368200
H	-2.92534700	-5.28534000	-0.72411700
H	-3.85279000	-5.11743300	0.77391200
H	-2.08768000	-5.25491600	0.83655500
C	-4.78570000	3.13178800	-0.84414100
H	-5.20261600	3.59047900	-1.73845100
C	2.69243900	1.55454100	2.82684600
H	3.74875100	1.43815700	3.10250700
H	2.09766500	1.55699800	3.74412300
H	2.59688000	2.53239100	2.34186300
C	-3.78995900	1.45143900	-3.29765000
H	-4.02290600	2.49214100	-3.55906600
H	-3.93514400	0.83632000	-4.19632200
H	-2.72776200	1.40967900	-3.02157800
C	6.12377700	1.88525500	-0.12133100
H	7.17781300	1.65109700	0.01232900
C	-1.71341700	1.98447400	3.07565700
H	-1.01022900	1.80461500	2.25282600

H	-1.28663900	1.54064000	3.98557900
H	-1.78515500	3.06951400	3.22965600
C	-4.69233900	0.94838700	-2.13915100
H	-4.41924400	-0.09255800	-1.93488800
C	0.04227300	-2.56401200	3.01107800
H	-0.94978500	-2.82471900	2.62328900
H	-0.09211000	-1.97395400	3.92093700
H	0.55207300	-3.49571700	3.29228900
C	-3.10568300	1.36999100	2.77217300
H	-2.96418200	0.29462600	2.61790800
C	1.55821800	4.25264200	-0.10756200
H	1.77978800	4.28208300	0.96685000
H	0.48764800	4.45890100	-0.23989400
H	2.11832100	5.06682200	-0.58606100
C	1.57220800	2.85745100	-2.23661200
H	2.15673400	3.60548900	-2.78841800
H	0.50748100	3.08058200	-2.38846900
H	1.78389200	1.87668000	-2.68329700
C	-4.04903900	1.55034300	3.99081100
H	-4.19259200	2.61126800	4.23438500
H	-3.62559300	1.05887400	4.87732300
H	-5.03881500	1.11598100	3.80120200
C	-6.18165800	0.96333300	-2.57410000
H	-6.83565100	0.59486400	-1.77356800
H	-6.32882700	0.32426900	-3.45536700
H	-6.51352500	1.97661600	-2.83636100
H	1.04240100	-0.27872800	3.46184000

Tl₄

Tl	-0.67421700	-2.07075500	0.16802500
Tl	0.65915000	1.99928600	-0.23817300
Tl	2.56749300	-0.93211900	-0.54955900
Tl	-2.58057800	0.85748900	0.48332400
N	-0.02604800	-2.03030400	2.49819400
C	2.90974300	-6.40212300	-1.47755100
H	2.66518500	-7.09379000	-0.66235600
H	3.93745800	-6.05146200	-1.32602100
H	2.88426400	-6.97155700	-2.41621900
C	0.48092100	-3.01739300	3.25410000
C	6.85497700	1.41343300	-0.60880800
H	7.56693300	0.59806200	-0.78724100
H	6.93446600	1.67764900	0.45089100
H	7.16576500	2.27109200	-1.21137900
C	0.58137700	-4.38059600	2.85012500
H	0.97212100	-5.03852600	3.61888300
C	-6.62084300	1.63267400	-0.00447000
N	-2.67689900	-0.59171900	2.51120700
C	0.26777300	0.49931700	-3.09292800

H	-0.42924100	0.25399700	-3.90786500
H	0.00429700	-0.17718500	-2.26544400
C	5.17708700	2.66290900	2.83373300
H	5.71180300	2.48743000	3.77665400
H	4.52246200	3.53402100	2.96988600
H	5.92049400	2.91597100	2.06811600
C	-1.60951800	-0.30310500	3.49908700
H	-1.61268400	0.78045900	3.69847700
H	-1.78972900	-0.79567000	4.46227600
C	-6.69534000	1.88391500	1.50725800
H	-6.12515300	1.10057000	2.01678900
N	-0.19814600	-4.47296000	0.50446100
N	-4.86367800	-0.10459000	0.29473600
C	-3.30888100	-2.57477300	3.91435000
H	-2.28821600	-2.97197900	3.93051000
H	-4.00175700	-3.41726000	3.84802200
H	-3.49680100	-2.07019800	4.87238400
C	-5.70775700	0.68832800	-0.56652400
C	-0.52678800	-5.29697200	-0.64329600
C	4.23912800	4.80692500	-0.21557200
H	4.79760800	5.36567600	0.54781600
H	4.92121800	4.58070200	-1.04444000
H	3.92803600	3.85281500	0.22586800
C	0.22400000	-5.05421500	1.65053200
C	-3.74007800	0.21395300	-3.75005000
H	-4.36261200	0.58107400	-4.57590200
H	-3.05284500	-0.53636400	-4.16516600
H	-3.14846300	1.05716800	-3.37296100
C	1.99936900	5.83456800	0.40458400
C	4.91340800	1.54546500	-2.16552600
H	5.56842300	2.28812800	-2.60824200
C	3.01865700	5.61977400	-0.72099800
H	2.54080400	5.03414900	-1.51240900
C	1.00051300	-2.72071300	4.66846500
H	1.90254000	-2.09427400	4.62849700
H	1.26194400	-3.64814900	5.18386600
H	0.25610400	-2.19247800	5.27781800
C	0.35546100	-6.58107300	1.70286600
H	0.69820000	-6.91107400	2.68691400
H	1.05972600	-6.94752200	0.94757500
H	-0.60809000	-7.06000500	1.49250300
C	0.08249700	-6.42158400	-2.73488300
H	0.83300900	-6.69667100	-3.47327800
C	1.92635900	-5.20277700	-1.51702600
H	2.04538500	-4.63878400	-0.58620700
C	6.68544400	-1.49927000	3.31363900
H	7.16945300	-1.90005700	4.20121900
C	0.46582900	-5.65524800	-1.61370900

C	-3.52086700	-1.62071200	2.72807200
N	4.79088600	0.09799000	-0.17579200
C	-4.58862800	-0.41432200	-2.61815500
H	-3.89800100	-0.74844600	-1.83423000
C	-1.81005000	3.91714900	2.68438700
H	-1.03778700	3.13641700	2.69001600
H	-2.79582300	3.43399300	2.64114400
H	-1.74445700	4.45151700	3.64122100
C	5.85189400	-0.37477600	3.40786500
H	5.68653300	0.08655500	4.37923300
C	2.37862800	6.61393100	1.51753000
H	3.37145800	7.05840300	1.54210200
C	-3.58211900	-6.58727200	0.84998200
H	-4.06453800	-7.25566600	0.12439800
H	-4.33900000	-6.29114300	1.58903300
H	-2.80665500	-7.16287700	1.37037000
C	-1.24290200	-6.84025400	-2.91600100
H	-1.51757800	-7.43729500	-3.78244500
N	2.78405300	0.39611000	-2.62846200
N	0.29406800	4.39217100	-0.71661500
C	-7.39955200	2.42563600	-0.87206300
H	-8.09085200	3.15360700	-0.45337600
C	5.22784300	0.17386500	2.26767000
C	5.43394000	0.97215600	-0.97648600
C	3.49763600	6.95810500	-1.34395500
H	4.05649400	7.56086000	-0.61566100
H	2.65727200	7.56535500	-1.70242200
H	4.16385600	6.76415800	-2.19563500
C	-5.35750900	-1.17906700	0.94174500
N	0.12135600	1.88741300	-2.60950500
C	-6.02066500	3.23847400	1.85823900
H	-4.98699400	3.27095200	1.48931500
H	-6.00415300	3.39305700	2.94587000
H	-6.56272000	4.07837100	1.40342000
C	6.88831100	-2.10230900	2.06348300
H	7.52550100	-2.98157600	1.99271700
C	-5.56234800	0.58740900	-1.98381400
C	5.90068000	-3.76264900	-0.36571100
H	6.44829300	-4.38962600	0.35052100
H	5.96108800	-4.24746200	-1.34986100
H	4.85015400	-3.74138300	-0.05069100
C	-2.21140300	-6.47392200	-1.97140500
H	-3.24165100	-6.79203000	-2.11437400
C	1.50331700	6.82932300	2.59227200
H	1.81400000	7.43447700	3.44075900
C	-0.20327000	5.47217400	1.46843300
C	5.45553600	-0.43069700	0.99578600
C	3.73337300	1.29997600	-2.92739200

C	0.68898800	5.25468500	0.37847200
C	-6.37021900	1.39621500	-2.81037200
H	-6.27899500	1.31695700	-3.89091100
C	-0.32254700	2.85689900	-3.42616500
C	-1.87958900	-5.70225900	-0.83810900
C	-6.76959500	-1.67396100	0.60863700
H	-7.52326100	-1.04854700	1.10449300
H	-6.91134300	-2.70172500	0.95558400
H	-6.97272300	-1.62874100	-0.46604400
C	-0.44545200	6.44075000	-1.92070900
H	-1.01176600	6.77933000	-1.04591800
H	-1.00150200	6.70670500	-2.82370000
H	0.49822800	6.99900500	-1.92193300
C	-2.99144800	-5.33298100	0.15087100
H	-2.56262800	-4.69347600	0.93166400
C	-4.68333400	-1.91141800	1.95378500
C	-0.69702300	2.53554600	-4.88126300
H	0.11369500	2.01100400	-5.40237700
H	-0.91209000	3.45393100	-5.43313700
H	-1.58894300	1.89747200	-4.93159600
C	-0.18738900	4.93071300	-1.86151700
C	-0.16800700	-0.65677800	3.01885900
H	0.51237900	-0.43197100	3.85159300
H	0.10542400	0.04307600	2.21385700
C	0.22349500	6.25625500	2.56097200
H	-0.45721300	6.42555900	3.39273600
C	-0.48959600	4.22272000	-3.05459600
C	6.28387300	-1.59159700	0.89574500
C	1.69498100	0.12638800	-3.59568900
H	1.67861000	-0.95769200	-3.79832200
H	1.86125400	0.61657200	-4.56177000
C	-1.61974000	4.88720600	1.48855100
H	-1.76573900	4.32090300	0.56125200
C	-7.29138700	2.30378300	-2.26598000
H	-7.91280700	2.91183800	-2.91928700
C	-2.70263200	5.99887800	1.52426700
H	-3.70796100	5.55651700	1.50976700
H	-2.61560000	6.66838000	0.65930200
H	-2.61687600	6.61165300	2.43123800
C	6.49791900	-2.33244100	-0.42953900
H	5.96372400	-1.78756100	-1.21541300
C	3.62663700	2.15262900	-4.20269000
H	2.66160700	2.67059800	-4.25511900
H	3.73544600	1.54181400	-5.10954900
H	4.41579800	2.90811000	-4.21827700
C	4.34512900	1.41741500	2.42660400
H	3.88467600	1.62631100	1.45399400
C	-4.12148100	-4.53312100	-0.54792100

H	-4.62454100	-5.13841600	-1.31327200
H	-3.72718300	-3.63401500	-1.03720200
H	-4.87159400	-4.21249300	0.18529700
C	3.20353900	1.18235600	3.44810500
H	3.59436700	1.06712200	4.46792400
H	2.63638600	0.27760700	3.19996300
H	2.51120500	2.03512500	3.44957700
C	2.28075900	-4.25673200	-2.69549100
H	3.31695700	-3.90209400	-2.61472800
H	1.61379300	-3.38441700	-2.71426600
H	2.17545400	-4.77049200	-3.66005100
C	7.99361600	-2.40365700	-0.83536600
H	8.57884700	-2.97336700	-0.10145600
H	8.44106600	-1.40560400	-0.91527100
H	8.10209300	-2.90259600	-1.80803300
C	-5.33789600	-1.67087600	-3.13957400
H	-6.07723800	-1.39328900	-3.90301300
H	-5.86724000	-2.18445600	-2.32888200
H	-4.63319300	-2.38457000	-3.58752800
C	-8.14330100	1.84766700	2.05762200
H	-8.76387300	2.64102000	1.62111700
H	-8.13984200	1.99273700	3.14643400
H	-8.63071700	0.88777100	1.84451000
H	-0.88656800	4.84921500	-3.84618900
H	-5.21584200	-2.79928000	2.27875000

B3LYP-D3/LANL2DZ

In₂^{OP}

In	3.19436800	-0.36452300	-1.10563000
In	-3.19434300	0.36539700	1.10533800
C	-5.64006800	0.16886900	-2.84451100
H	-6.44314600	0.86343400	-2.57267900
H	-6.06155700	-0.84135500	-2.77594100
H	-5.34790200	0.35587900	-3.88112400
C	0.31802200	-0.70864200	0.03400500
H	-0.33722400	-1.36191400	0.62387500
H	0.34013800	-1.12574200	-0.98198400
C	-5.99854500	-3.67426200	-1.35148300
H	-6.84714400	-4.20996900	-0.90694600
H	-5.25656700	-4.42219900	-1.66092900
H	-6.36148700	-3.15909400	-2.25008100
C	4.86375100	3.42285600	-0.91475000
H	5.69667900	3.90630000	-1.44220100
H	4.13651200	4.19928300	-0.64079600
H	4.38321300	2.72937300	-1.61753800
C	6.33836000	1.55643800	-0.03886900
C	-3.19958900	0.60371900	-2.48947100

H	-3.21330200	0.71120300	-3.56812800
C	5.36924600	2.67700200	0.34820200
H	4.49817800	2.22487400	0.83497400
C	-8.50488700	-0.87705300	0.95807200
H	-9.47541300	-1.14381200	1.36974000
N	-4.65408700	0.16392600	-0.56635400
C	6.39338700	-2.97696400	-1.55640900
H	5.63842800	-2.45634000	-2.15969900
H	6.09743400	-4.03078600	-1.46469000
H	7.34443200	-2.93640800	-2.10369100
C	-7.60156900	-1.88099500	0.57467700
H	-7.87992000	-2.92568900	0.69326800
C	7.60242800	1.88056800	-0.57281200
H	7.88117700	2.92524800	-0.69057600
N	-1.70773000	0.65217800	-0.55130800
N	4.65402000	-0.16413400	0.56624700
C	-6.33772700	-1.55680800	0.04022900
C	-4.45138100	0.31921200	-1.89895400
C	5.99963000	3.67344300	1.35372300
H	6.84827600	4.20924700	0.90939300
H	6.36254600	3.15784700	2.25208800
H	5.25776100	4.42134200	1.66351900
N	1.70753000	-0.65188300	0.55069700
C	-8.14823200	0.47241400	0.81133900
H	-8.84949200	1.24754300	1.11206300
C	-6.39378300	2.97765800	1.55435100
H	-7.34455800	2.93708800	2.10210200
H	-6.09831000	4.03153800	1.46175800
H	-5.63833700	2.45776700	2.15766500
C	8.50547000	0.87658200	-0.95675600
H	9.47618900	1.14329600	-1.36799700
C	6.89381200	-0.84184400	-0.28240800
C	-5.98741300	-0.18507100	-0.10035200
C	-1.92222800	0.73936600	-1.88260000
C	5.98752200	0.18472600	0.10063400
C	1.92182500	-0.73930300	1.88200400
C	5.63970400	-0.17017200	2.84455000
H	6.44298400	-0.86425400	2.57210200
H	5.34750600	-0.35824700	3.88096000
H	6.06092800	0.84023500	2.77698400
C	0.76070500	-1.02214400	2.83898600
H	-0.05333100	-0.29546900	2.73185700
H	1.10116700	-0.99427700	3.87701000
H	0.33483400	-2.01739300	2.65141200
C	4.45110300	-0.31986400	1.89877500
C	8.14828200	-0.47285800	-0.81112700
H	8.84932000	-1.24802000	-1.11228500
C	3.19914600	-0.60412700	2.48906300

C	-6.89401500	0.84146300	0.28207500
C	-0.31814900	0.70904500	-0.03480700
H	-0.34017100	1.12617500	0.98117100
H	0.33701300	1.36231500	-0.62477600
C	6.53458500	-2.32478500	-0.15576000
H	5.56307000	-2.40156400	0.34495500
C	7.56509000	-3.10008200	0.70437100
H	7.24696300	-4.14342000	0.83115900
H	7.67388000	-2.65168700	1.70021600
H	8.55558500	-3.10771300	0.23137300
C	-6.53536200	2.32444000	0.15422300
H	-5.56408500	2.40121600	-0.34695300
C	-0.76132100	1.02243400	-2.83977400
H	0.05275900	0.29575900	-2.73294400
H	-0.33543100	2.01765100	-2.65209700
H	-1.10199800	0.99474500	-3.87773200
C	-5.36833600	-2.67729800	-0.34635100
H	-4.49739300	-2.22514700	-0.83332700
C	-4.86262600	-3.42256700	0.91684900
H	-5.69541200	-3.90594900	1.44457900
H	-4.38213400	-2.72872800	1.61931900
H	-4.13529000	-4.19898300	0.64312500
C	-7.56652800	3.09877700	-0.70598100
H	-8.55676200	3.10655100	-0.23243900
H	-7.67577600	2.64954700	-1.70139900
H	-7.24873400	4.14209200	-0.83379000
H	3.21269200	-0.71184500	3.56769800

ln₂^{dim}

ln	-1.16859200	0.60519700	-0.83594200
ln	2.18285100	1.36417800	-1.29201000
C	2.68702600	-1.07569300	2.63836100
H	3.78133400	-1.12572700	2.66595000
H	2.33277200	-2.05990600	2.31194700
H	2.31852500	-0.89034500	3.65026200
C	-0.64461200	3.62552100	-1.12483200
H	-1.03312500	4.60467400	-1.43349400
H	-0.27089700	3.13924500	-2.03584200
C	0.91460400	-3.79608900	0.18396300
H	1.28303700	-4.71927400	-0.28227000
H	-0.18257800	-3.83677100	0.19898500
H	1.26813000	-3.78057000	1.22275400
C	-0.72142600	-1.80996800	2.78389700
H	-0.71465500	-2.88878700	2.98610900
H	-0.20938200	-1.30286400	3.61067200
H	-0.14452100	-1.63126400	1.87206900
C	-2.87706400	-1.94814300	1.45650900
C	1.39476100	1.02530500	2.21221600

H	1.13120900	0.88660500	3.25444900
C	-2.16656300	-1.27640300	2.63449500
H	-2.10082900	-0.20115600	2.43280700
C	5.15507700	-3.22213300	-0.94817900
H	5.79922000	-4.02260300	-1.30475400
N	2.62696700	-0.04637500	0.38384500
C	-3.68254100	-1.50161300	-3.24510700
H	-2.60851200	-1.32783100	-3.10068000
H	-4.01331200	-0.91845100	-4.11502300
H	-3.82098200	-2.56595800	-3.47621100
C	3.75996000	-3.37290500	-0.97802800
H	3.32795500	-4.29484900	-1.36054400
C	-3.06995000	-3.34527600	1.47390400
H	-2.71726400	-3.92153900	2.32615000
N	1.13125000	2.58375900	0.34403600
N	-3.06019500	0.21373200	0.24009400
C	2.90480900	-2.34736700	-0.52424300
C	2.22631300	0.01404300	1.67277200
C	-2.95019900	-1.46488100	3.95946200
H	-3.00573500	-2.52551400	4.23764600
H	-3.97698500	-1.08673500	3.88125500
H	-2.45044600	-0.92881600	4.77742200
N	-1.68713700	2.74478700	-0.54275600
C	5.71458700	-2.03051700	-0.46144500
H	6.79587800	-1.91381700	-0.44362500
C	6.28219600	1.05427600	-0.61969600
H	7.09828800	0.44300500	-1.02736700
H	6.71313800	1.99498900	-0.25049900
H	5.59364200	1.28780200	-1.44144800
C	-3.70320400	-4.00444300	0.40935500
H	-3.83857500	-5.08299000	0.43741300
C	-3.98811500	-1.86583900	-0.75185500
C	3.48511800	-1.14576100	-0.02990800
C	0.89488000	2.21747500	1.62163300
C	-3.33962500	-1.20996100	0.33203200
C	-2.74012500	3.27598800	0.11017200
C	-5.22827000	0.58030500	1.38697100
H	-5.82045600	0.01980500	0.65318600
H	-5.83974800	1.39738300	1.77881900
H	-5.00119300	-0.11390700	2.20294800
C	-2.88034600	4.79469500	0.24201600
H	-1.97592100	5.24590500	0.66839500
H	-3.72375200	5.05080700	0.88797300
H	-3.05246200	5.26058200	-0.73754600
C	-3.94837700	1.10372900	0.74287900
C	-4.15646700	-3.26474900	-0.69370400
H	-4.64344500	-3.77850400	-1.51929200
C	-3.77994500	2.50769800	0.70068500

C	4.89771000	-0.98003800	0.00549900
C	0.57234000	3.85543000	-0.17495100
H	1.35100100	4.35717200	-0.76848300
H	0.28635500	4.54843100	0.62382900
C	-4.48688000	-1.10025100	-1.98072700
H	-4.32422200	-0.03020200	-1.80996400
C	-6.00535800	-1.30849100	-2.21218800
H	-6.34877300	-0.69948400	-3.05892900
H	-6.58774600	-1.02402700	-1.32632900
H	-6.23422700	-2.35758500	-2.43994500
C	5.54798900	0.30604600	0.52366800
H	4.75634700	0.96578700	0.89598400
C	0.04199100	3.09038000	2.54819200
H	-0.96090800	3.23786500	2.13172300
H	0.49656200	4.07769600	2.70425500
H	-0.06556100	2.61597900	3.52668900
C	1.38865700	-2.54392300	-0.59661100
H	0.90859800	-1.66875000	-0.14623000
C	0.91036900	-2.61234300	-2.06914300
H	1.35249900	-3.47474700	-2.58626800
H	1.19294700	-1.70378000	-2.61482400
H	-0.18312400	-2.70559000	-2.11066400
C	6.51752500	0.02804200	1.70137800
H	7.36491900	-0.59248100	1.38194700
H	6.01111700	-0.49514100	2.52260700
H	6.92153100	0.97110400	2.09336700
H	-4.57165300	3.08154800	1.16905600

In₄

In	-1.33279000	1.33090800	-0.34046000
In	1.27368300	-1.38496900	0.31042200
In	1.49376000	1.66823200	0.93611200
In	-1.56182900	-1.70691000	-0.97138300
N	-0.48452200	1.66514300	-2.34906500
C	-1.30729200	5.72355100	2.85325500
H	-1.51970600	6.49446000	2.10194300
H	-0.26612600	5.84437600	3.18127400
H	-1.95642700	5.91293200	3.71826200
C	-0.12384000	2.86877800	-2.82857900
C	5.94483700	2.66357000	1.15055500
H	5.88434700	3.73371500	0.92136300
H	6.32903400	2.17057500	0.25140100
H	6.66091200	2.51788300	1.96332600
C	-0.55534800	4.10509900	-2.26816000
H	-0.15294000	4.99329500	-2.74120100
C	-3.43845100	-4.21475700	1.07425800
N	-2.32682300	-0.88284200	-2.90109600
C	-0.05188300	-0.58570900	2.96843300

H	-0.86728900	-0.81537100	3.66476500
H	-0.49304100	0.05116100	2.19319800
C	5.98501900	0.32463800	-2.02044400
H	6.25168200	0.62240200	-3.04351900
H	6.13764600	-0.75816100	-1.93166900
H	6.67826900	0.82786000	-1.33489000
C	-1.34691400	-0.21324000	-3.80370000
H	-0.95017700	-0.96338900	-4.50942800
H	-1.81980900	0.57859100	-4.39777000
C	-3.02046600	-5.16169400	-0.05553400
H	-3.07889500	-4.61313700	-1.00235100
N	-2.05023300	3.37639600	-0.47628000
N	-3.60022500	-2.29154500	-0.49420200
C	-3.98745700	-0.53323200	-4.72682600
H	-3.96710300	0.56567600	-4.72898400
H	-5.00104700	-0.85044900	-4.98279200
H	-3.31014100	-0.87806300	-5.51805500
C	-3.73703700	-2.84353000	0.83984200
C	-3.16473600	3.67829800	0.39591700
C	5.29072200	-1.54681700	1.31386700
H	6.12208900	-1.30998300	0.63637500
H	5.59251100	-1.28311300	2.33543200
H	4.44262900	-0.90714200	1.04949700
C	-1.51780500	4.34109900	-1.26194800
C	-3.83319200	0.43424200	2.74900800
H	-4.32749600	0.30198700	3.72136000
H	-3.96815800	1.47896100	2.44927300
H	-2.76156000	0.25373900	2.87888200
C	4.52724300	-3.41750200	-0.21587600
C	4.45128000	1.51107000	2.79133500
H	5.36963800	1.49226800	3.36605400
C	4.90571300	-3.04406800	1.22032900
H	4.02713600	-3.18696300	1.85741500
C	0.79206900	2.98244300	-4.04809100
H	1.75340800	2.49053400	-3.85688900
H	1.00135300	4.03089200	-4.27171900
H	0.34142500	2.52680300	-4.93972100
C	-1.98725500	5.77915300	-1.07243400
H	-1.46938700	6.45615400	-1.75675600
H	-1.80773800	6.11239000	-0.04424200
H	-3.06726600	5.85747200	-1.24973000
C	-4.05245200	4.29961200	2.57624000
H	-3.89346100	4.62086600	3.60314700
C	-1.52415900	4.29924100	2.28504300
H	-0.81007500	4.14743200	1.46881500
C	4.15080400	4.23026900	-3.10492200
H	4.29033600	4.73761900	-4.05690800
C	-2.93834400	4.10053800	1.73452900

C	-3.58156700	-1.07573700	-3.35396100
N	3.56305200	2.23753700	0.62642100
C	-4.42161500	-0.49973700	1.66806100
H	-3.96356600	-0.21203700	0.71641700
C	0.99219000	-3.21953100	-3.51292800
H	1.20236100	-2.18359400	-3.22552600
H	-0.08144300	-3.30409200	-3.72734100
H	1.54629100	-3.43426400	-4.43692100
C	4.41027500	2.85547600	-2.99413500
H	4.75306800	2.30161800	-3.86539000
C	5.53207000	-3.53253400	-1.19760400
H	6.57010800	-3.35990800	-0.92281200
C	-5.65081400	4.00817500	-2.28067500
H	-6.65192900	4.05633900	-1.83237900
H	-5.76821500	3.70394000	-3.32963800
H	-5.22582800	5.02032200	-2.26251900
C	-5.35952600	4.07686800	2.11490100
H	-6.20631200	4.22502500	2.78092400
N	2.09338800	0.81114600	2.92577700
N	2.12662700	-3.39332700	0.37938000
C	-3.52846400	-4.70832000	2.39274000
H	-3.29936800	-5.75346900	2.58719900
C	4.23379200	2.17442500	-1.77135300
C	4.57140300	2.11252100	1.51970500
C	6.03742200	-3.94122700	1.77960300
H	6.98464500	-3.77690600	1.24965400
H	5.78447700	-5.00604200	1.69156300
H	6.20880100	-3.71477300	2.84048700
C	-4.64108000	-2.31522900	-1.35488100
N	0.48534200	-1.79913700	2.31091600
C	-1.55196500	-5.62693200	0.12129700
H	-0.87447400	-4.76903800	0.17738200
H	-1.24538200	-6.26059700	-0.72249800
H	-1.43062800	-6.20499900	1.04741100
C	3.70548600	4.94551500	-1.98294200
H	3.49996800	6.00987900	-2.07251400
C	-4.09974400	-1.97707500	1.91167000
C	1.65181900	5.73796900	0.22633100
H	1.66731400	6.46637500	-0.59623900
H	1.29647400	6.25315900	1.12922800
H	0.93581900	4.95315000	-0.03534300
C	-5.56868900	3.65181900	0.79274700
H	-6.58243600	3.47605800	0.43939500
C	5.21601400	-3.87281800	-2.52315600
H	6.00454600	-3.96100900	-3.26688700
C	2.83806200	-3.96912800	-1.93725800
C	3.79766800	2.91495200	-0.63646800
C	3.33486700	0.90392800	3.43877000

C	3.17056900	-3.62651400	-0.59830200
C	-4.19175600	-2.51931500	3.21053400
H	-4.48294800	-1.87588800	4.03669400
C	0.39468900	-2.99792600	2.90935400
C	-4.48468800	3.45380500	-0.08680500
C	-5.92573200	-3.03571300	-0.95196300
H	-5.80920400	-4.11215000	-1.13584500
H	-6.77681600	-2.68086900	-1.54027800
H	-6.14994100	-2.91536500	0.11067300
C	2.38899700	-5.76246100	1.05320200
H	2.22913400	-6.10894500	0.02638700
H	1.94544000	-6.48442500	1.74409500
H	3.47378300	-5.74377900	1.21808000
C	-4.74112700	3.00442500	-1.52828700
H	-3.77903100	2.97475100	-2.05005900
C	-4.61735800	-1.75869900	-2.65385900
C	-0.35343100	-3.14623200	4.23417800
H	0.04808200	-2.47565900	5.00454700
H	-0.27931000	-4.17147700	4.60548300
H	-1.41739400	-2.91448600	4.10110400
C	1.79413400	-4.37233500	1.25542800
C	-0.13816200	0.42714000	-3.08377300
H	0.63526700	0.59105000	-3.84164100
H	0.28700300	-0.29151200	-2.37322000
C	3.87827400	-4.09489900	-2.88253300
H	3.63523200	-4.36162800	-3.90860000
C	0.95554000	-4.19467800	2.37725300
C	3.52609000	4.30981700	-0.73697200
C	1.01483800	0.20928100	3.76007600
H	0.49066700	1.01864100	4.29443400
H	1.42135500	-0.47091600	4.51602600
C	1.38996900	-4.19437700	-2.37615400
H	0.73417300	-3.98430000	-1.52487600
C	-3.91293200	-3.87477800	3.45362600
H	-3.98930500	-4.27514200	4.46221900
C	1.14064700	-5.66082500	-2.80961000
H	0.08618200	-5.80072600	-3.08394100
H	1.37583300	-6.36261100	-1.99983200
H	1.75734200	-5.92986900	-3.67767500
C	3.05963600	5.13614800	0.46619300
H	2.98931100	4.47003300	1.33297000
C	3.64521600	0.32831100	4.82489200
H	3.51709900	-0.76286400	4.83339000
H	2.98718400	0.74811600	5.59604900
H	4.67796200	0.54563700	5.10727000
C	4.50720700	0.66962400	-1.70481500
H	4.29146500	0.32926700	-0.68910200
C	-5.33441700	1.57475100	-1.57780700

H	-6.28764100	1.52014300	-1.03604900
H	-4.64970900	0.84485800	-1.13376600
H	-5.51460800	1.26640600	-2.61586200
C	3.57003800	-0.11445600	-2.65592000
H	3.74766100	0.15633500	-3.70649900
H	2.52517400	0.09298300	-2.41086500
H	3.73508300	-1.19324900	-2.54887900
C	-1.20446000	3.23533100	3.36581400
H	-0.16313200	3.33611700	3.70031300
H	-1.33675800	2.22524600	2.96385200
H	-1.86537100	3.34464600	4.23677600
C	4.07637500	6.25319600	0.81778100
H	4.17231700	6.97434700	-0.00455800
H	5.07333000	5.84159100	1.02007500
H	3.74586500	6.80227800	1.70979900
C	-5.95073200	-0.26415900	1.54749300
H	-6.46904100	-0.61042700	2.45240200
H	-6.37362500	-0.79091900	0.68541800
H	-6.15146200	0.80690700	1.42182000
C	-3.96957100	-6.38267000	-0.16108700
H	-3.90391100	-7.01588000	0.73334200
H	-3.69997400	-7.00084900	-1.02795000
H	-5.01578100	-6.07049300	-0.27107900
H	0.75121900	-5.09395000	2.94692100
H	-5.55074700	-1.84703500	-3.19810500

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C	5.56484600	-0.05690800	3.07213900
H	6.36193800	0.67855800	2.90767800
H	6.01825800	-1.04737000	2.94072600
H	5.21277000	0.03273600	4.10321400
C	-0.30924200	-0.70478800	-0.11684800
H	0.37696300	-1.28615800	-0.74884700
H	-0.34079700	-1.22525500	0.85159700
C	6.01051600	-3.80047400	1.27820300
H	6.87779100	-4.30043300	0.82743500
H	5.26273500	-4.57068800	1.51023300
H	6.33895800	-3.34625900	2.22174100
C	-4.93761500	3.39213500	0.99785700
H	-5.78120100	3.84063500	1.53898500
H	-4.20185700	4.18274400	0.79739000
H	-4.47490500	2.65135100	1.66472100
C	-6.39454800	1.59635500	-0.04764500
C	3.14321200	0.40022400	2.61688900
H	3.11555300	0.43259000	3.70091100
C	-5.41123200	2.73590200	-0.32544200
H	-4.52940800	2.31014300	-0.81592500
C	8.57394800	-0.84819700	-0.78539400

H	9.54752900	-1.08166800	-1.20992000
N	4.70813800	0.07088400	0.75387000
C	-6.44020500	-3.04410000	1.05314800
H	-5.68473100	-2.57376500	1.69728200
H	-6.13666500	-4.08357900	0.86909000
H	-7.38611700	-3.05828400	1.61066000
C	7.66199500	-1.87786200	-0.50142100
H	7.93721100	-2.90957800	-0.71007900
C	-7.66198900	1.87788000	0.50141200
H	-7.93720300	2.90960200	0.71004700
N	1.68282600	0.60730000	0.65385900
N	-4.70814500	-0.07089100	-0.75387000
C	6.39454700	-1.59634900	0.04762400
C	4.42566700	0.14944500	2.07150900
C	-6.01054100	3.80044500	-1.27829400
H	-6.87781100	4.30041500	-0.82752700
H	-6.33899500	3.34620200	-2.22181300
H	-5.26276500	4.57065500	-1.51035700
N	-1.68283500	-0.60732100	-0.65388200
C	8.22015900	0.48494900	-0.52110400
H	8.92692100	1.28113500	-0.74487000
C	6.44025600	3.04414900	-1.05303200
H	7.38618600	3.05835000	-1.61051300
H	6.13671400	4.08362200	-0.86894600
H	5.68480100	2.57384000	-1.69720800
C	-8.57393400	0.84822200	0.78542700
H	-9.54750900	1.08170200	1.20996200
C	-6.96333600	-0.80977400	-0.02894000
C	6.04469400	-0.24099500	0.31061000
C	1.88001400	0.58714200	1.98436600
C	-6.04469600	0.24099600	-0.31060100
C	-1.88003400	-0.58716900	-1.98438700
C	-5.56487300	0.05688000	-3.07213400
H	-6.36196400	-0.67858500	-2.90766400
H	-5.21280400	-0.03277000	-4.10321100
H	-6.01828400	1.04734200	-2.94072300
C	-0.69825600	-0.79218500	-2.94492300
H	0.09796200	-0.05633400	-2.77430300
H	-1.02290300	-0.69861100	-3.98411900
H	-0.25738600	-1.79065800	-2.81814200
C	-4.42568700	-0.14946800	-2.07151100
C	-8.22014600	-0.48493100	0.52116800
H	-8.92690300	-1.28111300	0.74496800
C	-3.14323700	-0.40025500	-2.61690100
C	6.96334100	0.80978000	0.02899200
C	0.30923800	0.70476800	0.11681600
H	0.34079700	1.22523300	-0.85162900
H	-0.37697100	1.28613900	0.74881200

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H	-0.66370200	-0.04312300	2.03946000

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H	0.87272800	-5.05696900	2.42507400
H	-5.12592600	-1.20137700	-3.12359300

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