Supporting information for:

First homoleptic MIC and heteroleptic NHC-MIC coordination cages from 1,3,5-triphenylbenzene-bridged tris-MIC and tris-NHC ligands

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General methods. The 1,3,5-triphenylbenzene-bridged-tris-imidazolium salt **5** and the metal complex **4** were synthesized as previously reported.[1] 1,3,5-Tris(4-ethynylphenyl)benzene was obtained as described in the literature.[2] All manipulations were performed under nitrogen atmosphere using standard Schlenk techniques. Solvents were dried using a solvent purification system (MBraun SPS). All reagents were used as received from commercial suppliers. NMR spectra were recorded on Varian Innova 300 and 500 MHz spectrometers, using $CDCl_3$ and CD_2Cl_2 as solvents. Electrospray mass spectra (ESI-MS) were recorded on a Micromass Quatro LC instrument; nitrogen was employed as drying and nebulizing gas. Accurate mass measurements were performed by use of a Q-TOF premier mass spectrometer with electrospray source (Waters, Manchester, UK) operating at a resolution of ca. 16 000 (fwhm). Elemental analyses were carried out on a EuroEA3000 Eurovector Analyzer.

Synthesis of the 1,3,5-triphenylbenzene-bridged tris-(1,2,3)triazolium salt 1 In a Schlenk tube, a mixture of wrapped with aluminum foil containing 1,3,5-tris-(4-ethynylphenyl)benzene (270 mg, 0.71 mmol), 1,3-dimesityltriazene (1.50 g, 4.10 mmol) and KPF_6 (990 mg, 5.38 mmol) in CH_2Cl_2 was cooled down to -78 °C and stirred during 30 minutes. Then ^{t}BuOCl (486 mg, 0.53 mmol) was added dropwise over the period of one hour at -78 ^{0}C, and the reaction mixture was stirred at -78 ^{0}C during 6 hours. The reaction was allowed to slowly warm up and stirred at room temperature overnight. The resulting solution was filtrated, and the filtrate was evaporated. The resulting white solid was washed with diethyl ether and MeOH (yield: 1.1 g. 93%). ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 9.08 (s, 3H, C*H*N), 7.77 (m, 9H, CH_{Ar}), 7.60 (m, 6H, CH_{Ar}), 7.14 (d, 12H, *J*= 6Hz CH_{Ar}), 2.43 (bs, 18H, CH_3), 2.22 (bs, 18H, CH_3), 2.06 (bs, 18H, CH_3). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ (ppm) 144.7 (C_{Ar}), 144.0 (C_{Ar}), 143.9 (C_{Ar}), 143.1 (C_{Ar}), 140.7 (C_{Ar}), 134.4 (C_{Ar}), 134.1 (C_{Ar}), 131.3 (N*C*HN), 130.8 (C_{Ar}), 130.2 (C_{Ar}), 128.7 (C_{Ar}), 126.0 (C_{Ar}), 120.68 (C_{Ar}), 21.48 (CH$_3$), 21.40 (CH$_3$), 17.46 (CH$_3$), 17.28 (CH$_3$. ESI-MS(+) m/z calcd. for $[M]^{3+}$: 406,6; $[MPF_6]^{2+}$: 682,5. Elemental analysis calcd (%) for $C_{84}H_{84}N_9P_3F_{18}.3CH_2Cl_2$: C, 54.7; H, 4.7; N, 6.6 found C, 54.3; H, 5.0; N, 7.2.

Synthesis of compound 2. A mixture of **1** (100 mg, 0.085 mmol) and Ag_2O (30 mg, 0.13 mmol) in MeOH (7 mL) was heated at 60 °C overnight under exclusion of light. After cooling the reaction mixture to room temperature, the suspension was filtered through a pad of celite. The pad of celite was then washed with

CH_2Cl_2 to yield a clear solution, which was concentrated to dryness yielding a white solid. (yield: 114 mg. 42%).^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) 7.53-7.35 (m, 30H, CH_{Ar}), 7.06-7.00 (m, 24H, CH_{Ar}), 2.54 (bs, 18H, CH_3), 2.34 (bs, 18H, CH_3), 2.04 (bs, 72H, CH_3). ^{13}C{^{1}H} NMR (75 MHz, CD_2Cl_2): δ (ppm) 169.7 (dd, J (C-Ag^{107}) = 165.0 Hz, J (C-Ag^{109}) = 190.5Hz, $C_{carbene}$), 150.31 (C_{Ar}), 150.14 (C_{Ar}), 142.58 (C_{Ar}), 141.16 (C_{Ar}), 140.95 (C_{Ar}), 139.77 (C_{Ar}), 136.81 (C_{Ar}), 134.33 (C_{Ar}), 131.84 (C_{Ar}), 130.43 (C_{Ar}), 129.78 (C_{Ar}), 129.34 (C_{Ar}), 127.13 (C_{Ar}), 123.86 (C_{Ar}), 21.83 (CH_3), 21.50 (CH_3), 17.87 (CH_3). ESI-MS(+) m/z calcd. for $[M]^{3+}$: 919,2; $[MPF_6]^{2+}$: 1451,2. Elemental analysis calcd (%) for $C_{168}H_{162}N_{18}Ag_3P_3F_{18}$: C, 63.2; H, 5.1; N, 7.8 found C, 63.4; H, 5.3; N, 7.3.

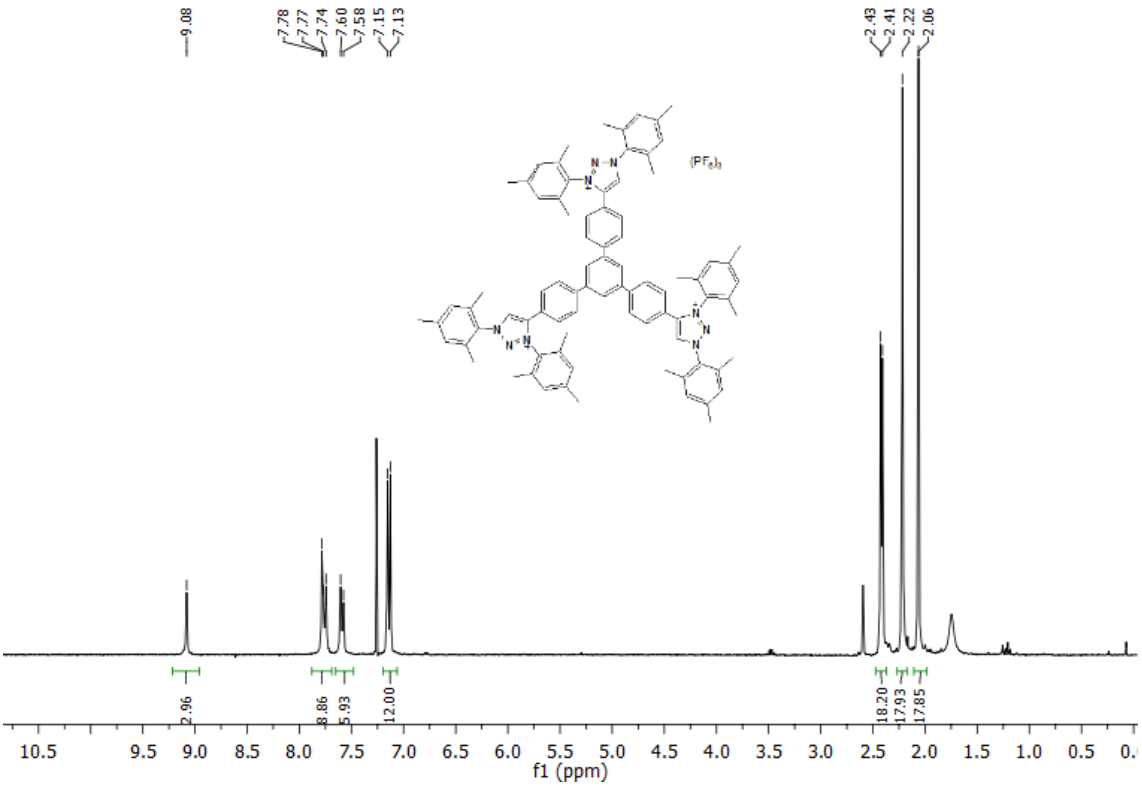
Synthesis of compound 3. A solution of **2** (55 mg, 0.017 mmol) and [AuCl(SMe_2)] (32 mg, 0.109 mmol) in acetonitrile (8 mL) was stirred at room temperature for 5 days. The resulting suspension was filtered through a pad of celite. The pad of celite was washed with CH_2Cl_2 to yield a clear solution, which was concentrated to dryness yielding a white solid. (yield: 38 mg. 58%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) 7.84 (sb, 6H, CH_{Ar}), 7.77-7.69 (bs, 24H, CH_{Ar}), 7.14-7.08 (m, 24H, CH_{Ar}), 2.43-2.39 (m, 36H, CH_3), 2.20 (bs, 36H, CH_3), 2.05 (bs, 36H, CH_3). ^{13}C{^{1}H} NMR (75 MHz, CD_2Cl_2): δ (ppm) 161.1 (Au-$C_{carbene}$), 147.9 (C_{Ar}), 142.7 (C_{Ar}), 141.8 (C_{Ar}), 141.8 (C_{Ar}), 136.4 (C_{Ar}), 135.0 (C_{Ar}), 134.8 (C_{Ar}), 131.8 (C_{Ar}), 130.5 (C_{Ar}), 130.0 (C_{Ar}), 129.6 (C_{Ar}), 128.1 (C_{Ar}), 126.1 (C_{Ar}), 21.7 (CH_3), 21.6 (CH_3), 17.9 (CH_3). ESI-MS(+) m/z calcd. for $[M]^{3+}$: 1008,1; $[MAuCl_2]^{2+}$: 1645,6. Elemental analysis calcd (%) for $C_{168}H_{162}N_{18}Au_3(AuCl_2)_3$: C, 52.7; H, 4.3; N, 6.6 found C, 53.5; H, 4.7; N, 6.2.

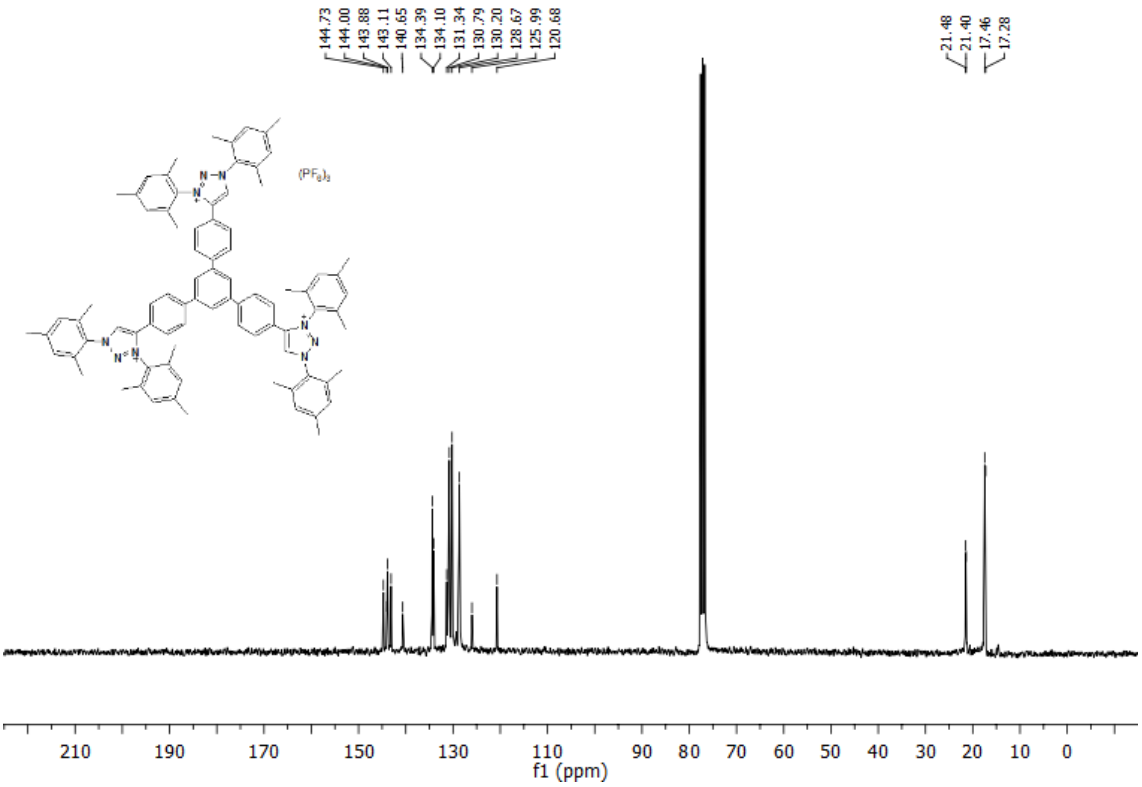
Synthesis of compound 6. A mixture of **1** (60 mg, 0.04 mmol), **5** (42 mg, 0.04 mmol) and Ag_2O (25 mg, 0.11 mmol) in MeOH (7 mL) was heated to 60 °C overnight under exclusion of light. The resultimg suspension was filtered through a pad of celite, and washed with CH_2Cl_2. Then the filtrate was concentrated to dryness, yielding a white solid (yield: 55 mg, 43%). ***Method i.*** A mixture of **2** (20 mg, 0.006 mmol) and **4** (12 mg, 0.006 mmol) in MeOH (5 mL) was heated to 60 °C overnight under exclusion of light. The resulting suspension was filtered through a pad of celite and washed with CH_2Cl_2. The filtrate was concentrated to dryness obtained a white solid (yield: 45%). ***Method ii.*** A mixture of **2** (30 mg, 0.015 mmol) and **5** (24 mg, 0.015 mmol) in MeOH (5 mL) was heated to 60 °C overnight under exclusion of light. The resulting suspension

was filtered through a pad of celite and washed with CH_2Cl_2. The filtrate was concentrated to dryness obtained a white solid (yield: 55%). ***Method iii.*** A mixture of **1** (30 mg, 0.009 mmol) and **4** (10 mg, 0.009 mmol) in MeOH (5 mL) was heated to 60 °C overnight under exclusion of light. The resulting suspension was filtered through a pad of celite and washed with CH_2Cl_2. The filtrate was concentrated to dryness obtained a white solid (yield: 45%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) 7.65-7.65 (m, 12H, CH_{Ar}), 7.55 (m, 6H, CH_{Ar}), 7.46 (m, 12H, CH_{Ar}), 7.20 (m, 12H, CH_{Ar}), 7.06 (m, 6H, CH_{Ar}), 3.72 (m, 6H, CH_2), 2.47 (bs, 9H, CH_3), 2.34 (bs, 9H, CH_3), 2.24 (bs, 18H, CH_3), 2.05 (bs, 9H, CH_3), 2.02 (bs, 18H, CH_3). ^{13}C{^{1}H} NMR (75 MHz, CD_2Cl_2): δ (ppm) 180.9-178.1 (dd, J (C-Ag^{107}) = 179.6 Hz, J (C-Ag^{109}) = 179.4 Hz, $C_{carbene}$), 170.8-168.3 (dd, J (C-Ag^{107}) = 169.6 Hz, J (C-Ag^{109}) = 169.6 Hz, $C_{carbene}$), 150.2 (C_{Ar}), 150.0 (C_{Ar}), 142.5 (C_{Ar}), 141.9 (C_{Ar}), 141.6 (C_{Ar}), 141.0 (C_{Ar}), 140.6 (C_{Ar}), 139.8 (C_{Ar}), 137.3 (C_{Ar}), 134.9 (C_{Ar}), 134.7 (C_{Ar}), 131.5 (C_{Ar}), 130.3 (C_{Ar}), 129.8 (C_{Ar}), 129.0 (C_{Ar}), 128.7 (C_{Ar}), 127.7 (C_{Ar}), 126.5 (C_{Ar}), 124.7 (C_{Ar}), 122.6 (C_{Ar}), 122.6 (C_{Ar}), 122.0 (C_{Ar}), 46.6 (CH$_2$), 21.4 (CH$_3$), 21.3 (CH$_3$), 17.7 (CH$_3$), 17.6 (CH$_3$), 17.1 (CH$_3$). ESI-MS(+) m/z calcd. for [M]$^{3+}$: 709,5; [MPF$_6$]$^{2+}$: 1136,8. Several attempts to obtain satisfactory elemental analysis of **6** failed, probably due to the large amount of fluorine present, and to the possibility that this cage-type complex retains solvent.

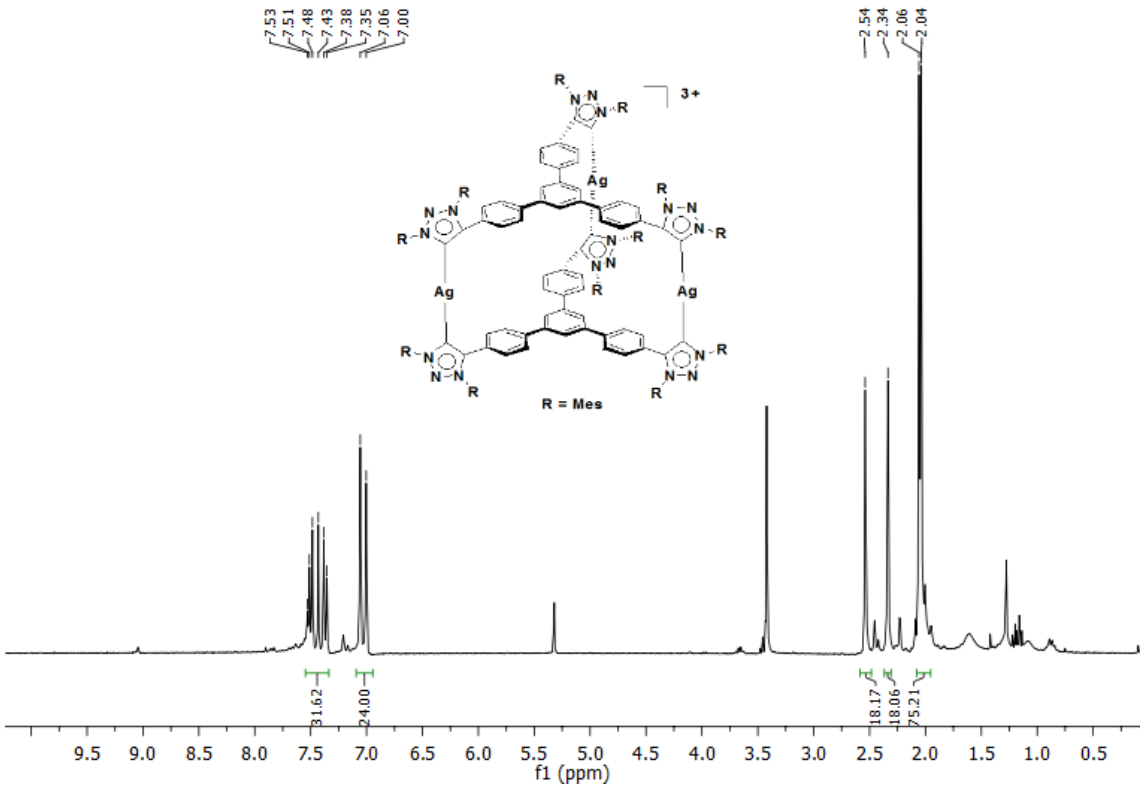
2. Spectra

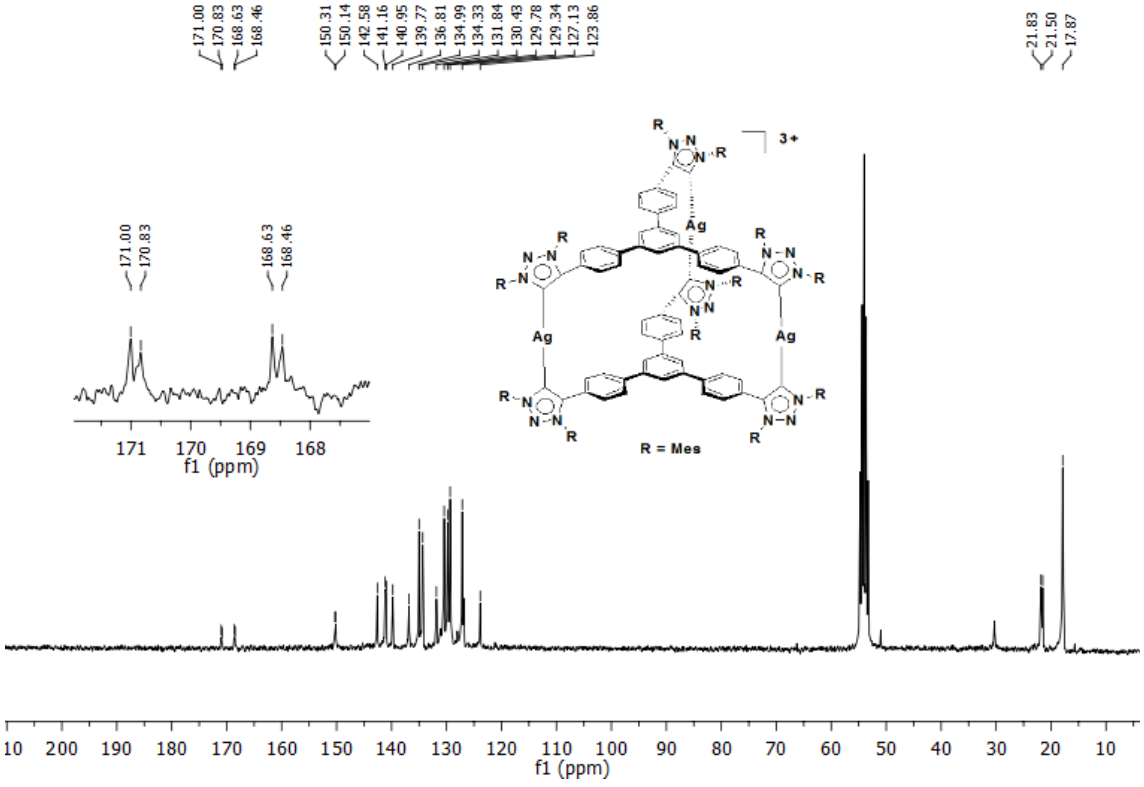
2.1. ^{1}H and ^{13}C NMR spectra of 1



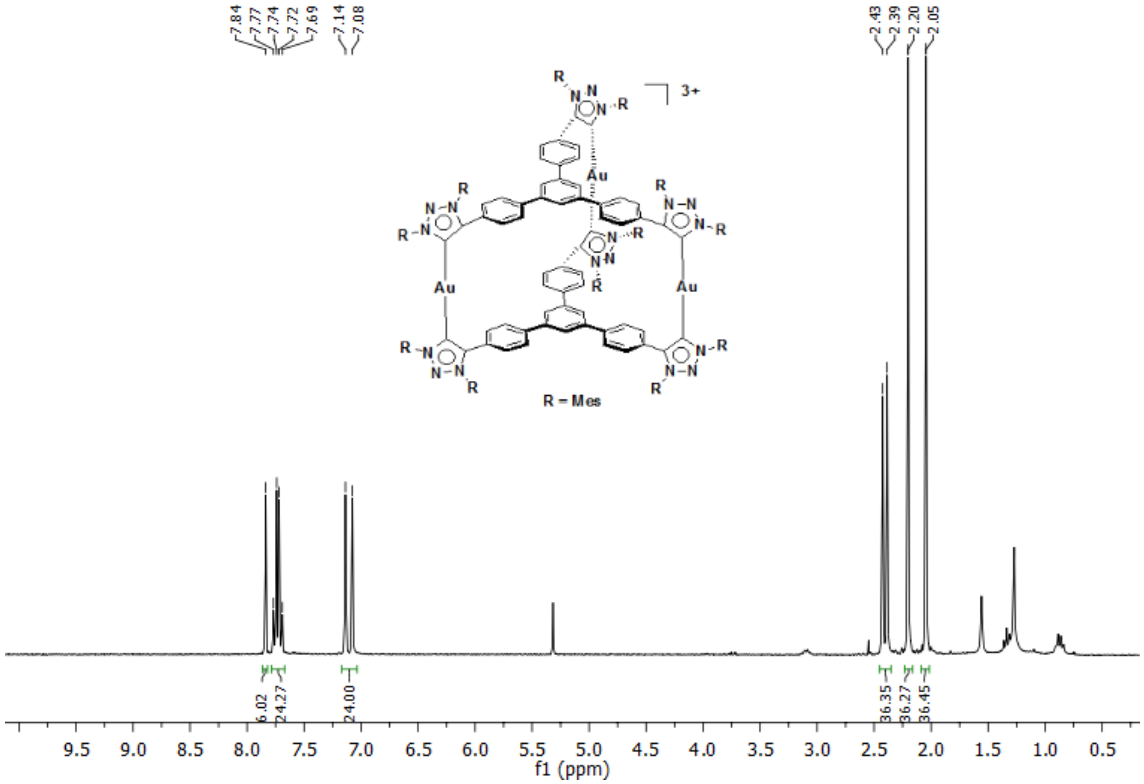


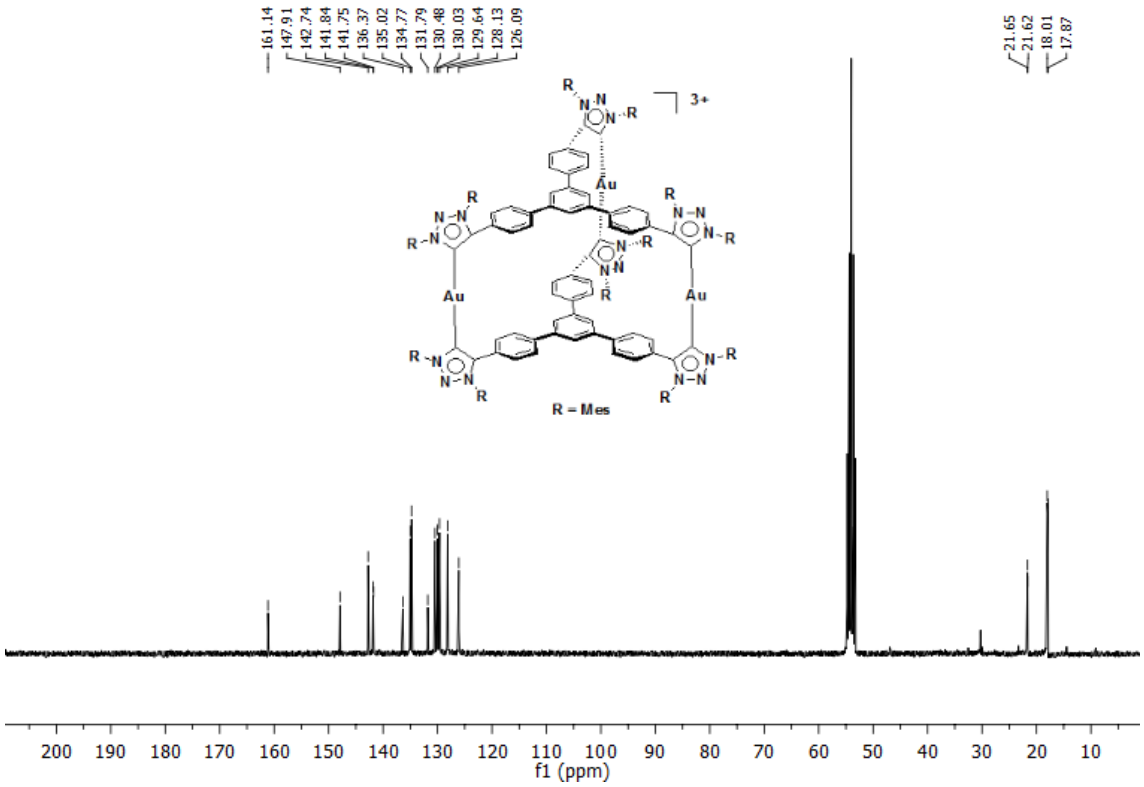
2.2. ^{1}H and ^{13}C NMR spectra of 2



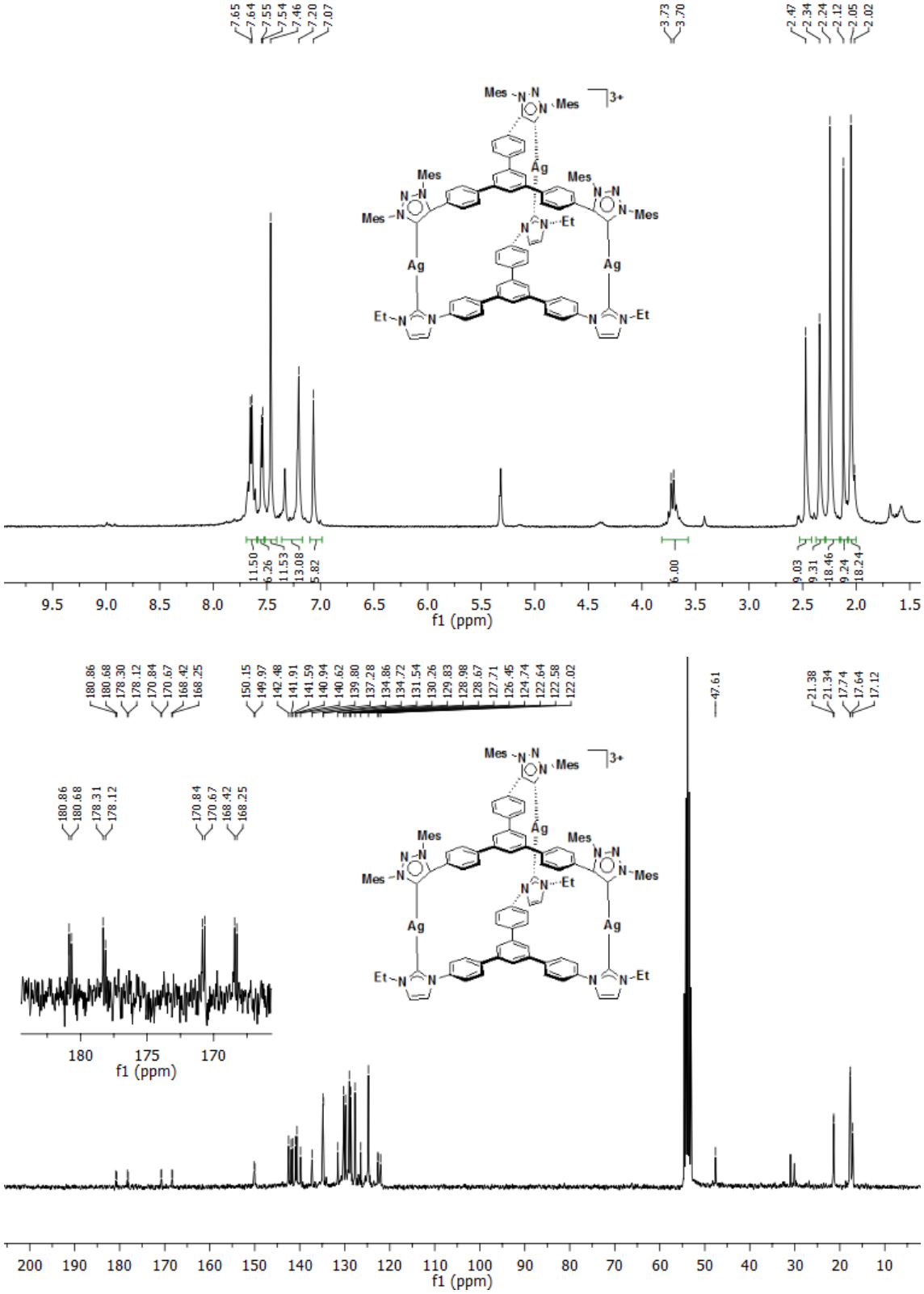


2.3. ^{1}H and ^{13}C NMR spectra of 3

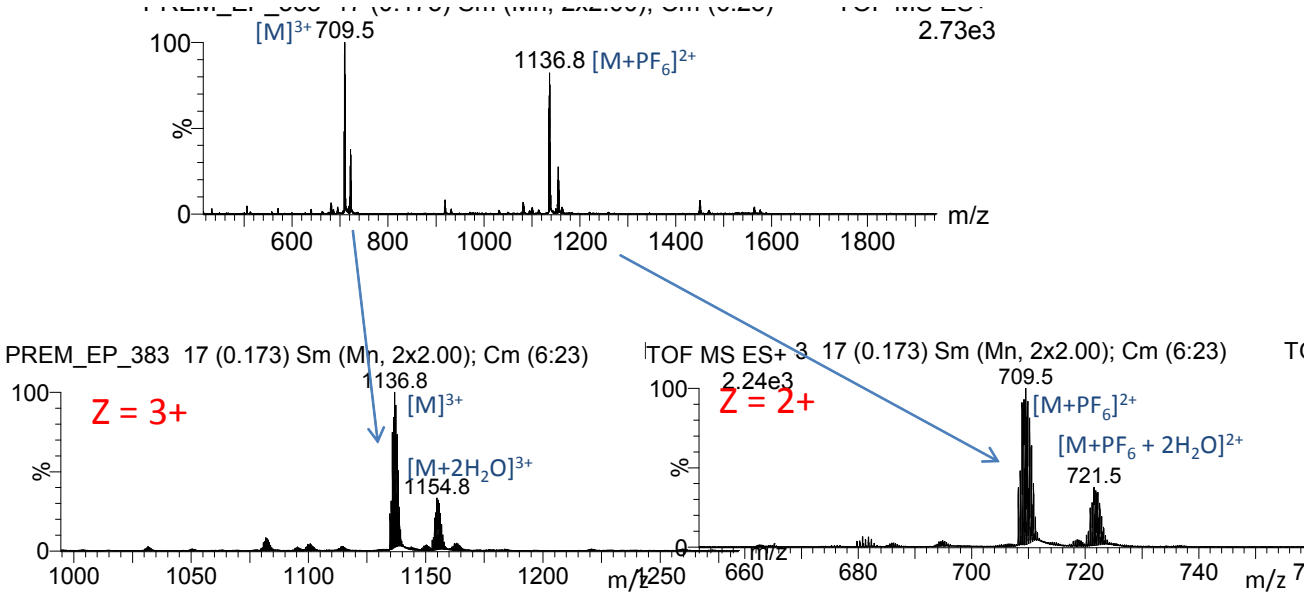




2.4. ^{1}H and ^{13}C NMR spectra of 6



3. ESI Mass spectrum of 6



4 X-Ray Diffraction studies

Single crystals of **2** suitable for X-ray crystallographyc analysis were obtained by slow vapour diffusion of diethylether into a DCM solution of **2**. Diffraction data were collected on a Agilent SuperNova diffractometer equipped with an Altas CCD detector using Cu Kα radiation (λ = 1.54184 Å). Single crystal was mounted on a MicroMount polymer tip (MiteGen) in a random orientation. The crystals were kept during data collection at 150 K for **2**. The structures were solved by direct methods in SHELXS-97[3] and refined by the full-matrix method based on F^2 with the program SHELXL-97 using the OLEX software package.[3-4] Key details of the crystal and structure refinement data for compound **2** are summarized below. Refinement (R= 0.0922) was obtained when SQUEEZE methodology was applied only after all residual solvent peaks present in the asymmetric unit were removed. Further crystallographic data may be found in the corresponding CIF file which was deposited at the Cambridge Crystallographic Data Centre CCDC, Cambridge, UK. The reference number for **2** was assigned as *CCDC 1406599*.

Compound *2*: $C_{168}H_{162}Ag_3F_{18}N_{18}P_3$ (M= 3191.67): trigonal, space group R-3 (no. 148), a = 35.4661(16) Å, b = 35.4661(16) Å, c = 26.1940(17) Å, α = 90°β = 90° γ = 120°, V = 28534(3)Å^3, Z = 6, T = 150.00 (14) K, μ(CuKα) = 3.228 mm^{-1},*Dcalc* = 1.114 g/cm^3, 36807 reflections measured (6.672° ≤ 2Θ ≤ 129.874°), 10546 unique (R_{int} = 0.1245, R_{sigma} = 0.0962), which were used in all calculations. The final R_1 was 0.0922 (I>=2u(I)) and wR_2 was 0.2886 (all data).

4. Computational details.

All calculations were carried out in Gaussian 09[5] (revision D.01) using the M06L functional,[6] tight optimizations, and the ultrafine integration grid (a pruned (99,590) grid). The basis sets, listed by their corresponding Gaussian 09 keyword, included QZVP[7] (with the QZVP ECP as implemented in Gaussian 09) for silver and TZVP[8] for all other atoms. The following density fitting basis sets were employed: QZVP (silver) and TZVPFit (all other atoms). The polarizable continuum model using the integral equation formalism (IEFPCM) was used for all calculations, with the radii and non-electrostatic terms of Truhlar and co-workers' SMD solvation model (scrf=smd).[9] The optimized geometries were verified to have no negative frequencies by frequency calculations, which also provided the enthalpies and free energies reported below. The energies were calculated at 298.15 K, under pressure (275 atm for benzene and 605 atm for methanol), following the approach of Martin and co-workers.[10]

Calculated energies for the ground-state structures (Hartree)

Compound	Sovent	E	H	G
NHC (carbene)	methanol	-535.958446	-535.738644	-535.782130
MIC (carbene)	methanol	-1171.456758	-1170.962326	-1171.042564
$[Ag(NHC)]^+$	methanol	-682.972172	-682.748679	-682.798568
$[Ag(MIC)]^+$	methanol	-1318.473701	-1317.975867	-1318.062726
$[Ag(NHC)_2]^+$	methanol	-1218.998969	-1218.553087	-1218.630025
$[Ag(NHC)_2]^+$	benzene	-1218.985555	-1218.538735	-1218.616004
$[Ag(MIC)_2]^+$	methanol	-2490.003772	-2489.009124	-2489.161157
$[Ag(MIC)_2]^+$	benzene	-2489.997866	-2489.001076	-2489.149935
$[Ag(NHC)(MIC)]^+$	methanol	-1854.501641	-1853.781108	-1853.895051
$[Ag(NHC)(MIC)]^+$	benzene	-1854.493038	-1853.771150	-1853.885411

Optimized ground-state geometries

NHC
0 1

C	2.69013200	6.24763900	0.35598700
N	2.39206900	5.40151000	1.39761600
N	1.56788500	6.16939500	-0.40045100
C	1.13042800	4.83344500	1.27502000
C	3.26674400	5.16170900	2.49041100
C	0.61361000	5.31736500	0.12799100
C	1.39479300	6.88024600	-1.66397100
H	0.73012100	4.13083800	1.98457000
C	2.74771800	4.88585500	3.75115600
C	4.64380300	5.20301000	2.29737200
H	-0.33292100	5.13281800	-0.35071600
H	2.18992500	7.62284100	-1.71032400
H	0.44491700	7.41663300	-1.62500400
C	1.44305100	5.95395800	-2.85532600
H	1.67646300	4.87463700	3.90706800
C	3.60812200	4.64695700	4.81199900
H	5.03510400	5.40600800	1.30937200
C	5.49408800	4.97512400	3.36733900
H	2.39862800	5.43100400	-2.90704400
H	1.31834800	6.52176000	-3.77694400
H	0.64950900	5.20705400	-2.81487400
H	3.19704000	4.43446300	5.79122700
C	4.98250600	4.69281100	4.62711200
H	6.56531000	5.00631200	3.21020900
H	5.65096800	4.50860600	5.45875900

MIC
0 1

N	-4.22255500	-0.65296000	-0.05620300
C	-3.19221900	0.20348700	0.25790200
N	-3.79741500	-1.88994300	-0.24194500
C	-5.63845700	-0.41406500	-0.14131000
C	-2.00308300	-0.53194400	0.28084100
C	-3.37315800	1.62723500	0.52552700
N	-2.47754400	-1.77177800	-0.03768800
C	-6.23630700	-0.39245800	-1.40317400
C	-6.34626100	-0.20476600	1.04058500
C	-2.54769800	2.23295600	1.47962200
C	-4.31611800	2.41619000	-0.14077700
C	-1.69460900	-2.97162100	-0.15868700
C	-7.60089600	-0.14070000	-1.45619600
C	-5.43577000	-0.61688700	-2.64357500
C	-7.71163300	0.04362400	0.92894300
C	-5.67164600	-0.23814200	2.37213900
C	-2.67102800	3.58118100	1.76823000
H	-1.81364000	1.62772000	1.99791600
C	-4.43916400	3.76479300	0.15628900
H	-4.94152300	1.98401400	-0.91124700
C	-0.99856800	-3.19807700	-1.34448800
C	-1.64983800	-3.84868900	0.92490300
C	-8.35455200	0.08063300	-0.30395500
H	-8.08749300	-0.11093900	-2.42548400
H	-4.50328500	-0.04849100	-2.63393300
H	-5.16128600	-1.66806400	-2.75598900
H	-6.00054100	-0.32808500	-3.52791900
H	-8.28555100	0.20716900	1.83475200
H	-4.98406400	-1.08146000	2.45985800
H	-5.08424800	0.66784700	2.54499500
H	-6.40213800	-0.31006200	3.17551100
C	-3.62234100	4.35181900	1.11247700
H	-2.02654600	4.03109300	2.51365200
H	-5.17224000	4.36204400	-0.37213900
C	-0.23299800	-4.35765900	-1.42658200
C	-1.07157500	-2.23177500	-2.48053000
C	-0.86779800	-4.99074900	0.79306000
C	-2.41940200	-3.57251700	2.17485200
C	-9.82401100	0.33352500	-0.39948300
H	-3.72220200	5.40575600	1.34137300
C	-0.15523400	-5.26337800	-0.37263200
H	0.31681400	-4.55497800	-2.34089600
H	-0.56422000	-1.29461200	-2.23993000
H	-0.60440900	-2.64318500	-3.37327100
H	-2.10367700	-1.97252300	-2.72558200
H	-0.81361800	-5.68406800	1.62596200
H	-2.11661700	-4.24405600	2.97598800
H	-2.27793600	-2.54580400	2.51842300
H	-3.49220100	-3.70764900	2.01930900
H	-10.04800900	1.11419500	-1.12790200
H	-10.35613500	-0.56136200	-0.72981900
H	-10.24501600	0.63303100	0.55892200
C	0.64762200	-6.51777000	-0.49652200
H	1.16087000	-6.76114600	0.43402200
H	0.00595600	-7.37040100	-0.73289000
H	1.39158500	-6.44515700	-1.28884500

[Ag(NHC)]$^{+}$
1 1

Ag	-0.04729800	-0.09812600	0.23297600
C	2.00720400	0.38448300	0.28440400
N	2.59995900	1.60755900	0.20266700
N	3.03482900	-0.47522700	0.43513300
C	3.97643300	1.49835700	0.30963400
C	1.90353400	2.84200000	0.05443000
C	4.24698100	0.18338400	0.44578100
C	2.88925800	-1.92980000	0.49855000
H	4.62459600	2.35475800	0.25702600
C	2.30539300	3.94533600	0.79640700
C	0.83964700	2.93409200	-0.83479500
H	5.18187400	-0.33916600	0.54771200
H	1.87146900	-2.12468800	0.83839900
H	3.57266300	-2.29575700	1.26454100
C	3.15566000	-2.58051600	-0.83683700
H	3.12992000	3.85739500	1.49280000
C	1.63039700	5.14700100	0.64806400
H	0.56328400	2.07616900	-1.43555300
C	0.16399800	4.13780400	-0.96426900
H	2.45454800	-2.22305800	-1.59179200
H	3.04267900	-3.66068000	-0.75348400
H	4.16808200	-2.37447700	-1.18454100

H	1.94104200	6.00688600	1.22811700
C	0.55671600	5.24543400	-0.22599200
H	-0.66240400	4.21198500	-1.65996800
H	0.03074300	6.18538300	-0.33617400

$[Ag(MIC)]^+$

1 1

C	-3.18195000	0.26815300	0.12936400
C	-2.00937900	-0.47761800	0.14846100
N	-4.20679000	-0.62031200	-0.07193200
C	-3.35274600	1.70672400	0.29415900
Ag	0.00952100	0.06015400	0.35830900
N	-2.46163600	-1.74761600	-0.04937100
N	-3.77932200	-1.86673500	-0.18339400
C	-5.62666900	-0.38766900	-0.12910700
C	-2.52356800	2.38044100	1.19689000
C	-4.30198700	2.43525500	-0.42770500
C	-1.66223800	-2.94141900	-0.12081500
C	-6.25764400	-0.45572200	-1.37270300
C	-6.29731400	-0.10499900	1.05851000
C	-2.64783200	3.74735300	1.37800000
H	-1.79021200	1.81758700	1.76414800
C	-4.42317900	3.80269400	-0.23855800
H	-4.93234200	1.93874200	-1.15402500
C	-0.96463500	-3.20099500	-1.29818000
C	-1.61469000	-3.77356300	0.99813200
C	-7.62439800	-0.21399600	-1.40141900
C	-5.48968200	-0.76281300	-2.61595700
C	-7.66672300	0.12860400	0.96998700
C	-5.58177800	-0.05013300	2.36773800
C	-3.60107000	4.46189800	0.66454000
H	-2.00367100	4.25522400	2.08506600
H	-5.15932100	4.35649800	-0.80789600
C	-0.18867100	-4.35631900	-1.33449900
C	-1.04338600	-2.27557100	-2.46695400
C	-0.82387300	-4.91194400	0.90783800
C	-2.38254700	-3.45054600	2.23746500
C	-8.34440100	0.08140700	-0.24388700
H	-8.13983700	-0.25324900	-2.35511500
H	-4.57387200	-0.17117100	-2.68433900
H	-5.18847400	-1.81207200	-2.64945800
H	-6.08925500	-0.56281700	-3.50157600
H	-8.21616900	0.34811600	1.87895400
H	-4.90583100	-0.89763200	2.49797600
H	-4.97517200	0.85559700	2.45351900
H	-6.28784600	-0.04937200	3.19540300
H	-3.70047200	5.53044700	0.81019000
C	-0.10627400	-5.22041200	-0.24720100
H	0.36026800	-4.58594300	-2.24144300
H	-0.51516100	-1.33924000	-2.26428400
H	-0.59601300	-2.72479600	-3.35124100
H	-2.07510500	-2.00749700	-2.70447000
H	-0.76730300	-5.57521500	1.76451200
H	-2.08991300	-4.10334300	3.05729400
H	-2.22377000	-2.41707300	2.55327300
H	-3.45704500	-3.57207600	2.08458000
C	-9.81601400	0.32815400	-0.31312700
C	0.72869100	-6.45795700	-0.30890800
H	-10.05510700	1.10014500	-1.04622800
H	-10.35180200	-0.57125100	-0.62375000
H	-10.21834200	0.63932000	0.64947900
H	1.49233700	-6.46019900	0.47112300
H	0.12310400	-7.35261600	-0.15266600
H	1.23107300	-6.55765100	-1.26962000

$[Ag(NHC)_2]^+$ in MeOH

1 1

Ag	4.27695400	7.45945300	0.00697300
C	2.52030100	6.40992000	0.51904700
C	6.06349500	8.47578300	-0.46674500
N	2.34108500	5.53740200	1.54940600
N	1.31539200	6.45525000	-0.08614200
N	7.12704700	8.73856200	0.34186000
N	6.42557600	8.98521000	-1.66223800
C	1.04127700	5.06232100	1.58239600
C	3.35162400	5.19616800	2.49450400
C	0.39937800	5.63979800	0.54376500
C	1.02974200	7.29157000	-1.25606500
C	8.13233700	9.39196200	-0.35089000
C	7.20643000	8.35618200	1.71255900
C	7.68141900	9.55169400	-1.61420800
C	5.56696800	8.93515200	-2.84940200
H	0.70824200	4.35064500	2.31639100
C	3.03157700	5.13205300	3.84434500
C	4.64553200	4.93131300	2.05897100
H	-0.61456100	5.54280800	0.19747400
H	1.30860000	8.31581400	-1.00307000
H	-0.04907500	7.27387000	-1.39925200
C	1.75685500	6.82471500	-2.49318000
H	9.04885000	9.69848300	0.12084900
C	6.11056800	8.54260900	2.54840000
C	8.38377000	7.80487700	2.20078400
H	8.13463600	10.01592600	-2.47239300
H	6.18798500	9.20335900	-3.70225000
H	5.25570500	7.89767700	-2.98314900
C	4.36948100	9.84529100	-2.72815600
H	2.02279200	5.35155900	4.17125000
C	4.01809300	4.80641300	4.76331500
H	4.87210600	4.95112600	0.99961300
C	5.62590700	4.61921600	2.98813600
H	2.83903900	6.85554800	-2.34597900
H	1.51411400	7.47576200	-3.33257600
H	1.47755700	5.80540600	-2.76079600
H	5.21117800	9.00713700	2.16298600
C	6.19454200	8.15627600	3.87705800
H	9.22592800	7.65630600	1.53637800
C	8.46011100	7.43383400	3.53503700
H	4.67021000	10.88653500	-2.61009400
H	3.75299800	9.76818100	-3.62323900
H	3.75468600	9.56671900	-1.86909300
H	3.77033400	4.76144000	5.81647700
C	5.31565900	4.55503200	4.33999300
H	6.63472300	4.41579800	2.65030900

H	5.34127900	8.30031200	4.52845800
C	7.36739000	7.60351200	4.37369900
H	9.37666300	7.00073800	3.91560400
H	6.08494800	4.30999300	5.06175100
H	7.42875900	7.30570700	5.41306600

$[Ag(NHC)_2]^+$ in benzene

1 1

Ag	4.28924100	7.44942600	0.02348600
C	2.51733000	6.41026600	0.52157200
C	6.07233700	8.47293100	-0.46815300
N	2.32496400	5.53713200	1.54697600
N	1.32109800	6.45518100	-0.10210200
N	7.13587500	8.75026500	0.33301700
N	6.41288000	8.99996500	-1.66329800
C	1.02722000	5.05869000	1.55813400
C	3.31956300	5.19026400	2.50999700
C	0.39774400	5.63808200	0.51309700
C	1.04871200	7.29194800	-1.27396500
C	8.12009900	9.42939300	-0.36287100
C	7.24064300	8.36260500	1.70281000
C	7.65748700	9.58954000	-1.62173400
C	5.54817100	8.93701600	-2.84429900
H	0.68662600	4.34318100	2.28416300
C	2.97287600	5.12077300	3.85282500
C	4.61900100	4.91912100	2.09820600
H	-0.61129300	5.54048500	0.15428600
H	1.33503500	8.31458100	-1.02241600
H	-0.02977000	7.28681800	-1.42156300
C	1.77350900	6.81318900	-2.50860300
H	9.03203700	9.75390200	0.10454000
C	6.15810000	8.53332900	2.55767900
C	8.43475200	7.83015200	2.17053800
H	8.09601900	10.06813200	-2.47911200
H	6.16083800	9.19922300	-3.70513600
H	5.24293900	7.89636700	-2.96866300
C	4.34819200	9.84487000	-2.72249800
H	1.96094800	5.35005500	4.16244900
C	3.93712900	4.77812800	4.78790000
H	4.86694600	4.94107700	1.04395000
C	5.57788000	4.59344400	3.04395200
H	2.85544900	6.84424200	-2.36166800
H	1.53030600	7.45239200	-3.35639600
H	1.49735000	5.79068900	-2.76471300
H	5.24613800	8.98703300	2.19026100
C	6.27182600	8.14937300	3.88422900
H	9.26675600	7.69176800	1.49167000
C	8.54152400	7.46376400	3.50319500
H	4.64422900	10.88703300	-2.60653400
H	3.72640300	9.76607000	-3.61323300
H	3.74047400	9.56792700	-1.85813400
H	3.66816000	4.72459100	5.83500100
C	5.23968700	4.51869400	4.38747200
H	6.59165800	4.38585600	2.72570800
H	5.42864100	8.27966000	4.55062000
C	7.46180200	7.61801300	4.36040100
H	9.47203300	7.04869100	3.86830500
H	5.99107400	4.25699600	5.12138300
H	7.54756800	7.32609400	5.39920700

$[Ag(MIC)_2]^+$ in methanol

1 1

N	4.21285400	0.72074800	-0.67129800
N	2.92963900	0.56121700	-0.99084800
N	4.19731900	0.69348200	0.65090300
C	2.93336600	0.52643900	1.15317700
C	2.07581700	0.43180800	0.06350100
C	2.57043900	0.62715300	-2.38275400
C	2.22581400	-0.54597700	-3.05100000
C	1.91293000	-0.43794900	-4.40430000
C	1.93933600	0.78334100	-5.07059800
C	2.25621500	1.93153200	-4.34657600
C	2.57916300	1.88156600	-2.99696500
C	5.44468300	0.84658700	1.35337300
C	6.31838000	-0.24142900	1.38587500
C	7.50054000	-0.08357600	2.09778500
C	7.80953200	1.10538800	2.75640400
C	6.90515500	2.16077300	2.68743100
C	5.70664500	2.05957800	1.98753300
H	1.65877500	-1.33933500	-4.95241000
H	2.26368700	2.89337800	-4.84850600
H	8.19302300	-0.91702500	2.14730900
H	7.13360500	3.09289700	3.19281700
C	2.59902100	0.52573200	2.57333300
C	1.45233200	1.21613400	2.98233600
C	3.38011400	-0.12081200	3.53403800
C	1.10917400	1.27581100	4.32205000
H	0.84503200	1.72088800	2.23863200
C	3.02778800	-0.06038100	4.87380600
H	4.25369100	-0.68537700	3.23295000
C	1.89847700	0.64169100	5.27251500
H	0.22247100	1.82005300	4.62396400
H	3.63787300	-0.57002800	5.60931800
H	1.62902100	0.68747300	6.32081300
C	2.18681300	-1.86308400	-2.35008800
H	1.32648300	-1.92097500	-1.67421600
H	2.10465800	-2.68172800	-3.06265100
H	3.07598700	-2.02867700	-1.73855000
C	1.63949500	0.87811000	-6.53117200
H	0.76388400	1.50295000	-6.71835300
H	2.46812300	1.33970600	-7.07158600
H	1.45673300	-0.09984600	-6.97261000
C	2.92477300	3.11791800	-2.23377900
H	2.67029400	4.00889000	-2.80442900
H	2.39498100	3.16277700	-1.27952800
H	3.99206000	3.16342300	-2.00749900
C	4.74221700	3.19770200	1.93266100
H	4.35455300	3.35607600	0.92483300
H	3.87875800	3.02007800	2.57993000
H	5.21345200	4.12078600	2.26397100
C	5.98433000	-1.52492000	0.70038900
H	4.96775000	-1.85328500	0.92865000
H	6.04418400	-1.42675000	-0.38569900
H	6.67030900	-2.31480200	0.99897600

C	9.09757300	1.24896400	3.49898200
H	9.37007300	0.32725000	4.01308000
H	9.91791300	1.48146800	2.81541600
H	9.05251900	2.05204400	4.23324700
Ag	0.02573000	-0.01001600	-0.01393900
C	-2.02639900	-0.44693100	0.04183300
N	-2.87162300	-0.55803100	-1.02158600
C	-2.89457900	-0.54602700	1.12268700
N	-4.15898400	-0.71070900	-0.71528000
C	-2.49891800	-0.61290000	-2.41050700
N	-4.15517500	-0.69760100	0.60721600
C	-2.57299500	-0.56177400	2.54575400
C	-2.13780900	0.56383400	-3.06363300
C	-2.50968000	-1.86142900	-3.03668900
C	-5.41018600	-0.84499000	1.29716500
C	-1.43437900	-1.26370500	2.95774000
C	-3.35794000	0.08059900	3.50616600
C	-1.80855900	0.46585700	-4.41383300
C	-2.09842100	1.87451300	-2.35076500
C	-2.17075800	-1.90128800	-4.38271600
C	-2.87305100	-3.10225000	-2.28922200
C	-6.27467100	0.25046200	1.32951300
C	-5.68758500	-2.05930700	1.92211900
C	-1.10278200	-1.33835400	4.29961700
H	-0.82407400	-1.76515200	2.21427000
C	-3.01746700	0.00469600	4.84821500
H	-4.22515300	0.65397500	3.20344300
C	-1.83557000	-0.74903000	-5.09173200
H	-1.54029700	1.37017100	-4.95034300
H	-1.24766400	1.91988100	-1.66191300
H	-1.99922500	2.69857500	-3.05487900
H	-2.99506000	2.04218600	-1.75084700
H	-2.17939800	-2.85821400	-4.89394700
H	-2.62180100	-3.98973500	-2.86664200
H	-2.35140700	-3.16131300	-1.33124500
H	-3.94247000	-3.14024100	-2.07195500
C	-7.46395900	0.09849700	2.03079000
C	-5.92314900	1.53587300	0.65658600
C	-6.89248200	-2.15426200	2.61183800
C	-4.73206900	-3.20504000	1.86961000
C	-1.89612500	-0.70854300	5.24956400
H	-0.22177300	-1.89064300	4.60359900
H	-3.63048700	0.51114700	5.58349600
C	-1.51521600	-0.83300700	-6.54857300
C	-7.78837400	-1.09158300	2.67986400
H	-8.14959100	0.93760300	2.08007700
H	-4.90719200	1.85552200	0.89970700
H	-5.96999200	1.44548600	-0.43078600
H	-6.60713900	2.32866300	0.95201100
H	-7.13280100	-3.08720800	3.11015100
H	-4.33554400	-3.36058000	0.86484500
H	-3.87384600	-3.03835700	2.52665400
H	-5.21412400	-4.12618700	2.19057100
H	-1.63572400	-0.76602300	6.29957800
H	-0.63559400	-1.45475400	-6.72732900
H	-2.33496700	-1.29267400	-7.10384600
H	-1.32769800	0.14832500	-6.98034400
C	-9.08306800	-1.22840300	3.41212900
H	-9.35467100	-0.30548100	3.92449100
H	-9.89929600	-1.45657800	2.72222000
H	-9.04798400	-2.03199100	4.14638600

$[Ag(MIC)_2]^+$ in benzene

1 1

N	4.23979300	0.67762600	-0.65078800
N	2.96616500	0.50769200	-0.99931400
N	4.19142900	0.69611500	0.67063700
C	2.91304700	0.54288200	1.14650500
C	2.08421000	0.41381000	0.03758500
C	2.65425100	0.51118400	-2.40548700
C	2.33768300	-0.69207200	-3.03202300
C	2.07998100	-0.64759500	-4.39938100
C	2.12797900	0.54043300	-5.12003300
C	2.41890800	1.72077200	-4.43909700
C	2.69073200	1.73459800	-3.07807600
C	5.42536100	0.86983800	1.39452700
C	6.31534500	-0.20469600	1.44586700
C	7.48439500	-0.02521600	2.17303100
C	7.76752200	1.17042700	2.83029600
C	6.84980800	2.21150000	2.73954800
C	5.66354500	2.09018600	2.02400100
H	1.84583300	-1.57342000	-4.91428100
H	2.44533700	2.65801400	-4.98490500
H	8.19008900	-0.84656300	2.23226500
H	7.05900100	3.15065200	3.23963400
C	2.54609700	0.58103300	2.55909600
C	1.38260600	1.26692600	2.92597400
C	3.31610100	-0.02322100	3.55581500
C	1.01283800	1.36416600	4.25583900
H	0.78165200	1.73767900	2.15541200
C	2.94024100	0.07770400	4.88595000
H	4.20576800	-0.58079800	3.29170300
C	1.79518600	0.77670100	5.24039300
H	0.11191900	1.90213300	4.52339700
H	3.54567200	-0.39536800	5.64863700
H	1.50831700	0.85675000	6.28158200
C	2.27100000	-1.97711800	-2.27472400
H	1.37982200	-2.01357200	-1.63916700
H	2.22812600	-2.82799600	-2.95150900
H	3.13070500	-2.11241600	-1.61617400
C	1.89054700	0.56339000	-6.59482200
H	1.12112000	1.28795900	-6.86536600
H	2.79426700	0.85773000	-7.13219200
H	1.58768700	-0.41064200	-6.97383800
C	3.01388600	3.00582500	-2.36308700
H	2.79353700	3.86991000	-2.98617700
H	2.44221000	3.10474500	-1.43749400
H	4.07038200	3.05477700	-2.09236500
C	4.69276100	3.22139400	1.94022100
H	4.33266200	3.37449000	0.92149700
H	3.81431600	3.04319000	2.56606800
H	5.14896700	4.14977400	2.27712200
C	6.01840300	-1.49579500	0.75555300
H	5.02678500	-1.87714100	1.01187900

H	6.04026700	-1.38287800	-0.32989000
H	6.74651300	-2.25754800	1.02486900
C	9.04440400	1.33945500	3.58652400
H	9.32583100	0.42796300	4.11322100
H	9.86886100	1.57960100	2.91120000
H	8.97969000	2.14671400	4.31434300
Ag	0.02678000	-0.00812200	-0.05437400
C	-2.03296700	-0.42403900	0.02084100
N	-2.90521800	-0.49174000	-1.02622100
C	-2.87449300	-0.56210700	1.11943200
N	-4.18415700	-0.65265400	-0.69350300
C	-2.57779000	-0.48722200	-2.42891700
N	-4.14964000	-0.69226700	0.62780200
C	-2.52112500	-0.63582800	2.53418100
C	-2.24719300	0.71752500	-3.04485100
C	-2.61284300	-1.70694400	-3.10839900
C	-5.39348200	-0.85579000	1.33618500
C	-1.36257000	-1.33497300	2.89224500
C	-3.29877500	-0.05841600	3.54108300
C	-1.97388700	0.67901600	-4.40941600
C	-2.18077100	1.99759500	-2.27925600
C	-2.32434100	-1.68740900	-4.46583300
C	-2.95090400	-2.97993000	-2.40346300
C	-6.26994400	0.23004900	1.38530400
C	-5.65327500	-2.07646500	1.95639800
C	-1.00410500	-1.46994900	4.22186300
H	-0.75626900	-1.78594100	2.11412500
C	-2.93447600	-0.19788700	4.87099000
H	-4.18624000	0.50713000	3.28704100
C	-2.01970500	-0.50488700	-5.13693700
H	-1.72845400	1.60626900	-4.91642000
H	-1.30141800	2.02071400	-1.62670000
H	-2.11553900	2.85167900	-2.95015000
H	-3.05129400	2.13886000	-1.63638700
H	-2.34928600	-2.62151600	-5.01705900
H	-2.73057600	-3.84219900	-3.02906000
H	-2.38821300	-3.08749600	-1.47328000
H	-4.01016600	-3.02322300	-2.14266800
C	-7.44812000	0.06149200	2.10032800
C	-5.94931200	1.52229600	0.70804700
C	-6.84742200	-2.18607500	2.66077000
C	-4.69584200	-3.21946600	1.87778300
C	-1.79377500	-0.90870900	5.21579200
H	-0.10667800	-2.01741700	4.48182700
H	-3.54586700	0.25457600	5.64138400
C	-1.76437600	-0.52140500	-6.60875200
C	-7.75250700	-1.13376500	2.74866600
H	-8.14350000	0.89169300	2.15805300
H	-4.95445600	1.88749600	0.97524600
H	-5.96455500	1.41929000	-0.37844900
H	-6.66865900	2.29195500	0.97849500
H	-7.07326300	-3.12501600	3.15404700
H	-4.31364100	-3.36312600	0.86583300
H	-3.83028600	-3.06211200	2.52684700
H	-5.17219900	-4.14613500	2.19073300
H	-1.51616400	-1.01842300	6.25677500
H	-0.98854400	-1.24174800	-6.87242800
H	-2.66023400	-0.81746400	-7.15816500
H	-1.46091700	0.45529400	-6.98032800
C	-9.03767900	-1.28987800	3.49360100
H	-9.31532300	-0.37514800	4.01663400
H	-9.85839700	-1.52364100	2.81153700
H	-8.98689600	-2.09667700	4.22306000

[Ag(NHC)(MIC)]$^{+}$ in methanol

1 1

Ag	-0.02006500	-0.05429000	0.22522900
C	-2.06089900	-0.53527800	0.10371100
C	2.03589600	0.39702100	0.29221200
N	-2.53162500	-1.79761000	-0.10027200
C	-3.22541300	0.22238000	0.09446500
N	2.63793500	1.61646200	0.21154200
N	3.06057400	-0.46736000	0.44423600
N	-3.85154300	-1.90383800	-0.22841600
C	-1.71717000	-2.98295000	-0.15490800
N	-4.26331500	-0.65055300	-0.10818600
C	-3.35717600	1.66359100	0.27401600
C	4.01323700	1.50205100	0.32215700
C	1.93149600	2.84403300	0.05441900
C	4.27655600	0.18439900	0.45776900
C	2.89575000	-1.92092500	0.50203100
C	-0.96266800	-3.21744000	-1.30300400
C	-1.66269300	-3.80154400	0.97455900
C	-5.67991700	-0.39384100	-0.14675600
C	-2.48711300	2.30177800	1.16583100
C	-4.29265100	2.43142800	-0.42451000
H	4.66661300	2.35487700	0.27363900
C	2.29796600	3.95120600	0.80843700
C	0.87994800	2.92050300	-0.85266100
H	5.20918900	-0.34207600	0.56115400
H	1.88896500	-2.10520300	0.88275400
H	3.60486700	-2.30418400	1.23547900
C	3.09443300	-2.56692600	-0.84837600
C	-0.12473000	-4.32919000	-1.29723000
C	-1.02331800	-2.30349300	-2.48147500
C	-0.80580700	-4.89428600	0.92736100
C	-2.47457200	-3.50027600	2.19113200
C	-6.32765900	-0.42288500	-1.38314100
C	-6.33212500	-0.11988900	1.05361500
C	-2.55795700	3.67057900	1.35926600
H	-1.76091600	1.70972400	1.71236900
C	-4.35645100	3.80224600	-0.22701800
H	-4.95649800	1.96270300	-1.13964700
H	3.11276000	3.87607400	1.51789400
C	1.59787000	5.13904200	0.65722400
H	0.62965000	2.05959400	-1.46096300
C	0.17908000	4.10922100	-0.98489800
H	2.36137800	-2.19978800	-1.56921400
H	2.97865700	-3.64763900	-0.76505900
H	4.09144100	-2.36477500	-1.24090200
C	-0.02740100	-5.17220700	-0.19533800
H	0.47173800	-4.53469200	-2.17977800
H	-0.53241200	-1.34944300	-2.26366400
H	-0.52394900	-2.74456000	-3.34206500

H	-2.05080900	-2.06831300	-2.76515400
H	-0.73894300	-5.53947100	1.79699300
H	-2.19917400	-4.15730700	3.01360900
H	-2.33458200	-2.46833500	2.52144600
H	-3.54238700	-3.63071700	2.00504700
C	-7.69012700	-0.15522200	-1.39038400
C	-5.58294700	-0.71634500	-2.64324500
C	-7.69770000	0.14121600	0.98688000
C	-5.60176900	-0.10391400	2.35553900
C	-3.49403100	4.42535500	0.66457400
H	-1.88094200	4.14855100	2.05687700
H	-5.08104600	4.38705300	-0.78002000
H	1.87971000	6.00147900	1.24821100
C	0.53559800	5.22001700	-0.23258400
H	-0.64452900	4.16655000	-1.68652300
C	0.90437300	-6.34007300	-0.20405000
C	-8.39113700	0.12942400	-0.21897200
H	-8.21702200	-0.16458800	-2.33861800
H	-4.65450500	-0.14485500	-2.70848800
H	-5.30803700	-1.77133500	-2.70778400
H	-6.18857300	-0.47976000	-3.51564900
H	-8.23139500	0.35435500	1.90671900
H	-4.96317000	-0.98129000	2.47403300
H	-4.95413800	0.77283000	2.44065300
H	-6.29870900	-0.07729400	3.19046300
H	-3.54889200	5.49656300	0.81557800
H	-0.01376900	6.14716800	-0.33997100
H	1.64498600	-6.26175400	0.59472500
H	0.37126600	-7.27862300	-0.04099300
H	1.43996800	-6.41968700	-1.14890100
C	-9.85947400	0.39998200	-0.26502900
H	-10.09864000	1.17368500	-0.99614000
H	-10.41412000	-0.49199600	-0.56416100
H	-10.24145700	0.71866300	0.70338900

[Ag(NHC)(MIC)]$^{+}$ in benzene

1 1

Ag	-0.01677100	-0.03802900	0.21397900
C	-2.05451300	-0.53600200	0.08309000
C	2.04290800	0.42452900	0.30163200
N	-2.52616700	-1.80166900	-0.11075700
C	-3.21896000	0.22256400	0.07019000
N	2.64292800	1.64643400	0.25677600
N	3.07041100	-0.44209400	0.42991100
N	-3.84552800	-1.90641300	-0.23751100
C	-1.72347000	-2.99671100	-0.15339400
N	-4.25812500	-0.65330000	-0.12656500
C	-3.36004900	1.66336300	0.24914700
C	4.01727000	1.53066800	0.36441800
C	1.94984900	2.88789800	0.13276300
C	4.28391700	0.21130600	0.46704400
C	2.91766800	-1.89752600	0.45608200
C	-0.98486500	-3.26130400	-1.30497500
C	-1.68334000	-3.80759400	0.98200400
C	-5.67647500	-0.39881300	-0.17405000
C	-2.50589900	2.30834400	1.15050400
C	-4.30069000	2.42267300	-0.45152300
H	4.66751100	2.38618900	0.33590300
C	2.34028700	3.96988900	0.91134500
C	0.90350200	3.00979700	-0.77368300
H	5.21782200	-0.31399200	0.55973800
H	1.88892200	-2.09734600	0.76243600
H	3.57563100	-2.28639900	1.23360500
C	3.21850100	-2.52169900	-0.88613700
C	-0.17252900	-4.39146100	-1.29373700
C	-1.04606100	-2.36186700	-2.49546000
C	-0.85134400	-4.91880400	0.93985600
C	-2.48990300	-3.48432200	2.19677800
C	-6.32176300	-0.46165600	-1.41061600
C	-6.33350700	-0.09774100	1.01705300
C	-2.59983400	3.67386300	1.35388700
H	-1.77626000	1.72264400	1.69915000
C	-4.38746300	3.78999600	-0.24512900
H	-4.95760500	1.94724500	-1.16829900
H	3.14627600	3.85954000	1.62584300
C	1.67659500	5.17951800	0.77779400
H	0.62928600	2.16794500	-1.39731500
C	0.23879100	4.22012000	-0.88845200
H	2.53924300	-2.14653700	-1.65262900
H	3.10402400	-3.60351500	-0.83078500
H	4.23889300	-2.31119900	-1.20648100
C	-0.09033200	-5.22840100	-0.18593800
H	0.40857500	-4.62342000	-2.18000700
H	-0.58609000	-1.39113100	-2.28420000
H	-0.52418400	-2.79948600	-3.34384800
H	-2.07442000	-2.15891800	-2.80000200
H	-0.79931200	-5.56173500	1.81192800
H	-2.23125400	-4.14353000	3.02249400
H	-2.32922600	-2.45528800	2.52655300
H	-3.55929500	-3.59412200	2.00774500
C	-7.68309300	-0.19203900	-1.42877200
C	-5.57862600	-0.80380300	-2.66046400
C	-7.69783600	0.16225300	0.93841000
C	-5.61149300	-0.05632200	2.32355900
C	-3.54278800	4.41842300	0.65877900
H	-1.93657800	4.15708400	2.06027000
H	-5.11828800	4.36712300	-0.79716200
H	1.97978300	6.02276600	1.38485700
C	0.62487500	5.30704800	-0.11794300
H	-0.57910200	4.31308800	-1.59198000
C	0.79932600	-6.42916100	-0.19383500
C	-8.38812800	0.12288500	-0.26790400
H	-8.20800800	-0.22992800	-2.37712000
H	-4.64941300	-0.23722000	-2.75447300
H	-5.30572900	-1.86067800	-2.68256700
H	-6.18337500	-0.60082900	-3.54159300
H	-8.23488600	0.39577000	1.85104800
H	-4.97399900	-0.93113100	2.46389400
H	-4.96838900	0.82397500	2.40063300
H	-6.31358600	-0.01922800	3.15348700
H	-3.61838600	5.48641600	0.82035000
H	0.10713800	6.25261200	-0.21650100
H	1.53863700	-6.38390000	0.60836600

H	0.23183100	-7.34825100	-0.03906000	H	-10.40998500	-0.50821700	-
H	1.33585600	-6.52722000	-1.13602300	0.60227500			
C	-9.85646500	0.39079000	-0.32407700	H	-10.24238800	0.73136000	0.63489300
H	-10.09664700	1.14761500	-1.07186100				

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