Supporting Information

Pre-Inverse-Crowns: Synthetic, Structural and Reactivity Studies of Alkali Metal Magnesiates Primed for Inverse Crown Formation

Antonio J. Martínez-Martínez, David R. Armstrong, Ben Conway, Ben J. Fleming, Jan Klett, Alan. R. Kennedy, Robert E. Mulvey, Stuart D. Robertson and Charles T. O'Hara*

WestCHEM, Department of Pure and Applied Chemistry, University of Strathclyde,

Glasgow, G1 1XL (UK)

[*] To whom correspondence should be addressed. E-mail: charlie.ohara@strath.ac.uk

Supporting Information Contents

Table S1. Selected crystallographic and refinement data for **3**-**6**, and **8**.

Compound	**3**	**4**	**5**	**6**	**8**
Formula	$C_{22}H_{45}KMgN_2$	$C_{88}H_{180}K_4Mg_4N_8$	$C_{168}H_{342}K_6Mg_6N_2$	$C_{189}H_{282}K_6Mg_6N_2$	$C_{62}H_{106}Mg_2N_6Na_4$
Fw	401.01	1604.04	2911.00	3102.73	1076.10
Cryst. System	Monoclinic	Monoclinic	Trigonal	Trigonal	Orthorhombic
Space Group	$P2_1$	Cc	R-3	R-3	$Pna2_1$
Wavelength/Å	1.5418	1.5418	0.71073	1.5418	1.5418
a/Å	12.8807(5)	25.779(3)	37.852(2)	37.8751(15)	16.9437(6)
b/Å	26.5173(9)	25.754(3)	37.852(2)	37.8751(15)	16.1245(5)
c/Å	16.1073(6)	16.135(2)	11.5850(6)	11.7865(4)	23.5059(8)
α/°	90	90	90	90	90
β/°	105.997(4)	94.132(11)	90	90	90
γ/°	90	90	120	120	90
Volume/Å^3	5288.6(3)	10684(2)	14374.9(13)	14642.8(10)	6422.0(4)
Z	6	4	3	3	4
Temp./K	123(2)	123(2)	123(2)	123(2)	123(2)
Refls. Collect.	20246	37909	14300	20485	24813
$2\theta_{max}$	111.48	140	53.98	139.94	140
R_{int}	0.0499	0.0797	0.0314	0.0297	0.0352
Goodness of fit	0.805	1.718	1.021	1.053	1.017
$R[F^2>2\sigma]$, F	0.0468	0.1495	0.0621	0.0842	0.0575
R_w (all data), F^2	0.0975	0.4047	0.1734	0.2627	0.1523

EXPERIMENTAL SECTION

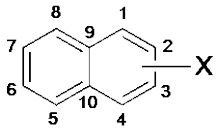
General Procedures. All reactions and manipulations were performed under a protective atmosphere of dry pure argon gas using standard Schlenk techniques. Products were isolated inside an argon-filled dry box. Solvents were dried by heating to reflux over sodium benzophenone ketyl and distilled under nitrogen prior to use. *cyc*-C_6D_{12} and d_8-THF were degasified and stored over 4 Å molecular sieves prior to use. 2,2,6,6-tetramethylpiperidine [TMP(H)] was purchased from Merck KGaA, distilled from CaH_2 and stored over 4 Å molecular sieves. *n*-BuLi, Me_3SiCH_2Li and *n,s*-Bu_2Mg solution were purchased from Aldrich. *n*-BuNa,[1] and Me_3SiCH_2K[2] were prepared according to literature methods.

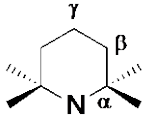
NMR spectra were recorded on a Bruker DPX 400 MHz spectrometer, operating at 400.13 and 100.62 MHz for ^{1}H and ^{13}C NMR, respectively. The NMR assignments were performed, in some cases, with the help $^{13}C\{^{1}H\}$-DEPT135, COSY, HMQC and HMBC experiments. Despite several attempts, satisfactory elemental analyses of the compounds **3**-**8**, carried out using a Perkin Elmer 2400 elemental analyser, could not be obtained due to their high air- and moisture-sensitive nature. Mass spectra for **9** and **10** were recorded on an Agilent 5975C GCMS running in CI mode with methane as reagent gas, helium carrier gas He at 1ml /min and an Agilent DB-5MS UI column.

Crystal Structure Determinations. Single-crystal data were recorded at 123(2) K on Oxford Diffraction Gemini and Xcalibur Diffractometers with Cu-$K\alpha$ (λ = 1.5418 Å; for **3**, **4**, **6**, and **8**) and Mo-$K\alpha$ (λ = 0.71073 Å; for **5**) radiation, respectively. The structures were refined to convergence on F^2 and against all independent reflections by full-matrix least-squares using SHELXL programs.[3] For structures **3** and **4** the SQUEEZE routine of PLATON was used to remove the effects of disordered solvent molecules.[4] For **3**, approximately 557 electron equivalents were removed from 2092 Å^3 of "void" space. This approximated to 11.6 molecules of cyclohexane per unit cell. For **4**, approximately 204 electron equivalents were removed from 1234 Å^3 of "void" space. This solvent was too disordered to identify. Measurement with several samples of **4** were attempted. All samples were polycrystalline and gave diffraction patterns with many non-indexed peaks. This clearly leads to a low quality structural model for **4**, but one which does show atomic connectivity. The butyl group of **5** was modeled as disordered over two sites, as was the naphthalenide ligand in **6** and the two TTHP anions in **8**. The geometries of the disordered groups were restrained to approximate typical values. Selected crystallographic parameters are given in Table S1 and full details are given in the deposited cif files. CCDC-964188 (**3**), CCDC-964189 (**4**), CCDC-964190 (**5**), CCDC-964191 (**6**) and CCDC-964192 (**8**) 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.

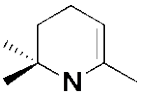
Computational Details. All structures were optimized at the B3LYP[5-8]/6-31G* level of theory.[9, 10] Geometry optimizations were carried out with standard procedures based on analytical energy gradients. All calculations were performed within the Gaussian 03 package.[11]

Chart 1. Atom numbering and abbreviations used for NMR assignments.





TMP = 2,2,6,6-tetramethylpiperidide



TTHP = 2,2,6-trimethyl-1,2,3,4-tetrahydropyridine

Synthesis of $[KMg(TMP)_2Bu]_\infty$ (3), $[KMg(TMP)_2Bu]_4$ (4), $[KMg(TMP)_2Bu]_6$ (5). In a Schlenk tube, freshly prepared KCH_2SiMe_3 (0.24 g, 2 mmol) was suspended in 8 mL of the appropriate solvent (cyclohexane for **3**, and methylcyclohexane for **4** and **5**), and then reacted with TMP(H) (0.34 mL, 2 mmol) for 1 h, forming KTMP *in situ* as a yellow suspension. In a second Schlenk tube, *n,s*-Bu_2Mg (2 mL from a 1M commercial solution in *n*-heptane, 2 mmol) in 3 mL of the appropriate solvent (cyclohexane for **3**, and methylcyclohexane for **4** and **5**) was reacted with TMP(H) (0.34 mL, 2 mmol) for 1 h to give *n*-BuMgTMP *in situ* as a pale yellow solution. This *n*-BuMgTMP solution was cannulated into the newly formed KTMP suspension, forming a yellow/orange solution which was stirred for 1 h. For **3**, cyclohexane was replaced by deuterated cyclohexane (*ca* 1 mL, *cyc*-C_6D_{12}) and transferred via syringe to a NMR tube and after 48 h at room temperature, a small crop of colourless prism crystals of **3** was obtained. For **4**, the methylcylcohexane solution was concentrated *in vacuo* (*ca* 5 mL) and after 2 days at room temperature, a crop of colourless block crystals of **4** (0.401 g, 50%) was obtained. For **5**, the methylcyclohexane was replace by cyclohexane (*ca* 1 mL) and then transferred via syringe to an NMR tube which was allowed to cool at 8 °C for 48 h, depositing a small crop of colourless block crystals of **5**. Crystals of **3**, **4** and **5** were suitable for an X-Ray diffraction study. The synthesis and crystallisation for **3** and **5** are optimized for X-ray crystallography quality crystal growth rather than yield of isolated product. The NMR spectra of isolated crystalline **3**, **4** and **5** are coincident and the respective *in situ* mixtures resemble the same compounds. ^{1}H NMR (400.13 MHz, 300 K, *cyc*-C_6D_{12}): δ -0.83 (m, 2 H, Mg-CH_2, *n*-Bu), 0.78 (t, 3 H, ^{3}J(H,H) = 7.0 Hz, CH_3, *n*-Bu), 1.19-1.34 (v br s, 12 H, β-CH_2-TMP + CH2-*n*-Bu + CH_2-*n*-Bu), 1.27 (s, 24 H, CH_3, TMP), 1.80 (br s, 4 H, γ-CH_2, TMP). ^{13}C{^{1}H} NMR (100.62 MHz, 300 K, *cyc*-C_6D_{12}): δ 14.7 (CH_3, *n*-Bu), 18.5 (Mg-CH_2), 20.0 (γ-TMP), 34.2 (CH_2, *n*-Bu), 34.4 (CH_2, *n*-Bu), 36.3 (br s, CH_3-TMP), 42.2 (β-TMP).

Synthesis of $[KMg(TMP)_2(2\text{-}C_{10}H_7)]_6$ (6). In a Schlenk tube, freshly prepared KCH_2SiMe_3 (0.24 g, 2 mmol) was suspended in methylcyclohexane (8 mL), and then reacted with TMP(H) (0.34 mL, 2 mmol) for 1 h, forming KTMP *in situ* as a yellow suspension. In a second Schlenk tube, *n,s*-Bu_2Mg (2

mL from a 1M commercial solution in *n*-heptane, 2 mmol) in methylcyclohexane (3 mL) was reacted with TMP(H) (0.34 mL, 2 mmol) for 1 h, forming *n*-BuMgTMP as a pale yellow solution. This *n*-BuMgTMP solution was cannulated into the newly formed KTMP suspension, forming a yellow/orange solution. Naphthalene (0.256 g, 2 mmol) was then added, dissolving after 2 min. This solution was then refluxed at 100°C for 1 h to give a pale yellow suspension. The solvent was then removed *in vacuo* until dryness, and replaced by toluene (10 mL). After vigorous heating, an orange solution was achieved, and this immediately placed in a Dewar containing hot water overnight to give yellow needle crystals of **6**·C_7H_8 suitable for an X-ray diffraction study (0.385 g, 41%). The ^{1}H NMR spectrum of the reaction crude shows that the metallation is almost quantitative. ^{1}H NMR (400.13 MHz, 300 K, d_8-THF): δ 1.26 (s, 24 H, CH_3, TMP), 1.29 (t, 8 H, ^{3}J(H,H) = 6.1 Hz, β-TMP), 1.73 (m, 4 H, γ-TMP), 2.30 (s, 3H, Me, C_7H_8), 7.01 (t, 1 H, ^{3}J(H,H) = 7.2 Hz, C8), 7.09 (t, 1 H, ^{3}J(H,H) = 6.9 Hz, C7), 7.12 (m, 3H, C_7H_8), 7.18 (t, 2H, ^{3}J(H,H) = 7.4 Hz, C_7H_8), 7.31 (d, 1 H, ^{3}J(H,H) = 7.4 Hz, C4), 7.49 (d, 1 H, ^{3}J(H,H) = 7.8 Hz, C9), 7.57 (d, 1H, ^{3}J(H,H) = 7.9 Hz, C6), 8.20 (d, 1 H, ^{3}J(H,H) = 7.5 Hz, C3), 8.37 (s, 1 H, C1). ^{13}C{^{1}H} NMR (100.62 MHz, 300 K, d_8-THF): δ 21.7 (γ-TMP), 21.3 (Me, C_7H_8), 36.2 (CH_3, TMP), 42.5 (β-TMP), 52.9 (C-N, TMP), 121.9 (C4), 121.85 (C8), 122.8 (C7), 127.8 (C9), 128.0 (C6), 128.9 (C_7H_8), 129.6 (C_7H_8), 140.6 (C1), 142.1 (C3).

Synthesis of [NaMg(TMP)$_2$^{n}Bu] (7). In a Schlenk tube, NaTMP was prepared *in situ* by reaction of *n*-BuNa (0.32 mg, 4 mmol) with TMP(H) (0.68 mL, 4 mmol) in methylcyclohexane (10 mL) for 1h, forming a pale yellow suspension. In a separate Schlenk tube, *n,s*-Bu_2Mg (4 mL from a 1M *n*-heptane commercial solution, 4 mmol) was reacted with TMP(H) (0.68 mL, 4 mmol) for 1h, forming a pale yellow solution. This *n*-BuMgTMP solution was cannulated into the newly formed NaTMP suspension, obtaining a pale yellow solution. The reaction mixture was stirred for 1h, concentrated under vacuum to *ca* 5 mL and immediately placed in a fridge operating at 8 °C. After 48 h, pale yellow block crystals of **7** were obtained (0.932 g, 2.42 mmol, 61%). ***Alternative synthesis of 7.*** Freshly prepared *n*-BuNa (0.32 g, 4 mmol) was suspended in methylcyclohexane (10 mL) in an argon-filled Schlenk tube. The suspension was placed in an ultrasonic bath for 30 min to obtain a more reactive fine suspension and TMP(H) (1.36 mL, 8 mmol) was then added. The resulting pale yellow suspension was stirred for 30 min and then *n,s*-Bu_2Mg (4 mL from a 1M *n*-heptane commercial solution, 4 mmol) was added via syringe to give a pale yellow solution. The reaction mixture was stirred for 30 min, concentrated under vacuum (*ca* 5 mL) and immediately placed in a fridge operating at 4°C. After 48 h, pale yellow block crystals of **7** were obtained (0.874 g, 2.27 mmol, 57%).

Attempts to analyse the crystalline material by X-ray diffraction studies were futile due to the high disorder nature present within the structure of **7**. Unfortunately, attempts to study by X-ray diffraction different samples of single crystals of **7** have so far been unsuccessful due to the disorder found within

the structure. The NMR spectra of isolated crystalline **7** and the respective *in situ* mixture resemble the same compound. ^{1}H NMR (400.13 MHz, 300 K, *cyc*-C_6D_{12}): δ -0.80 (br m, 2 H, Mg-CH_2, *n*-Bu), 0.89 (t, 3 H, $^{3}J(H,H)$ = 7.0 Hz, CH_3, *n*-Bu), 1.03-1.34 (several m, 10 H, β-CH_2-TMP + CH_2-*n*-Bu), 1.25 (s, 24 H, CH_3, TMP), 1.69 (m, 6H, CH_2-*n*-Bu + γ-CH_2-TMP). $^{13}C\{^{1}H\}$ NMR (100.62 MHz, 298K, *cyc*-C_6D_{12}): δ 14.5 (Mg-*C*H_2-*n*-Bu + Me-*n*-Bu), 20.0 (γ-TMP), 32.4 (*C*H_2, *n*-Bu), 36.7 (br s, *C*H_3-TMP), 39.2 (*C*H_2, *n*-Bu), 42.2 (β-TMP), 52.8 (N-C, TMP).

[$Na_2Mg(TMP)_3{}^{n}Bu$] (7·NaTMP). When **7** is treated with an equimolar amount of NaTMP, equimolar amounts of [$NaMg(TMP)_2{}^{n}Bu$] (**7**), NaTMP and [$Na_2Mg(TMP)_3{}^{n}Bu$] in hydrocarbon solvent are identified in *cyc*-C_6D_{12} solution by ^{1}H NMR. Small amount of TMPH are also detected. ^{1}H NMR (400.13 MHz, 300 K, *cyc*-C_6D_{12}): δ -0.80 (br m, 2 H, Mg-CH_2, *n*-Bu, [$Na_2Mg(TMP)_3{}^{n}Bu$]), -0.43 (v br s, 2 H, Mg-CH_2, *n*-Bu, [$Na_2Mg(TMP)_3{}^{n}Bu$]), 0.90 (m, 6 H, *n*-Bu, [$Na_2Mg(TMP)_3{}^{n}Bu$] + [$Na_2Mg(TMP)_3{}^{n}Bu$]), 1.03-1.34 (several m, 24 H, β-CH_2-TMP + CH_2-*n*-Bu, [$Na_2Mg(TMP)_3{}^{n}Bu$] + [$Na_2Mg(TMP)_3{}^{n}Bu$]), 1.04 (s, 12 H, CH_3-TMP, NaTMP), 1.25 (s, 64 H, CH_3-TMP, [$Na_2Mg(TMP)_3{}^{n}Bu$] + [$Na_2Mg(TMP)_3{}^{n}Bu$] + NaTMP), 1.69 (m, 16 H, CH_2-*n*-Bu + γ-CH_2-TMP, [$Na_2Mg(TMP)_3{}^{n}Bu$] + [$Na_2Mg(TMP)_3{}^{n}Bu$] + NaTMP).

Synthesis of [$Na_4Mg_2(TMP)_4(TTHP)_2(1,4\text{-}C_{10}H_6)$] (8). Freshly prepared *n*-BuNa (0.32 g, 4 mmol) was suspended in methylcyclohexane (10 mL) in an argon-filled Schlenk tube. The suspension was placed in an ultrasonic bath for 30 min to obtain a more reactive fine suspension and TMP(H) (1.36 mL, 8 mmol) was then added. The resulting pale yellow suspension was stirred for 1h and then *n,s*-Bu_2Mg (4 mL from a 1M commercial solution in *n*-heptane, 4 mmol) was added to give a pale yellow solution, which was stirred for 30 min. Naphthalene (256.3 mg, 2 mmol) was then added and after 2 min of stirring it was dissolved. The reaction mixture was refluxed at 100°C overnight to give a pale brown suspension which was filtered. The solid collected was dried under vacuum to give **8** as a pale brown solid (1.13 g, 1.02 mmol, 51%). ***Alternative Synthesis of 8 from an in situ mixture of 7·NaTMP***. Freshly prepared *n*-BuNa (0.481 g, 6 mmol) was suspended in methylcyclohexane (10 mL) in an argon-filled Schlenk tube. The suspension was placed in an ultrasonic bath for 30 min to obtain a more reactive fine suspension and TMP(H) (1.6 mL, 9 mmol) was then added. The resulting pale yellow suspension was stirred for 1h and then *n,s*-Bu_2Mg (3 mL from a 1M commercial solution in *n*-heptane, 3 mmol) was added to give a pale yellow solution, which was stirred for 30 min. Naphthalene (192.3 mg, 1.5 mmol) was then added and after 2 min of stirring it was dissolved. The reaction mixture was refluxed at 100°C overnight to give a pale brown suspension which was filtered. The solid collected was dried under vacuum to give **8** as a pale brown solid (1.23 g, 1.14 mmol, 76%).

Crystals of **8** suitable for an X-ray diffraction study were obtained by filtration of a hot suspension of **8** (0.5 g, 0.46 mmol) in toluene (20 mL), and allowing the filtrate to cool slowly to ambient temperature (185 mg, 0.17 mmol, 37%). The NMR spectra of isolated pale brown solid and crystals of

8 are coincident and resemble its X-ray structure retains its configuration *cyc*-C_6D_{12} solution. ^{1}H NMR (400.13 MHz, 300 K, *cyc*-C_6D_{12}): δ 0.06 (s, 12H, C*Me*$_2$, TTHP), 0.81 (s, 12H, Me, TMP), 1.04 (s, 12H, Me, TMP), 1.23-1.58 (several m, 28H, TMP + TTHP), 1.28 (s, 6H, C*Me*, TTHP), 1.53 (s, 24H, Me, TMP), 1.90 (m, 6 H, TTHP + TMP), 7.29 (m, 2H, H7+H6), 7.92 (s, 2H, H2+H3), 7.95 (m, 1H, H5+H8). ^{13}C{^{1}H} (100.62 MHz, 300 K, *cyc*-C_6D_{12}): δ 18.9 (Me), 19.3 (Me), 20.4 (Me), 30.1 (Me), 31.9 (TMP), 32.9 (CH2, TTHP), 33.0 (TMP), 36.7 (TMP), 37.4 (TTHP), 38.2 (TMP), 38.8 (RMP), 39.7 (TMP), 40.8 (TTHP), 41.9 (br s, TMP), 42.2 (TMP), 42.7 (CH2, TTHP), 125.6 (C9+C10), 126.1 (C6+C7), 136.5 (C8+C5), 140.0 (C2+C3).

Synthesis of 2-Iodonaphthalene (9) by Reaction of 6 with Iodine. In a Schlenk tube, magnesiate **6** (933 mg, 0.33 mmol) was suspended in 10 methylcyclohexane (10 mL). In a second Schlenk tube, an excess of iodine (5.08 g, 20 mmol) was dissolved in THF (10 mL). Both samples were then cooled to -78°C in a dry ice/acetone cooling bath and stirred for 15 min, Then, the cold magnesiate suspension was added dropwise to the stirring cold iodine THF solution via syringe. The reaction mixture was stirred at -78°C for 3h, followed by stirring at room temperature for 12 h. Then, saturated aqueous NH_4Cl (10 mL) was added along with the addition of saturated $Na_2S_2O_3$ until bleaching occurred (15 mL). The organic layer was separated from the aqueous layer and dried over anhydrous $MgSO_4$ for 30 min. After filtration, the solvent was removed *in vacuo* and the resultant oily crude was extracted with *n*-hexane (1 mL). The *n*-hexane extract was subjected to flash column chromatography on silica with *n*-hexane as eluent. 2-iodonaphthalene **9** was obtained as an off-white solid (425 mg, 1.68 mmol, 84%). R_F (*n*-hexane) 0.9.

Synthesis of 2-Iodonaphthalene (9) by Reaction of Crude Solution of 6 with Iodine. In a Schlenk tube, freshly prepared KCH_2SiMe_3 (0.24 g, 2 mmol) was suspended in methylcyclohexane (8 mL), and then reacted with TMP(H) (0.34 mL, 2 mmol) for 1 h, forming KTMP *in situ* as a yellow suspension. In a second Schlenk tube, *n*-Bu_2Mg (2 mL from a 1M commercial solution in *n*-heptane, 2 mmol) in methylcyclohexane (3 mL) was reacted with TMP(H) (0.34 mL, 2 mmol) for 1 h, forming *n*-BuMgTMP as a pale yellow solution. This *n*-BuMgTMP solution was cannulated into the newly formed KTMP suspension, forming a yellow/orange solution which was stirred for 30 min. Naphthalene (0.256 g, 2 mmol) was then added, dissolving after 2 min. This solution was then refluxed at 100°C for 1 h to give **6** a pale yellow suspended in methylcyclohexane. In a second Schlenk tube, an excess of iodine (5.08 g, 20 mmol) was dissolved in THF (10 mL). Both samples were then cooled to -78°C in a dry ice/acetone cooling bath and stirred for 15 min, and then the cold magnesiate suspension was added dropwise to the stirring cold iodine solution via syringe. The reaction mixture was stirred at -78°C for 3h, followed by stirring at room temperature for 12 h. Then, saturated aqueous NH_4Cl (10 mL) was added along with the addition of saturated $Na_2S_2O_3$ until bleaching occurred (15 mL). The organic layer was separated from the aqueous layer and dried over anhydrous $MgSO_4$ for 30 min. After filtration, the solvent was removed *in vacuo* and the resultant

oily crude was extracted with *n*-hexane (1 mL). The *n*-hexane extract was subjected to flash column chromatography on silica with *n*-hexane as eluent. 2-Iodonaphthalene **9** was obtained as an off-white solid (338 mg, 1.33 mmol, 67%). R_F (*n*-hexane) 0.9.

2-Iodonaphthalene[12-17] **(9)**: ^{1}H NMR (400.13 MHz, 300 K, $CDCl_3$): δ 7.49 (m, 2H, H^{6+7}), 7.57 (d, 1H, ^{3}J(H,H) = 8.6 Hz, H^4), 7.72 (m, 2H, H^{3+8}), 7.81 (m, 1H, H^5), 8.25 (d, 1H, ^{3}J(H,H) = 1.1 Hz, H^1). $^{13}C\{^1H\}$ NMR (100.62 MHz, 300 K, $CDCl_3$): δ 91.5 (C2), 126.4 (C6 or C7), 126.7 (C6 or C7), 126.8 (C8); 127.8 (C5), 129.4 (C4), 132.1 (C10), 134.4 (C3), 135.0 (C9), 136.6 (C1). GC-MS (CI) *m*/*z* calc. for $C_{10}H_7I$ $[M]^+$, 254.0; found 253.8.

Synthesis of 1,4-Diodonaphthalene (10) by Reaction of 8 with Iodine. In a Schlenk tube, magnesiate **8** (2.22 g, 2 mmol) was suspended in methylcyclohexane (20 mL). In a second Schlenk tube, an excess of iodine (5.08 g, 20 mmol) was dissolved in THF (20 mL). Both samples were then cooled to -78°C in a dry ice/acetone cooling bath and stirred for 15 min, Then, the cold magnesiate suspension was added drop wise to the stirring cold iodine THF solution via syringe. The reaction mixture was stirred at -78°C for 3h, followed by stirring at room temperature for 12 h. Then, saturated aqueous NH_4Cl (10 mL) was added along with the addition of saturated $Na_2S_2O_3$ until bleaching occurred (20 mL). The organic layer was separated from the aqueous layer and dried over anhydrous $MgSO_4$ for 30 min. After filtration, the solvent was removed *in vacuo* and the resultant oily crude was extracted with *n*-hexane (1 mL). The *n*-hexane extract was subjected to flash column chromatography on silica with *n*-hexane as eluent. 1,4-diiodonaphthalene **10** was obtained as an white solid (0.676 mg, 1.78 mmol, 89%). R_F (*n*-hexane) 0.85.

Synthesis of 1,4-Diiodonaphthalene (10) by Reaction of Crude Solution of 8 with Iodine. In a Schlenk tube, freshly prepared BuNa (0.32 g, 4 mmol) was suspended in methylcyclohexane (10 mL), and then reacted with TMP(H) (0.68 mL, 4 mmol) for 1 h, forming NaTMP *in situ* as a yellow suspension. In a second Schlenk tube, *n,s*-Bu_2Mg (2 mL from a 1M commercial solution in *n*-heptane, 2 mmol) in methylcyclohexane (10 mL) was reacted with TMP(H) (0.34 mL, 2 mmol) for 1 h, forming *n*-BuMgTMP as a pale yellow solution. This *n*-BuMgTMP solution was cannulated into the newly formed KTMP suspension, forming a yellow/orange solution which was stirred for 30 min. Naphthalene (256.3 g, 2 mmol) was then added, dissolving after 2 min. This solution was then refluxed at 100°C for 12 h to give **8** a pale yellow suspended in methylcyclohexane. In a second Schlenk tube, an excess of iodine (5.08 g, 20 mmol) was dissolved in THF (20 mL). Both samples were then cooled to -78°C in a dry ice/acetone cooling bath and stirred for 15 min, and then the cold magnesiate suspension was added dropwise to the stirring cold iodine solution via syringe. The reaction mixture was stirred at -78°C for 3h, followed by stirring at room temperature for 12 h. Then, saturated aqueous NH_4Cl (15 mL) was added along with the addition of saturated $Na_2S_2O_3$ until bleaching occurred (20 mL). The organic layer was separated from the aqueous layer and dried over

anhydrous $MgSO_4$ for 30 min. After filtration, the solvent was removed *in vacuo* and the resultant oily crude was extracted with *n*-hexane (1 mL). The *n*-hexane extract was subjected to flash column chromatography on silica with *n*-hexane as eluent. 2-Iodonaphthalene **10** was obtained as an off-white solid (0.653 mg, 1.72 mmol, 86%). R_F (*n*-hexane) 0.85.

1,4-Diiodonaphthalene[18] **(10)**: ^{1}H NMR (400.13 MHz, 300 K, $CDCl_3$): δ 7.61 (m, 2H, H^{6+7}), 7.78 (s, 2H, H^{2+3}), 8.06 (m, 2H, H^{5+8}). $^{13}C\{^1H\}$ NMR (100.62 MHz, 300 K, $CDCl_3$): δ 100.7 (C1+C4), 128.7 (C6+C7), 133.1 (C5+C8), 134.8 (C9+C10), 138.2 (C2+C3). GC-MS (CI) *m*/*z* calc. for $C_{10}H_6I_2$ $[M]^+$, 379.9; found 379.7.

NMR Spectra

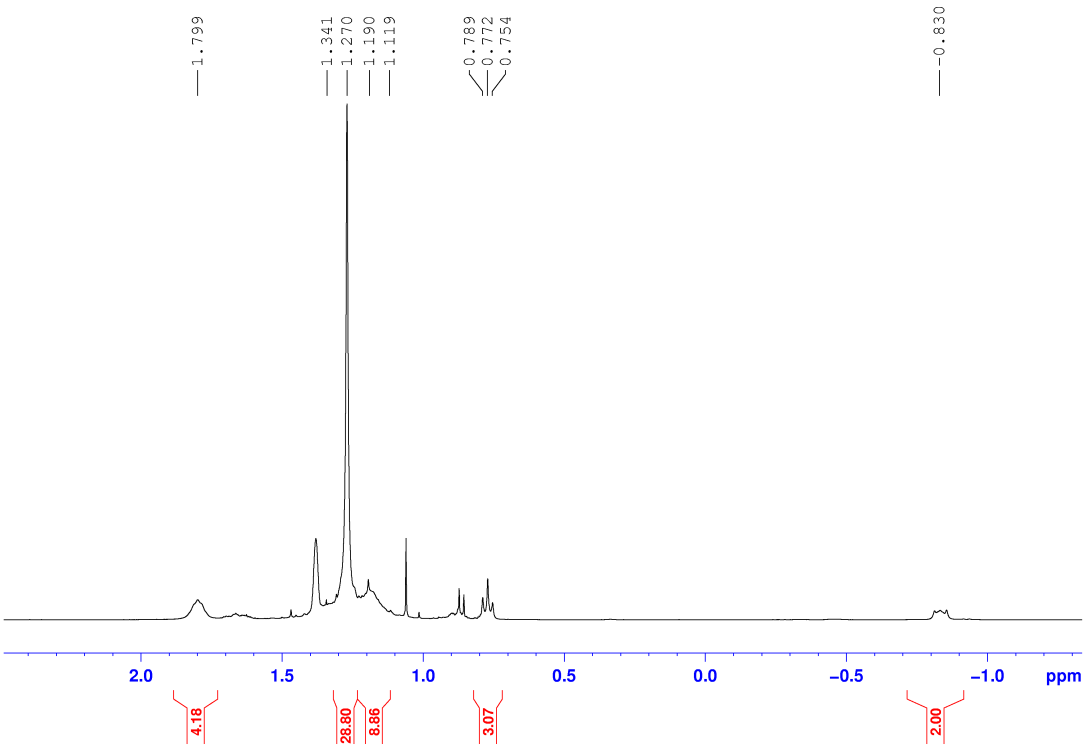


Figure S1. ^{1}H NMR spectrum of **3** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

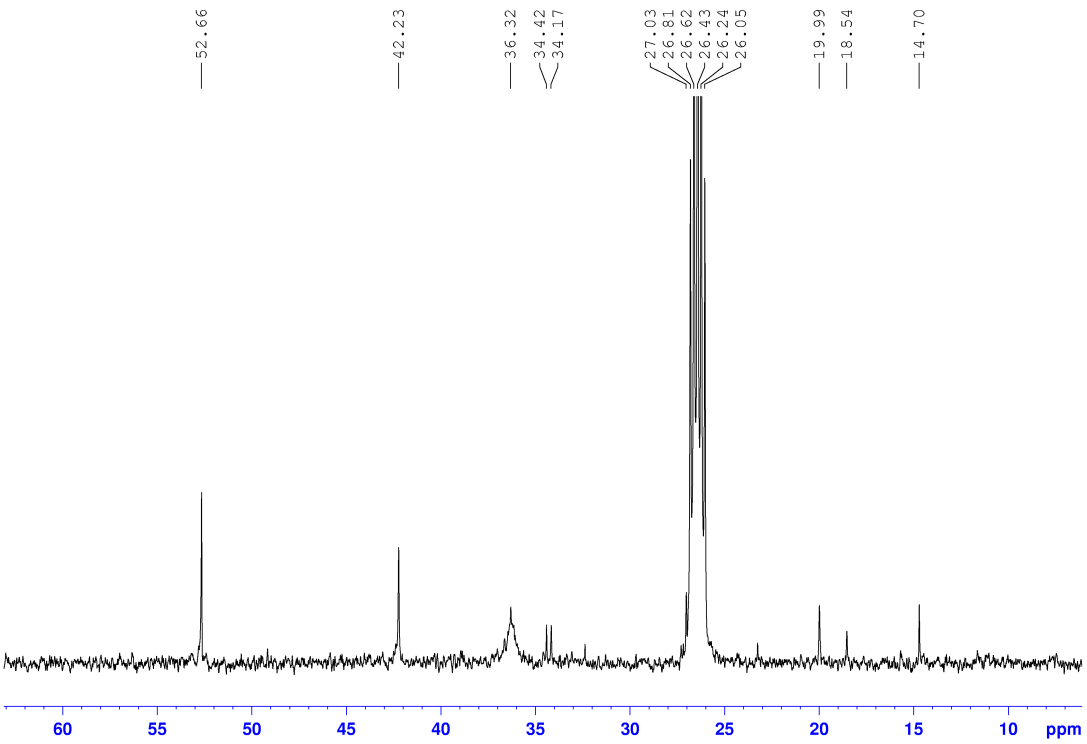


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **3** (100.62 MHz, 300K, *cyc*-C_6D_{12}).

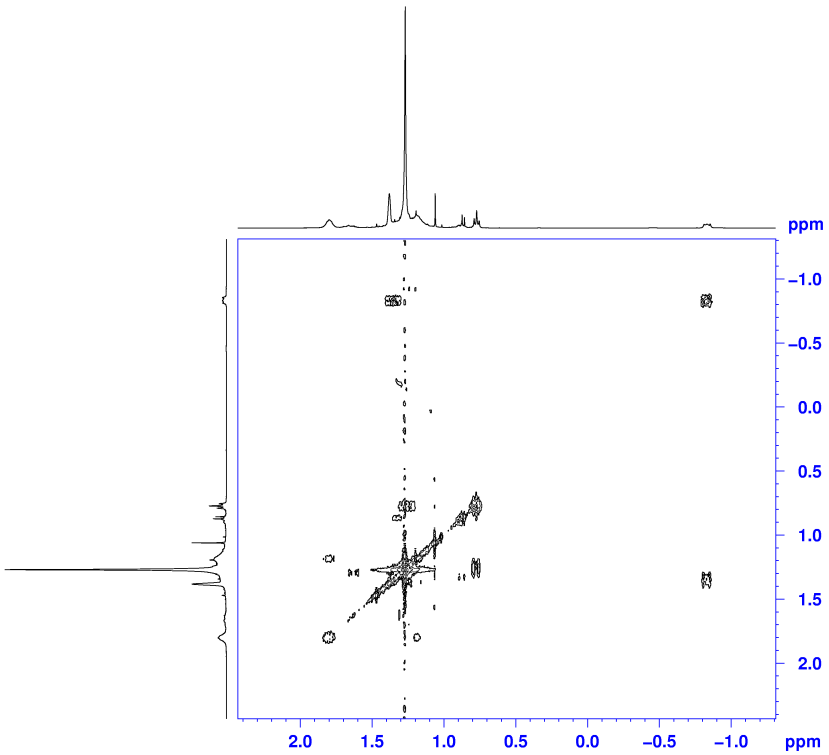


Figure S3. $^{1}H,^{1}H$-COSY NMR spectrum of **3** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

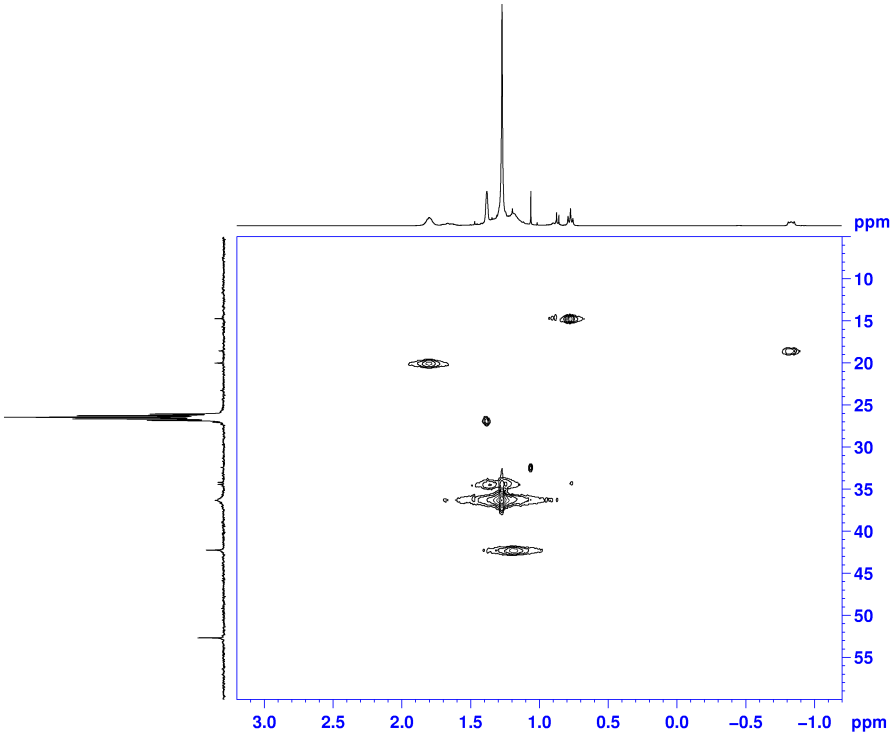


Figure S4. $^{1}H,^{13}C$-HSQC NMR spectrum of **3** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

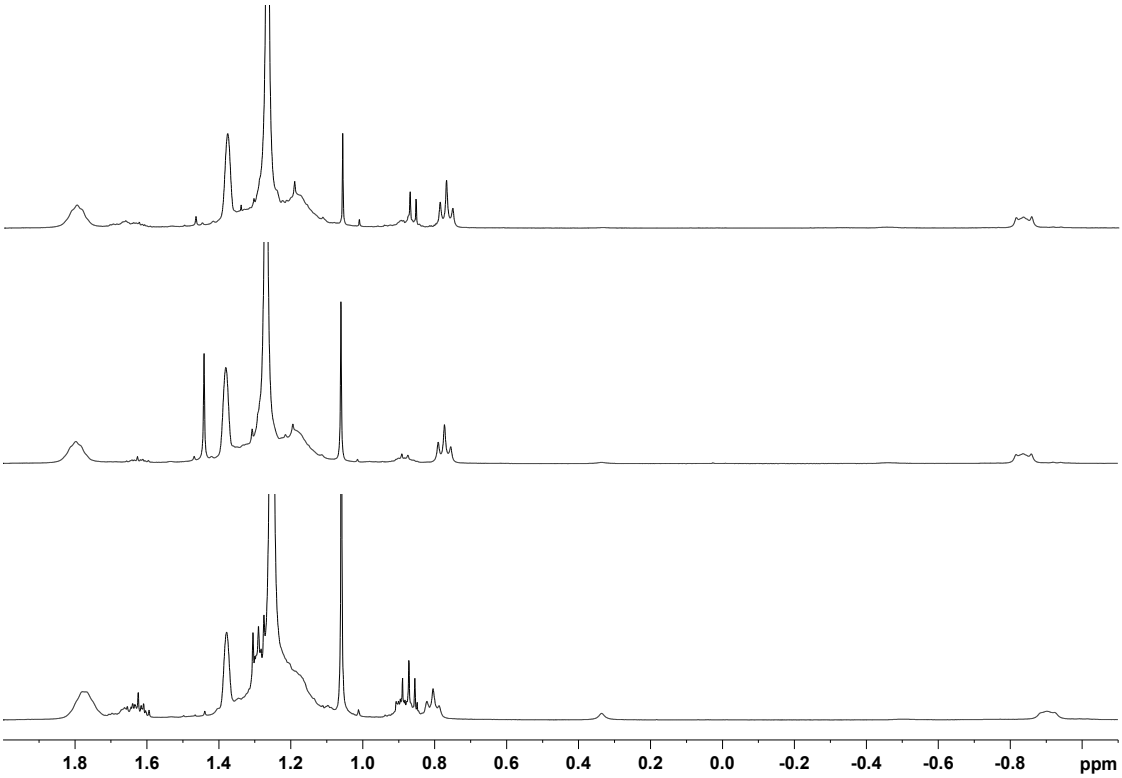


Figure S5. ^{1}H NMR spectrum of **4** (up), **5** (middle) and reaction crude from KTMP·TMPMgBu (down) *in situ* mixture (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

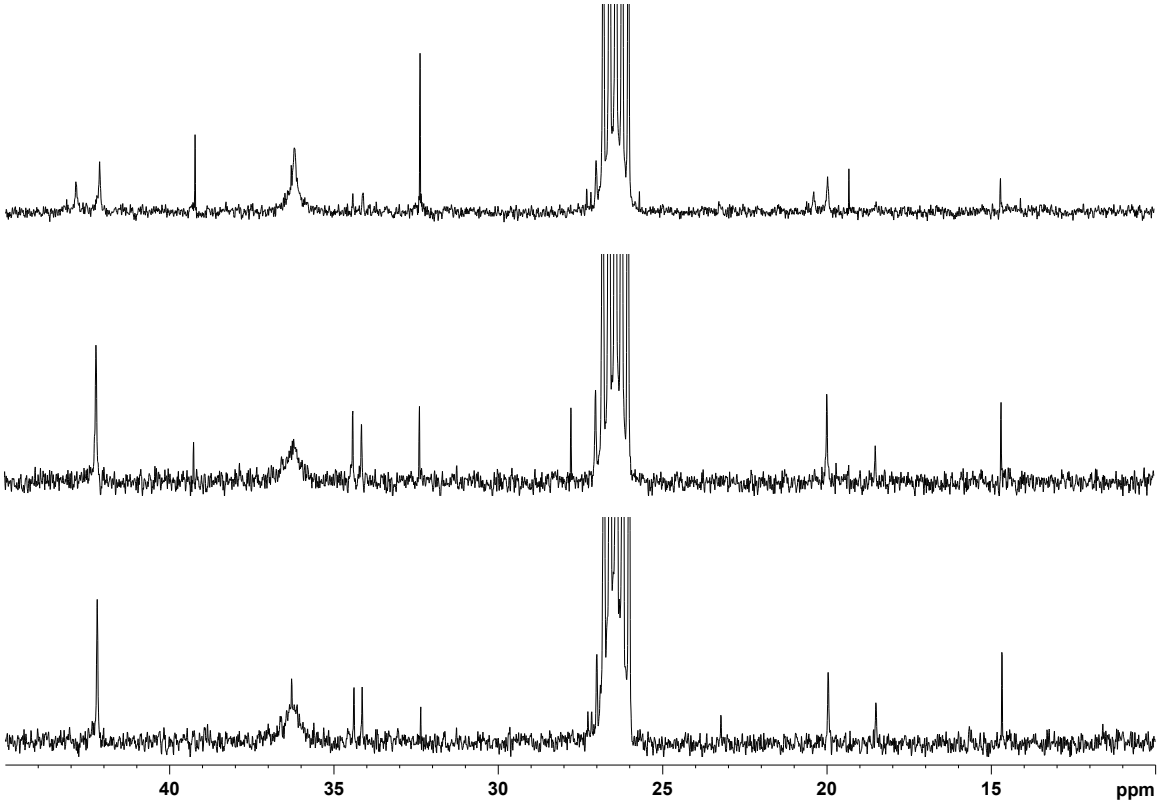


Figure S6. ^{13}C NMR spectrum of **4** (up), **5** (middle) and reaction crude from KTMP·TMPMgBu (down) *in situ* mixture (100.62 MHz, 300K, *cyc*-C_6D_{12}).

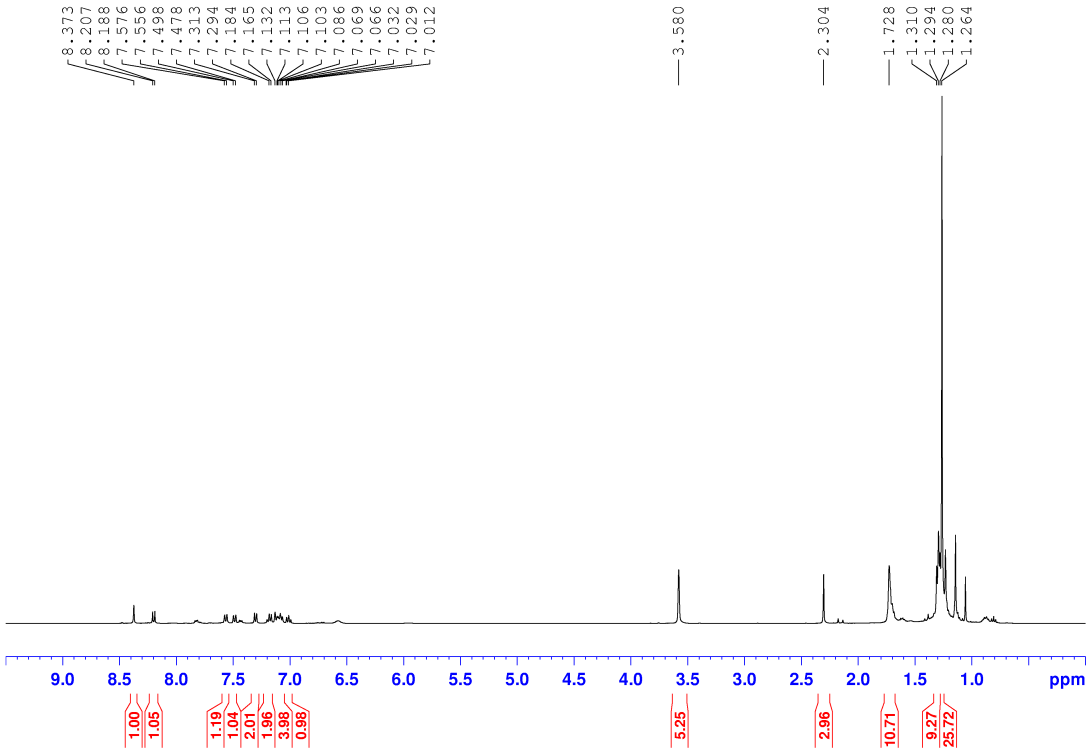


Figure S7. ^{1}H NMR spectrum of **6**·C_7H_8 (400.13 MHz, 300 K, d_8-THF).

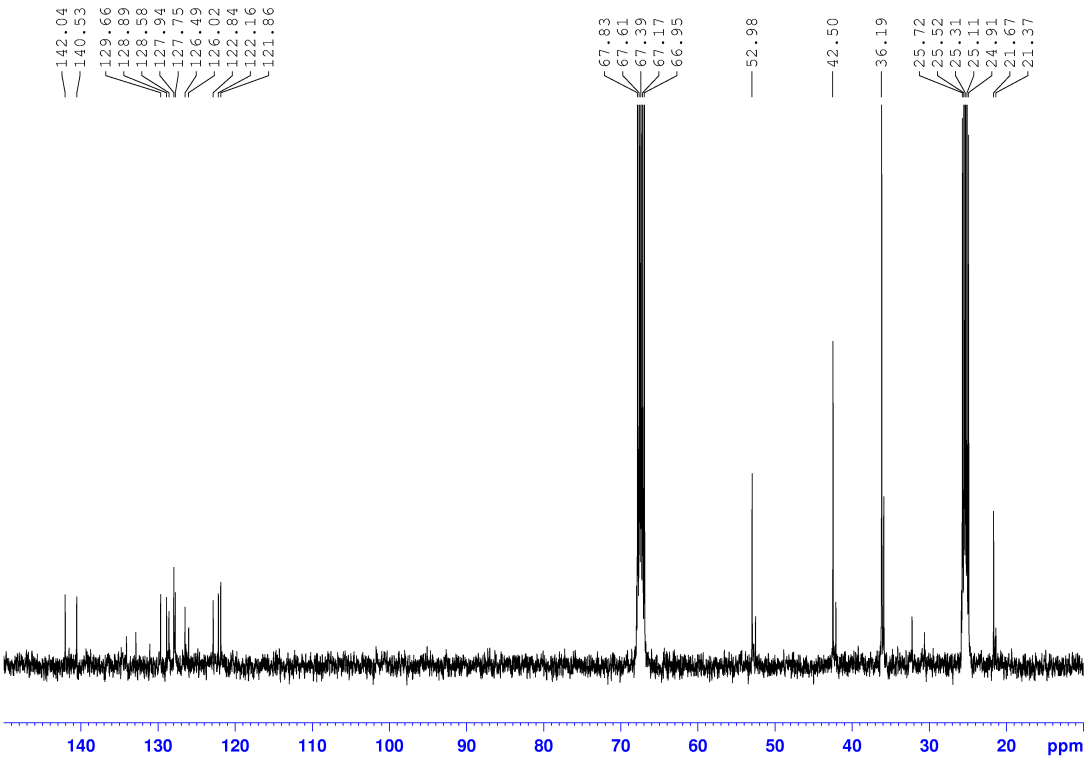


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **6**·C_7H_8 (100.62 MHz, 300K, d_8-THF).

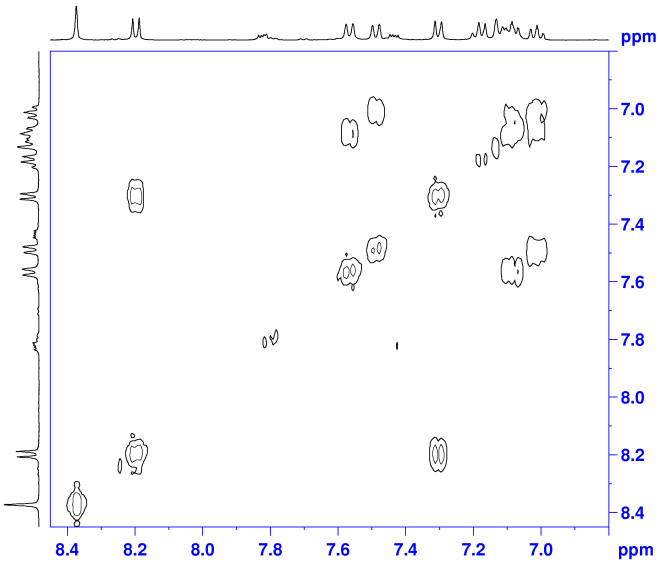


Figure S9. ^{1}H,^{1}H-COSY NMR spectrum of **6**·C_7H_8 (400.13 MHz, 300 K, d_8-THF).

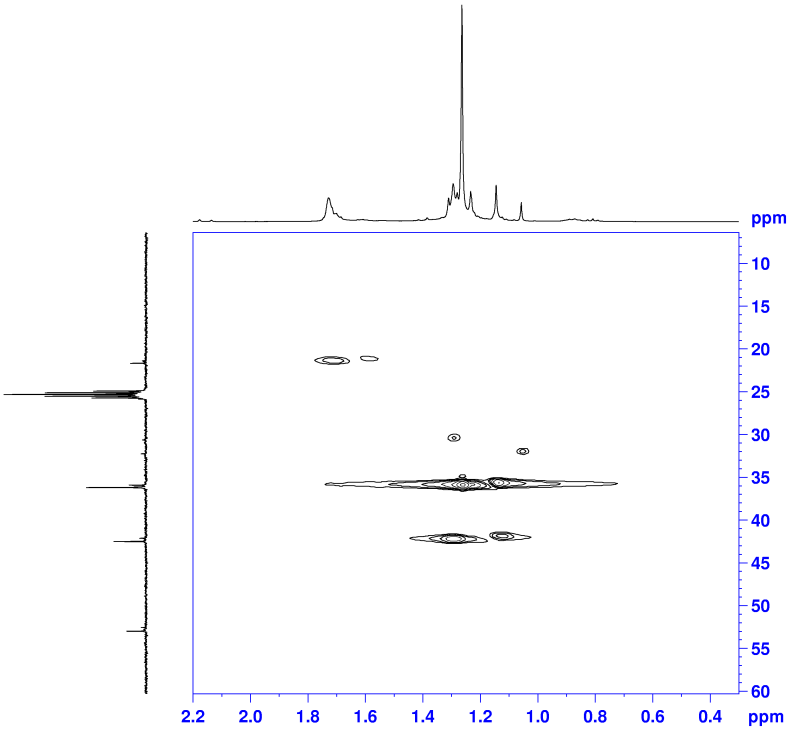


Figure S10. ^{1}H,^{13}C-HSQC NMR spectrum of **6**·C_7H_8 (400.13 MHz, 300 K, d_8-THF).

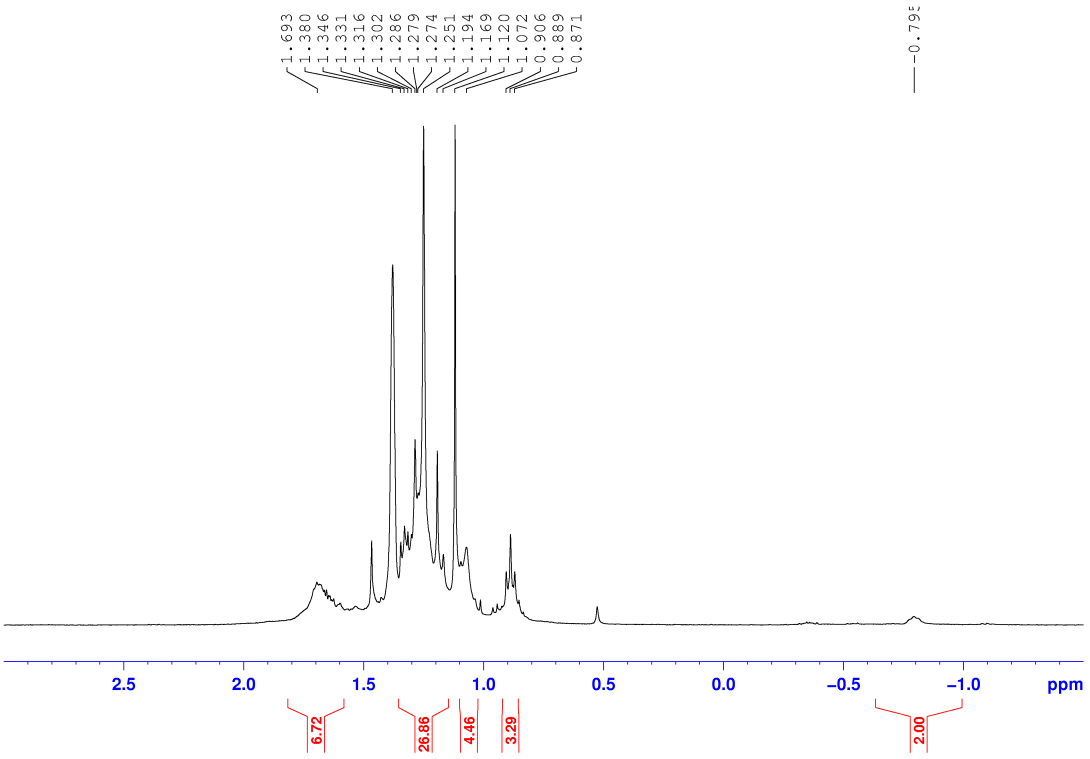


Figure S11. ^{1}H NMR spectrum of **7** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

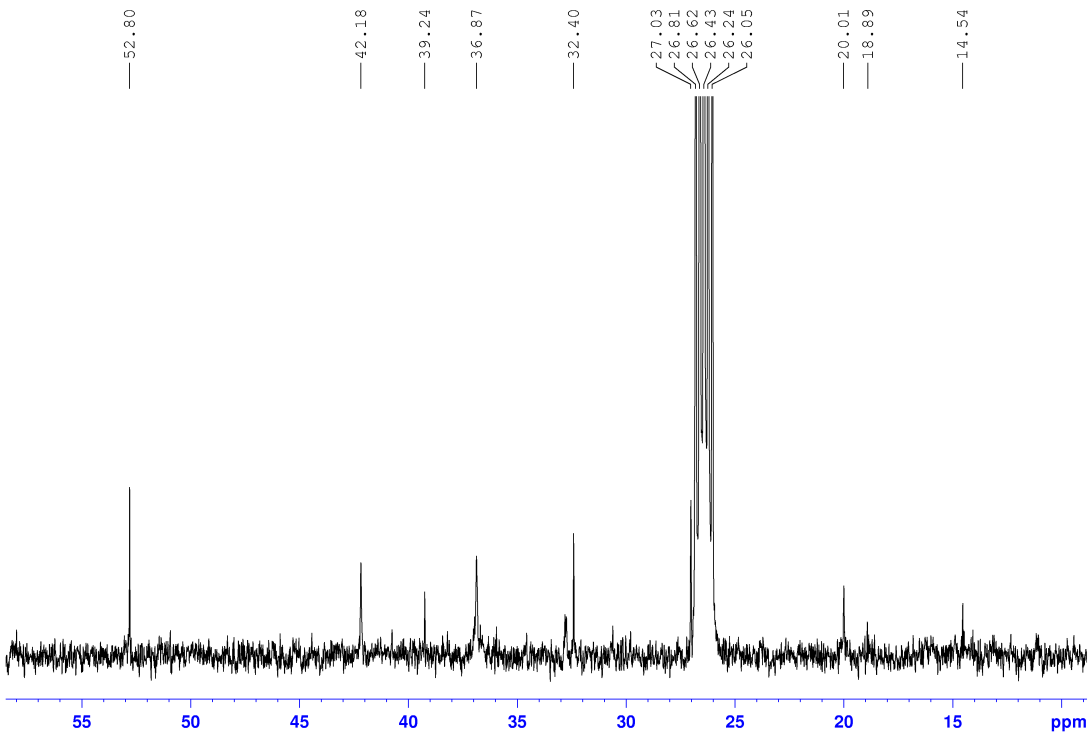


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of **7** (100.62 MHz, 300K, *cyc*-C_6D_{12}).

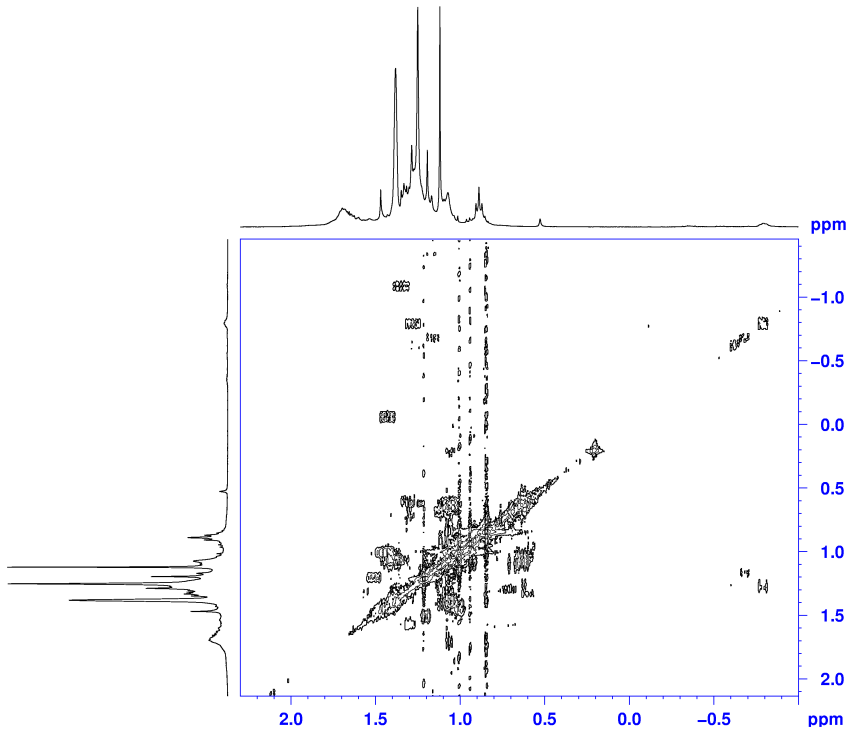


Figure S13. $^{1}H,^{1}H$-COSY NMR spectrum of **7** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

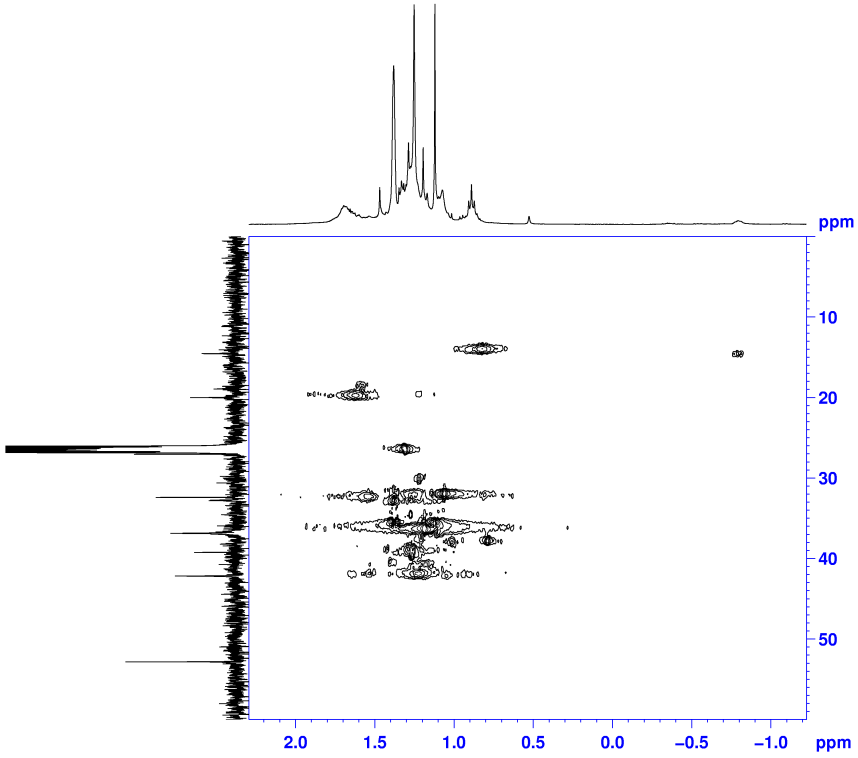


Figure S14. $^{1}H,^{13}C$-HSQC NMR spectrum of **7** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

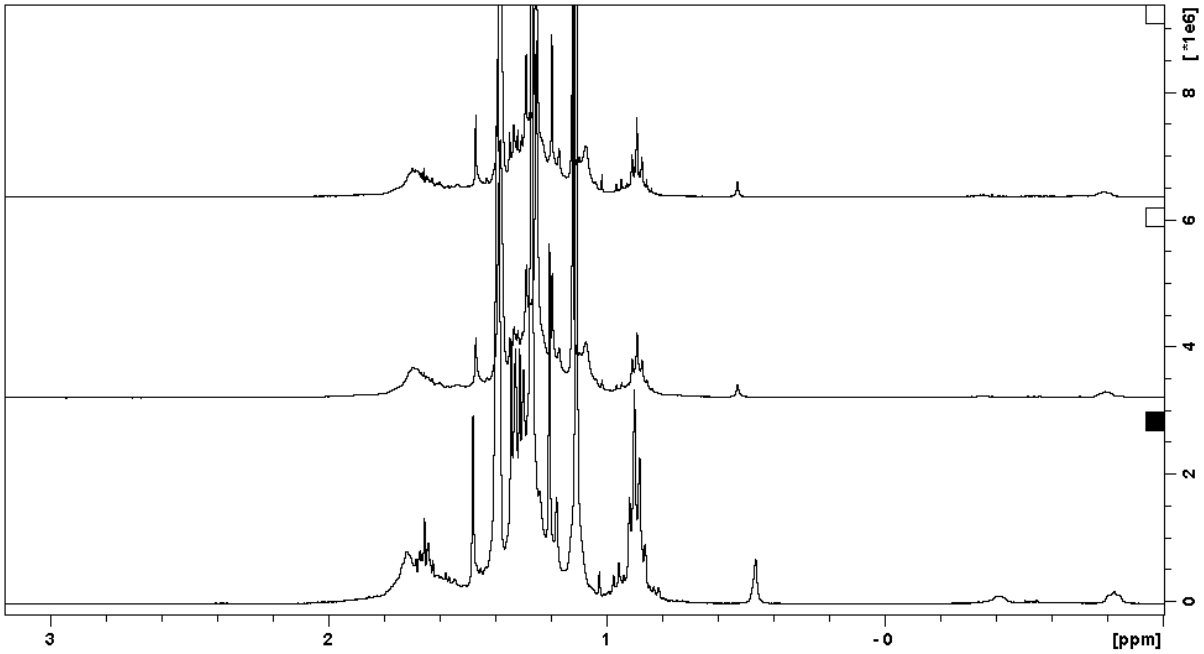


Figure S15. ^{1}H NMR spectrum of **7** (up) and reaction crude from NaTMP·TMPMgBu *in situ* mixture (middle) and reaction crude from **7**·NaTMP (down) *in situ* mixture (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

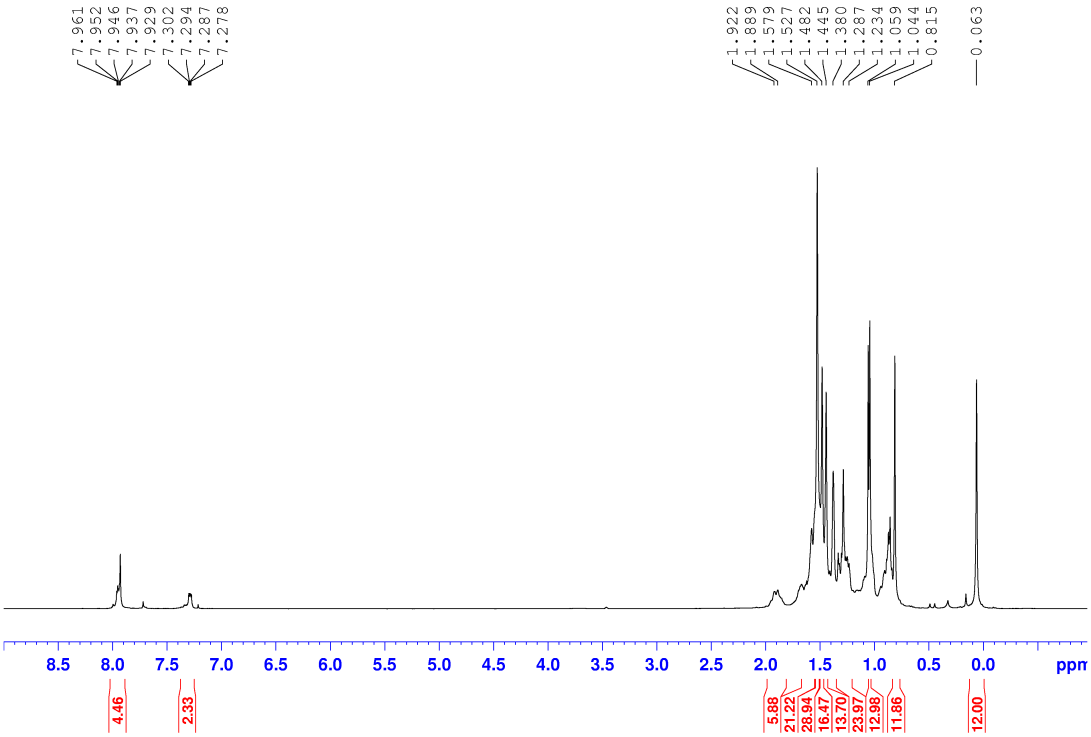


Figure S16. ^{1}H NMR spectrum of **8** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

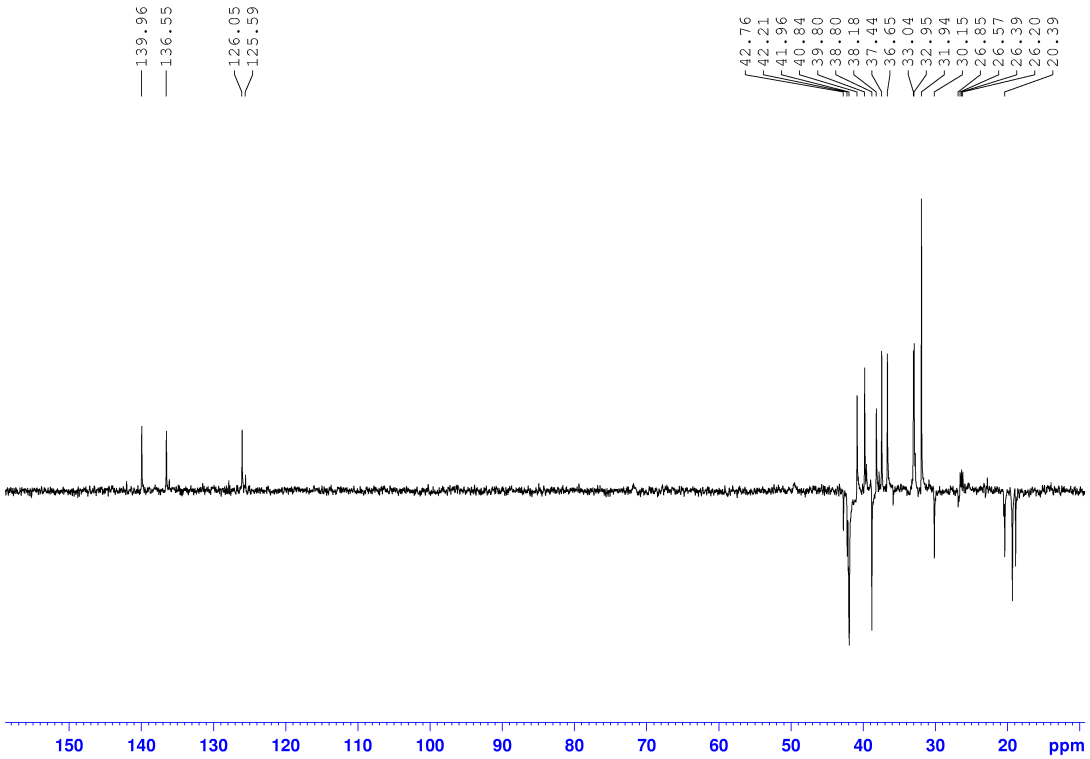


Figure S17. $^{13}C\{^{1}H$, DEPT135$\}$ NMR spectrum of **8** (100.62 MHz, 300K, *cyc*-C_6D_{12}).

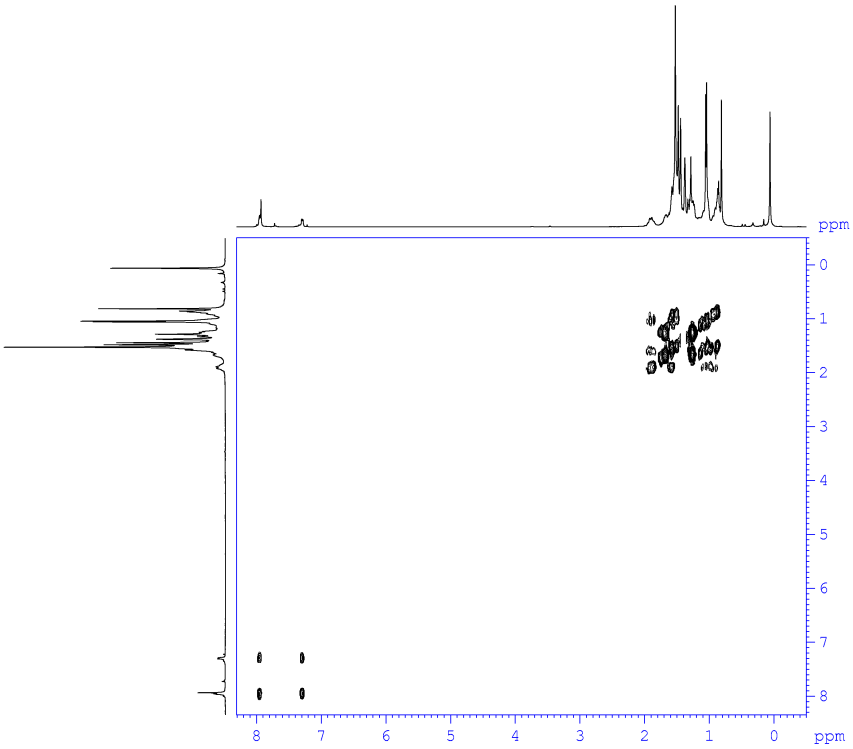


Figure S18. $^{1}H,^{1}H$-COSY NMR spectrum of **8** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

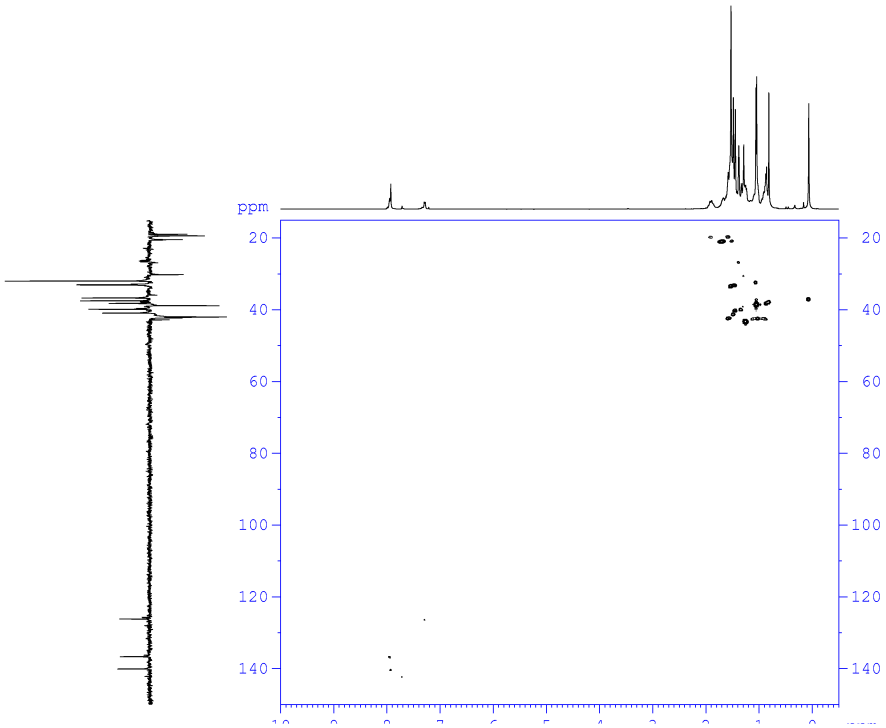


Figure S19. $^{1}H,^{13}C$-HSQC NMR spectrum of **8** (400.13 MHz, 300 K, *cyc*-C_6D_{12}).

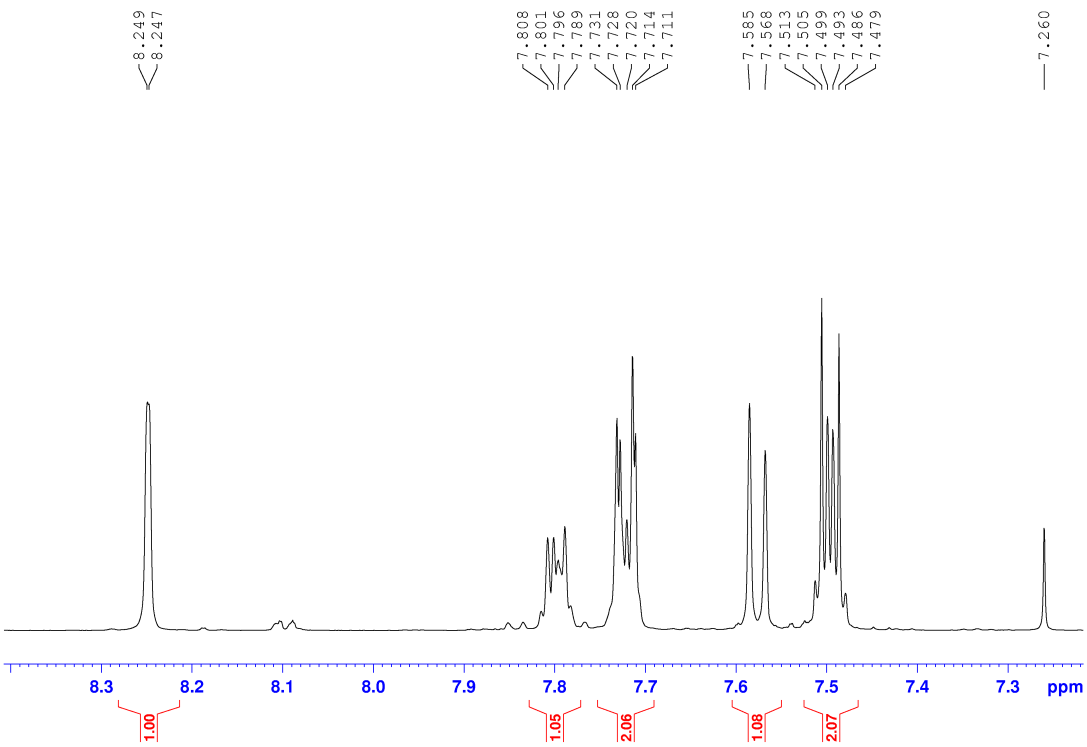


Figure S20. ^{1}H NMR spectrum of **9** (400.13 MHz, 300 K, $CDCl_3$).

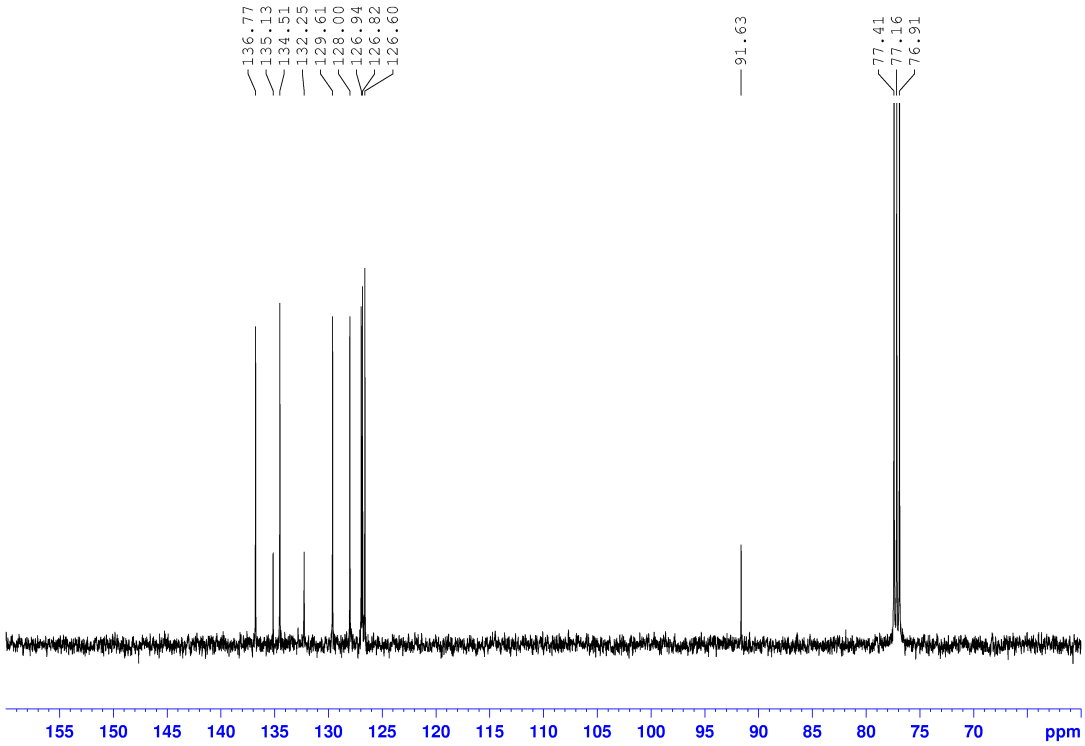


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of **9** (100.62 MHz, 300K, $CDCl_3$).

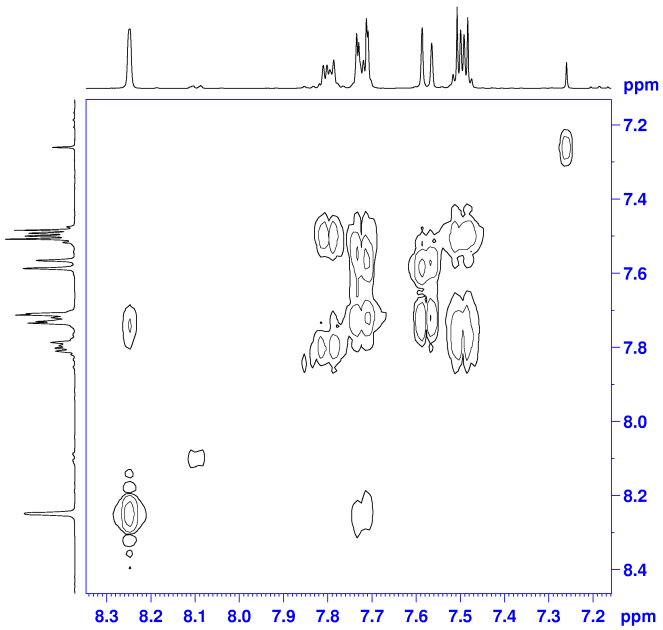


Figure S22. $^{1}H,^{1}H$-COSY NMR spectrum of **9** (400.13 MHz, 300 K, $CDCl_3$).

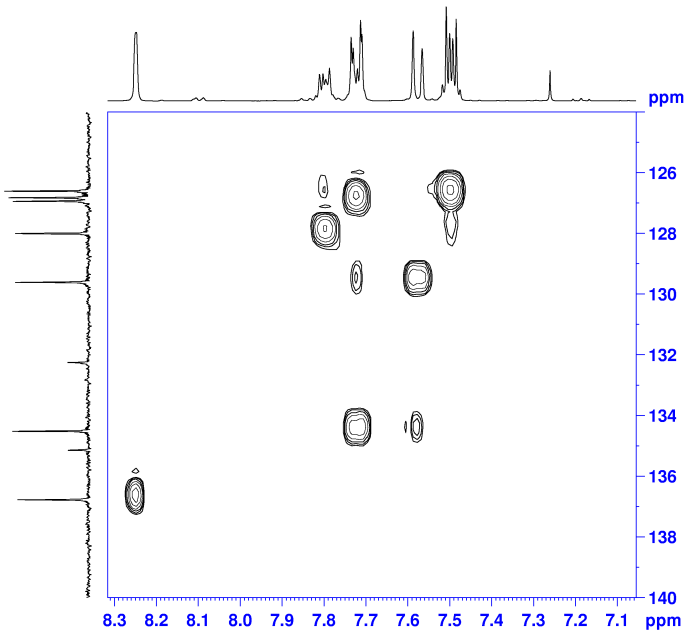


Figure S23. $^{1}H,^{13}C$-HSQC NMR spectrum of **9** (400.13 MHz, 300 K, $CDCl_3$).

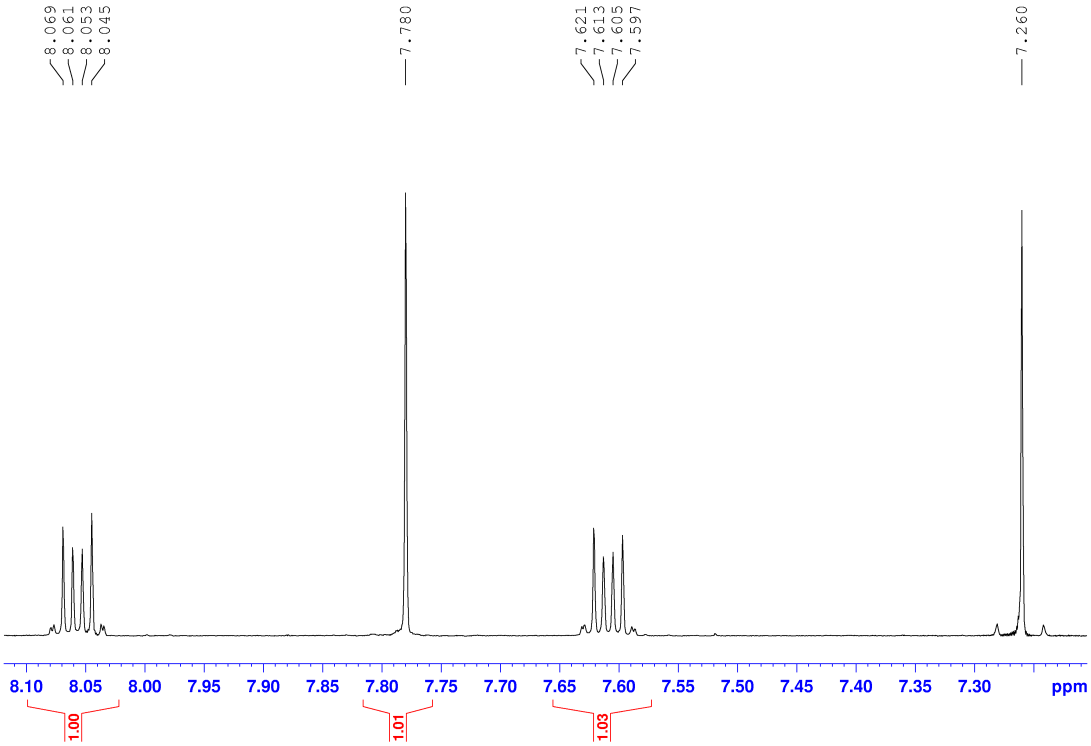


Figure S24. ^{1}H NMR spectrum of **10** (400.13 MHz, 300 K, $CDCl_3$).

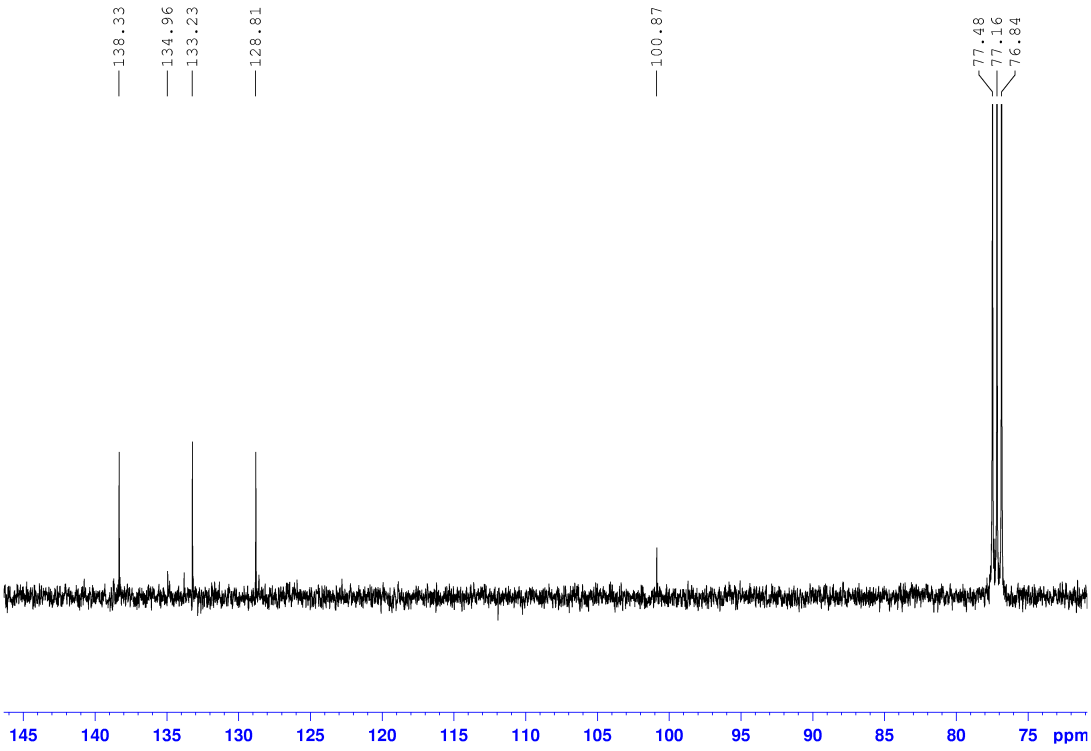


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of **10** (100.62 MHz, 300K, $CDCl_3$).

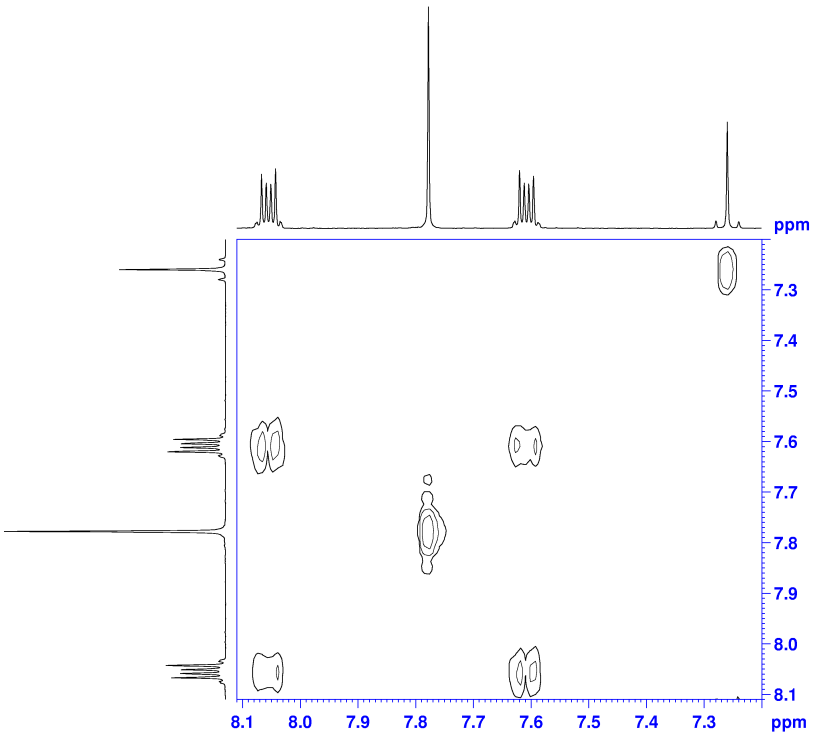


Figure S26. $^{1}H,^{1}H$-COSY NMR spectrum of **10** (400.13 MHz, 300 K, $CDCl_3$).

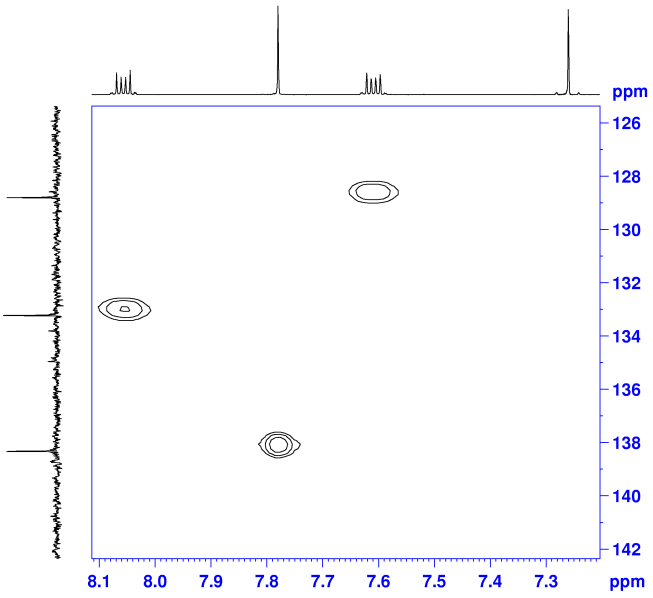
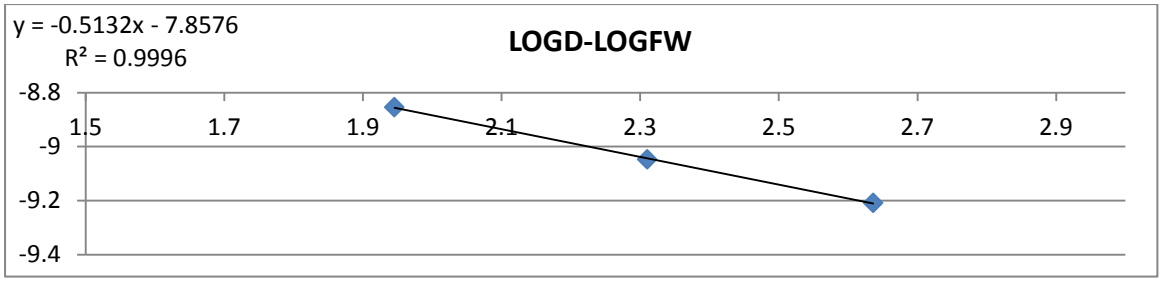


Figure S27. $^{1}H,^{13}C$-HSQC NMR spectrum of **10** (400.13 MHz, 300 K, $CDCl_3$).



			D1	D2	D3	FW	LOGFW	LOGD	Dav
Standards	Tetraphenylnaphthalene	**TPhN**	6.19E-10	6.34E-10	6.04E-10	432.55	2.636036316	-9.208309351	6.19E-10
	Phenylnaphthalene	**PhN**	8.65E-10	9.20E-10	9.06E-10	204.27	2.310204589	-9.0473044	8.97E-10
	TMS	**TMS**	1.40E-09			88.22	1.945567053	-8.854182286	1.40E-09
Sample	[KMgTMP2Bu]6	**5**	2.55E-10	2.52E-10	2.48E-10	**2478.742653**	3.39423144	-9.599519575	2.51E-10

entry	Possible species	fw(g/mol)	fw(g/mol) predicted (1H)	error %
1	[KMgTMP2Bu]6 (**5**)	2406.06	2478.74	-3.02

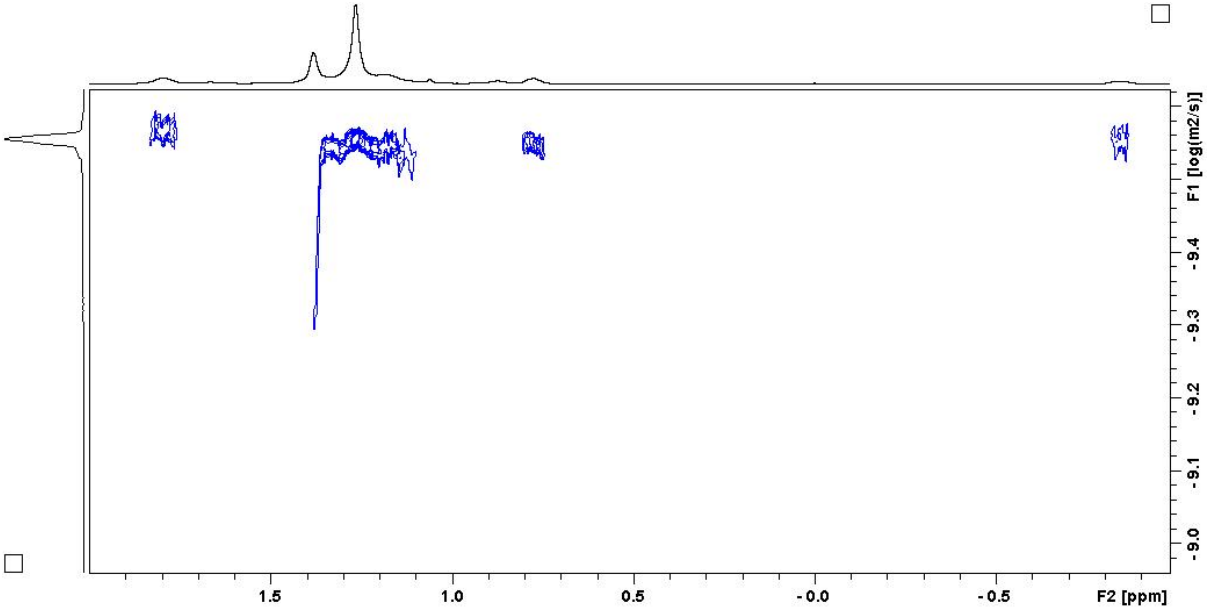
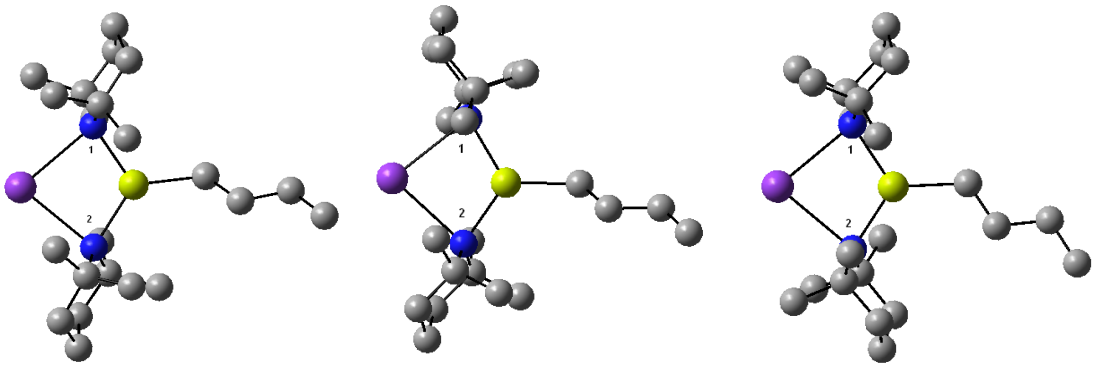


Figure S28. DOSY NMR spectrum of a 1:1 mixture of KTMP and ^{n}BuMgTMP (400.13 MHz, 300 K, *cyc*-C_6D_{12}) and calibration data.

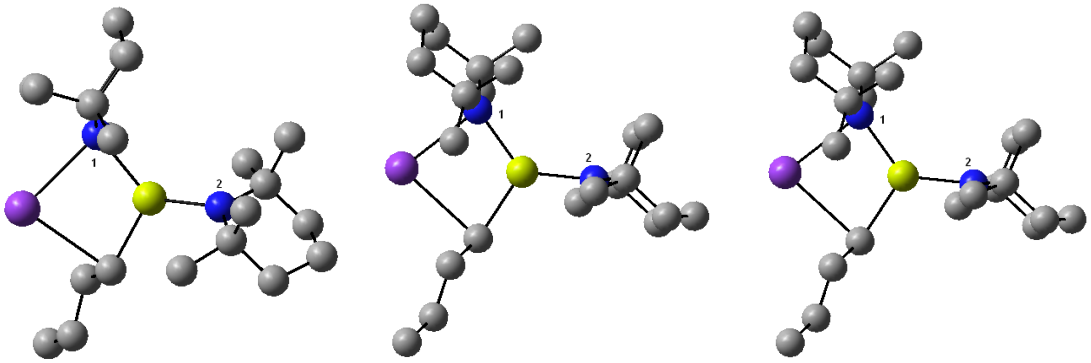
Electronic Energies, Selected Bond Distances/Angles, and XYZ Files for Optimized Structures



Model 1
E = -1774.9918934

Model 2
E = -1774.9897475

Model 3
E = -1774.9918603



Model 4
E = -1774. 9891223

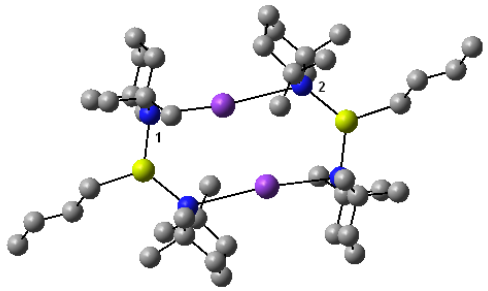
Model 5
E = -1774.990077

Model 6
E = -1774.9902278

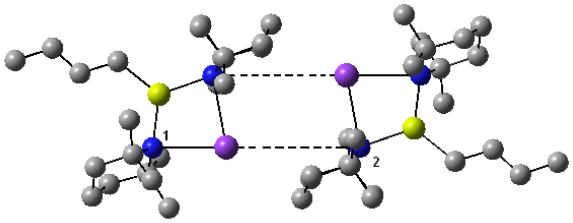
Figure S28. Optimized Geometries and Energies (a.u.) for [K(μ-TMP)$_2$Mg(^{n}Bu)] (Model 1-3) and [K(μ-TMP)(μ-^{n}Bu)MgTMP] (Model 4-6). Hydrogen atoms omitted for clarity.

Table S2. Principal Bond Lengths (Å) and Angles (°) for Models 1-6.

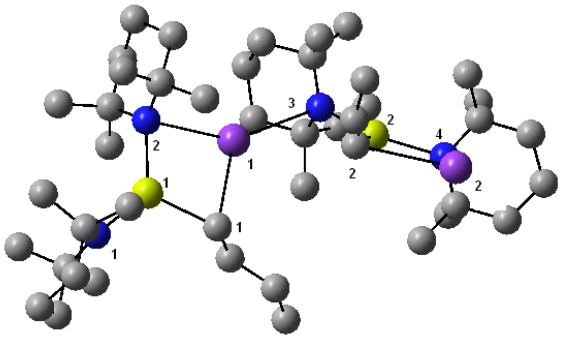
Bond Distances and Angles	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6
K-N_1	2.834	2.814	2.807	2.746	2.764	2.759
K-C				2.878	2.865	2.868
K-N_2	2.780	2.820	2.820			
Mg-N_1	2.123	2.167	2.155	2.148	2.146	2.146
Mg-C	2.152	2.152	2.151	2.240	2.231	2.231
Mg-N_2	2.177	2.164	2.157	2.030	2.022	2.024
N-K-C	79.7			80.0	80.3	79.4
N-K-N		80.8	80.2			
K-N_1-Mg	82.7	82.2	82.9	84.6	85.1	86.0
K-C-Mg				79.9	81.2	81.9
K-N_2-Mg	83.1	82.1	82.5			
C-Mg-N_1	118.2	120.9	120.4	111.0	112.0	110.5
N_1-Mg-N_2	113.7	114.9	114.4	131.1	132.2	131.3
C-Mg-N_2	127.8	123.9	125.1	116.9	115.6	118.2



Model 7
E = -3549.983362



Model 8
E = -3549.9934285

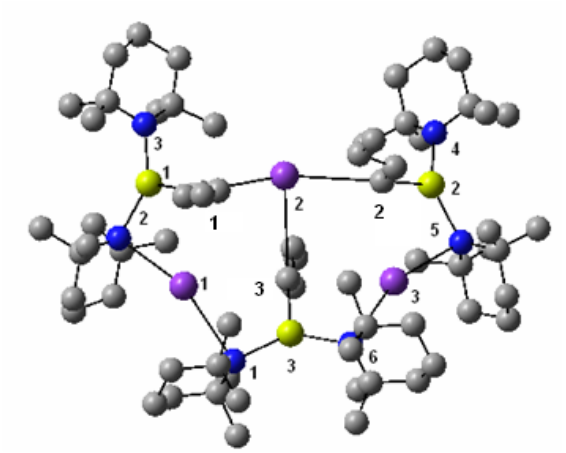


Model 9
E = -3549.9983491

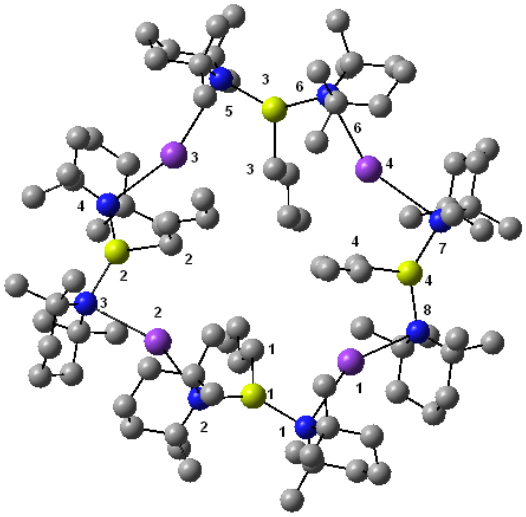
Figure S29. Optimized Geometries and Energies (a.u.) for $[K(\mu\text{-TMP})_2Mg(^{n}Bu)]_2$ (Model 7-9). Hydrogen atoms omitted for clarity.

Table S3. Principal Bond Lengths (Å) and Angles (°) for Models 7-9.

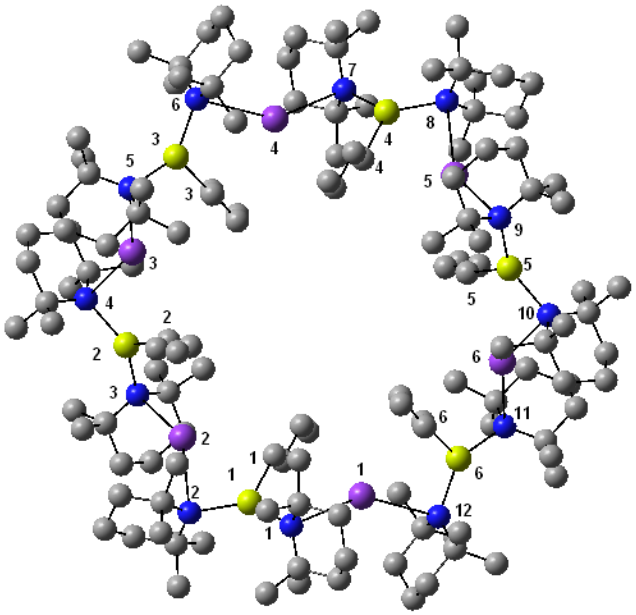
Bond Distances and Angles	Model 7	Model 8	Model 9
$K\text{-}N_1$	2.863	2.849	2.807
$K\text{-}C_1$			3.001
$K\text{-}N_2$	3.239	2.840	2.899
$K_1\text{-}N_3$			3.272
$K_1...C_2$			3.702
$K_2\text{-}C_2$			2.917
$K_2\text{-}N_4$			2.796
$Mg_2\text{-}N_3$			2.072
$Mg_2\text{-}N_4$			2.120
$Mg_2\text{-}C_2$			2.227
$Mg\text{-}N_1$	2.143	2.116	2.039
$Mg\text{-}C_1$	2.173	2.156	2.218
$Mg\text{-}N_2$	2.174	2.204	2.137
$N_2\text{-}K_1\text{-}C_1$			75.8
N-K-N	151.0	79.5	80.2
$K\text{-}N_1\text{-}Mg$	104.1	83.3	82.9
$K_1\text{-}N_2\text{-}Mg_1$			86.3
$K_1\text{-}C_1\text{-}Mg_1$			82.4
$K\text{-}N_2\text{-}Mg$	124.6	82.1	82.5
$K_1\text{-}N_3\text{-}Mg_2$			95.0
$N_4\text{-}K_2\text{-}C_2$			95.8
$C\text{-}Mg\text{-}N_1$	115.3	114.7	120.4
$N_2\text{-}Mg_1\text{-}C_1$			112.7
$N_1\text{-}Mg\text{-}N_2$	122.2	123.6	114.4
$K_2\text{-}N_4\text{-}Mg_2$			88.8
$K_2\text{-}C_2\text{-}Mg_2$			64.9
$N_4\text{-}Mg_2\text{-}C_2$			106.3
$C\text{-}Mg\text{-}N_2$	122.5	121.5	125.1



Model 10
E = -5325.0254799



Model 11
E = -7100.0557033



Model 12
E = -10650.083603

Figure S30. Optimized Geometry and Energy (a.u.) for $[K(\mu\text{-TMP})_2Mg(^n\text{Bu})]_3$ (Model 10), $[K(\mu\text{-TMP})_2Mg(^n\text{Bu})]_4$ (Model 11) and $[K(\mu\text{-TMP})_2Mg(^n\text{Bu})]_6$ (Model 12). Hydrogen atoms omitted for clarity.

Table S4. Principal Bond Lengths (Å) and Angles (°) for Models 10-12.

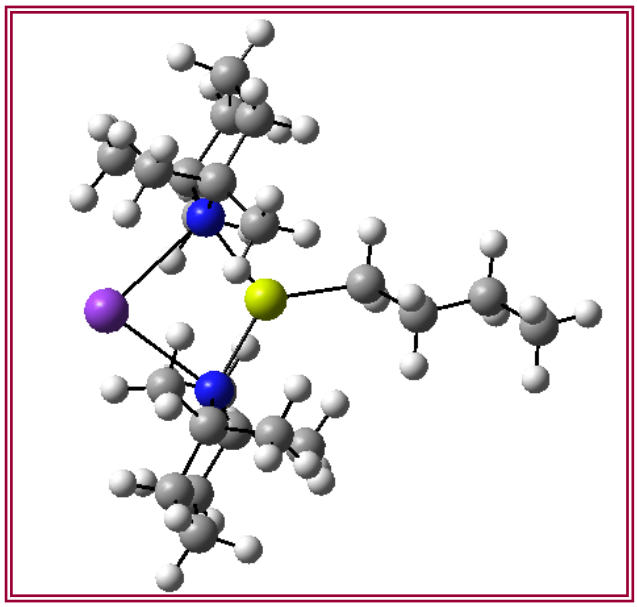
Bond Distances and Angles	Model 10	Model 11	Model 12
K1-N1	3.057	3.096	3.126
K1-N2	2.948		
K3-N4		3.077	3.145
K1-N8		3.094	
K3-N5		3.098	3.131
K5-N8			3.162
K1-N12			3.120
K5-N9			3.117
K1…C1	3.191	3.384	3.390
K1…C3	3.507		
K3…C2		3.281	3.359
K1…C4		3.285	
K3…C3		3.421	
K1…C6			3.267
K3…C3			3.291
K5…C5			3.275
Mg1-N2	2.109	2.103	2.099
Mg1-N3	2.046		
Mg1-N1		2.107	2.102
Mg3-N5		2.107	
Mg3-N6		2.101	2.098
Mg5-N9			2.099
Mg5-N10			2.099
Mg1-C1	2.238	2.209	2.215
Mg3-C3		2.209	2.214
Mg5-C5			2.216
K2-C1	3.182		
K2-C2	3.191		
K2-C3	3.374		
Mg2-N4	2.035		
Mg2-N5	2.112		
Mg2-C2	2.232		

K3-N5	2.947		
K3-N6	3.120		
K2-N2		3.088	3.145
K4-N6		3.082	3.155
K2-N3		3.096	3.131
K4-N7		3.107	3.119
K6-N10			3.181
K6-N11			3.116
K3…C2	3.287		
K3…C3	3.455		
K2…C1		3.304	3.380
K4…C3		3.265	3.380
K2…C2		3.419	3.295
K4…C4		3.451	3.327
K6…C5			3.402
K6…C6			3.266
Mg3-N6	2.096		
Mg3-N1	2.100		
Mg2-N3		2.102	2.101
Mg4-N7		2.107	2.100
Mg2-N4		2.106	2.098
Mg4-N8		2.102	2.099
Mg6-N11			2.099
Mg6-N12			2.099
Mg3-C3	2.225		
Mg2-C2		2.208	2.216
Mg4-C4		2.209	2.216
Mg6-C6			2.215

Table S5. Relatives Energies of Association (kcal·mol^{-1}) for [K(μ-TMP)$_2$Mg(^{n}Bu)]$_2$, [K(μ-TMP)$_2$Mg(^{n}Bu)]$_3$, [K(μ-TMP)$_2$Mg(^{n}Bu)]$_4$ and [K(μ-TMP)$_2$Mg(^{n}Bu)]$_6$.

	[K(TMP)$_2$Mg(^{n}Bu)]n	ΔE
Dimerisation	n = 2	-4.57
Trimerisation	n = 3	-10.42
Tetramerisation	n = 4	-13.83
Hexamerisation	n = 6	-13.83

XYZ Files for Optimized Structures

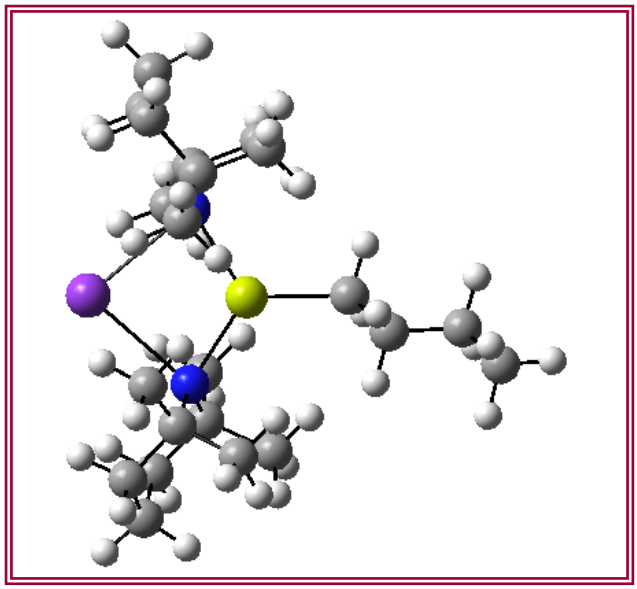


Model 1 E = -1774.9918934 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.746025	-0.967494	-2.482079
2	6	0	3.753573	-1.692376	-1.218111
3	6	0	-1.898605	-0.720845	-2.410396
4	6	0	3.155488	0.744966	-1.390771
5	6	0	2.572595	-0.689256	-1.211713
6	6	0	4.558731	-1.643834	0.077844
7	6	0	-3.901751	0.269303	-1.348498
8	6	0	-2.765204	-0.768467	-1.138057
9	6	0	-3.427568	-2.185529	-1.119283
10	6	0	3.612469	-1.930143	1.239203
11	6	0	-4.735549	0.477958	-0.087728
12	6	0	2.359569	-1.006671	1.288967
13	6	0	2.751020	0.356196	1.931359
14	6	0	-3.803468	0.924002	1.033914

15	6	0	-2.609119	-0.043253	1.282615
16	6	0	1.408261	-1.696224	2.298859
17	6	0	-1.627336	0.758704	2.165393
18	6	0	-3.100643	-1.241310	2.146840
19	1	0	2.369721	-0.891638	-3.380732
20	1	0	4.395820	-1.493999	-2.086576
21	1	0	1.316012	-1.979011	-2.465805
22	1	0	3.662141	0.837297	-2.360888
23	1	0	0.928992	-0.246632	-2.607315
24	1	0	-2.499253	-0.921889	-3.305728
25	1	0	3.353150	-2.711271	-1.344799
26	1	0	-1.442392	0.268669	-2.536888
27	1	0	-1.094385	-1.469035	-2.398081
28	1	0	2.359990	1.493680	-1.352569
29	1	0	5.369455	-2.384024	0.059462
30	1	0	3.889114	1.001266	-0.623142
31	1	0	-4.534840	-0.039842	-2.191784
32	1	0	-3.442742	1.227991	-1.626995
33	1	0	5.039585	-0.664978	0.197231
34	1	0	-4.029203	-2.350654	-2.022566
35	1	0	-2.677820	-2.991799	-1.103434
36	1	0	3.267532	-2.970976	1.132122
37	1	0	-5.509288	1.237148	-0.260926
38	1	0	-4.080989	-2.337149	-0.258321
39	1	0	3.474616	0.904528	1.326004
40	1	0	4.139298	-1.876106	2.201407
41	1	0	-5.268183	-0.443461	0.185488
42	1	0	-3.394702	1.906566	0.761270
43	1	0	1.298032	-2.770015	2.082702

44	1	0	1.868663	0.999721	2.039671
45	1	0	-1.266794	1.653253	1.641043
46	1	0	0.415974	-1.237080	2.313408
47	1	0	3.188019	0.221828	2.930217
48	1	0	-4.358368	1.063354	1.971933
49	1	0	-0.766168	0.161438	2.484263
50	1	0	-3.890804	-1.817592	1.657675
51	1	0	1.804812	-1.635947	3.318789
52	1	0	-2.267274	-1.926173	2.358697
53	1	0	-2.118711	1.105153	3.082389
54	1	0	-3.497074	-0.903217	3.113662
55	12	0	-0.025769	0.485335	-0.209715
56	7	0	1.671645	-0.865093	-0.028538
57	7	0	-1.905321	-0.470646	0.037995
58	19	0	-0.311362	-2.813829	-0.000184
59	6	0	-0.008678	2.551391	-0.810474
60	6	0	0.747973	3.594336	0.034109
61	1	0	-1.071738	2.853231	-0.851988
62	1	0	0.339764	2.646047	-1.856042
63	6	0	0.638869	5.045755	-0.468006
64	1	0	0.390094	3.570934	1.078091
65	1	0	1.817807	3.335069	0.091822
66	6	0	1.404089	6.059890	0.390353
67	1	0	1.005816	5.089974	-1.504041
68	1	0	-0.423254	5.328127	-0.512653
69	1	0	1.304686	7.081197	0.002152
70	1	0	1.036282	6.061288	1.424722
71	1	0	2.474980	5.821050	0.424889

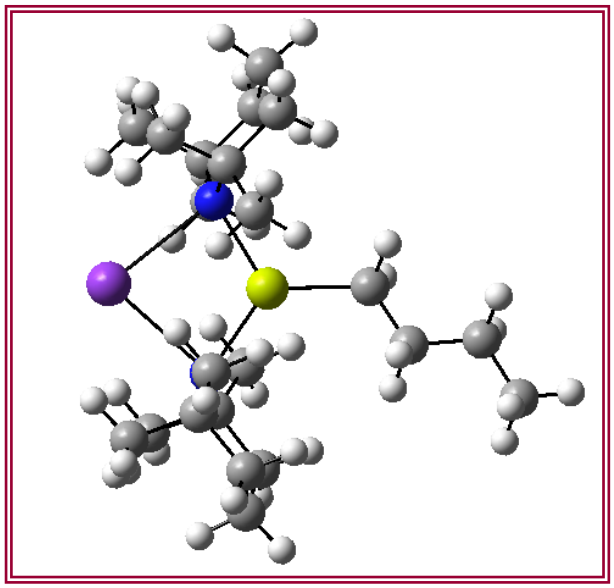


Model 2 E = -1774.9897475 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.345651	-1.225941	-2.402090
2	6	0	3.203624	-2.387407	-1.246051
3	6	0	-1.766240	0.151527	2.428471
4	6	0	3.248939	0.116270	-1.613246
5	6	0	2.342540	-1.096979	-1.237789
6	6	0	4.120036	-2.489911	-0.028258
7	6	0	-4.019707	-0.350560	1.530198
8	6	0	-2.680480	0.364659	1.211242
9	6	0	-2.931513	1.903582	1.162311
10	6	0	3.288584	-2.351196	1.245215
11	6	0	-4.965176	-0.386884	0.331701
12	6	0	2.394517	-1.078700	1.271038
13	6	0	3.281102	0.161523	1.597886
14	6	0	-4.243666	-1.011056	-0.860010
15	6	0	-2.886462	-0.330398	-1.193717

16	6	0	1.480947	-1.235109	2.502002
17	6	0	-2.215923	-1.235760	-2.246345
18	6	0	-3.155172	1.012900	-1.938510
19	1	0	1.870263	-1.406146	-3.347537
20	1	0	3.788154	-2.438831	-2.175072
21	1	0	0.647872	-2.059117	-2.252996
22	1	0	3.569435	0.045710	-2.661204
23	1	0	0.766219	-0.303250	-2.544834
24	1	0	-2.252631	0.493039	3.349556
25	1	0	2.526493	-3.257916	-1.251520
26	1	0	-1.506785	-0.905157	2.567595
27	1	0	-0.835365	0.728197	2.339752
28	1	0	2.700849	1.054773	-1.488440
29	1	0	4.657445	-3.447518	-0.030411
30	1	0	4.156417	0.177069	-1.010619
31	1	0	-4.503123	0.133020	2.390359
32	1	0	-3.797530	-1.386700	1.834840
33	1	0	4.890300	-1.709363	-0.066694
34	1	0	-3.203929	2.280827	2.157023
35	1	0	-2.028478	2.428225	0.834839
36	1	0	2.632984	-3.234919	1.327318
37	1	0	-5.870214	-0.960215	0.572701
38	1	0	-3.738695	2.187025	0.485167
39	1	0	4.130928	0.270942	0.923095
40	1	0	3.936744	-2.364045	2.132310
41	1	0	-5.304626	0.626838	0.084060
42	1	0	-4.048397	-2.071340	-0.626972
43	1	0	0.826512	-2.116621	2.435799
44	1	0	2.689635	1.080948	1.532013

45	1	0	-2.029888	-2.252282	-1.867929
46	1	0	0.856113	-0.354256	2.661935
47	1	0	3.688418	0.092300	2.615397
48	1	0	-4.887985	-1.002397	-1.750133
49	1	0	-1.271844	-0.820868	-2.605867
50	1	0	-3.821804	1.678528	-1.388308
51	1	0	2.082500	-1.372985	3.407681
52	1	0	-2.215884	1.551900	-2.101629
53	1	0	-2.868181	-1.353772	-3.119182
54	1	0	-3.619786	0.831281	-2.916812
55	12	0	0.015136	0.534808	-0.205491
56	7	0	1.567876	-0.953106	0.034380
57	7	0	-2.006957	-0.215214	0.008467
58	19	0	-0.655671	-2.660497	0.340915
59	6	0	0.382033	2.564370	-0.819209
60	6	0	1.306852	3.461126	0.026391
61	1	0	-0.588724	3.078377	-0.926412
62	1	0	0.787240	2.539001	-1.849050
63	6	0	1.513108	4.885336	-0.520851
64	1	0	0.915675	3.547553	1.054553
65	1	0	2.298868	2.992746	0.132285
66	6	0	2.431856	5.755529	0.344940
67	1	0	1.922927	4.817572	-1.539367
68	1	0	0.532470	5.372743	-0.622517
69	1	0	2.559757	6.760080	-0.077041
70	1	0	2.027691	5.871192	1.359058
71	1	0	3.428949	5.306266	0.439871



Model 3 E = -1774.9918603 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.304050	-0.784728	2.415911
2	6	0	3.522529	-0.710269	1.328591
3	6	0	-1.973856	-0.479110	-2.366438
4	6	0	2.291367	-2.891372	1.609921
5	6	0	2.120442	-1.377635	1.257105
6	6	0	4.397183	-1.051503	0.124846
7	6	0	-3.692733	1.063835	-1.493970
8	6	0	-2.899539	-0.231851	-1.164440
9	6	0	-3.904076	-1.428939	-1.164904
10	6	0	3.650186	-0.672785	-1.151499
11	6	0	-4.521751	1.563969	-0.313391
12	6	0	2.234931	-1.306232	-1.254747
13	6	0	2.380748	-2.798924	-1.681046
14	6	0	-3.604533	1.745184	0.893544

15	6	0	-2.786410	0.471421	1.246545
16	6	0	1.550439	-0.611106	-2.447067
17	6	0	-1.755644	0.914663	2.302432
18	6	0	-3.713814	-0.539703	1.986514
19	1	0	1.815932	-0.930214	3.374508
20	1	0	4.021445	-0.994198	2.265848
21	1	0	1.154194	0.294130	2.291702
22	1	0	2.705976	-3.009911	2.619443
23	1	0	0.318999	-1.261304	2.509988
24	1	0	-2.547741	-0.544834	-3.298303
25	1	0	3.378967	0.378510	1.358937
26	1	0	-1.252098	0.336346	-2.490939
27	1	0	-1.416814	-1.422030	-2.275256
28	1	0	1.325351	-3.420154	1.605689
29	1	0	5.350007	-0.509356	0.181101
30	1	0	2.951669	-3.425038	0.925643
31	1	0	-4.329179	0.897155	-2.374569
32	1	0	-2.967272	1.843025	-1.765750
33	1	0	4.655228	-2.119645	0.123280
34	1	0	-4.368910	-1.546090	-2.152514
35	1	0	-3.397884	-2.380411	-0.938984
36	1	0	3.532477	0.419111	-1.171105
37	1	0	-5.007445	2.515244	-0.566879
38	1	0	-4.711307	-1.317545	-0.440350
39	1	0	3.004825	-3.386984	-1.005073
40	1	0	4.238117	-0.944227	-2.039451
41	1	0	-5.334154	0.860114	-0.084925
42	1	0	-2.892273	2.550719	0.668107
43	1	0	1.366786	0.451750	-2.243714

44	1	0	1.393588	-3.281654	-1.729518
45	1	0	-1.020259	1.614357	1.883566
46	1	0	0.605390	-1.094393	-2.709371
47	1	0	2.828397	-2.877541	-2.680567
48	1	0	-4.180213	2.067123	1.772618
49	1	0	-1.230612	0.061171	2.739597
50	1	0	-4.607293	-0.811484	1.420813
51	1	0	2.189664	-0.657468	-3.336784
52	1	0	-3.165648	-1.466631	2.209133
53	1	0	-2.253145	1.440075	3.126244
54	1	0	-4.055181	-0.126014	2.944613
55	12	0	-0.016786	0.507667	-0.124813
56	7	0	1.410672	-1.105658	-0.024167
57	7	0	-2.072386	-0.108529	0.069057
58	19	0	-0.923223	-2.662299	0.267371
59	6	0	0.473875	2.573335	-0.469111
60	6	0	1.836265	3.118086	-0.003462
61	1	0	-0.320197	3.199459	-0.022528
62	1	0	0.383297	2.768912	-1.555167
63	6	0	2.100153	4.598421	-0.334596
64	1	0	1.943118	2.991254	1.087502
65	1	0	2.653151	2.521449	-0.442226
66	6	0	3.463101	5.109379	0.147274
67	1	0	2.018182	4.738467	-1.422605
68	1	0	1.300306	5.209774	0.108465
69	1	0	3.615778	6.166360	-0.103945
70	1	0	3.560427	5.009992	1.236267
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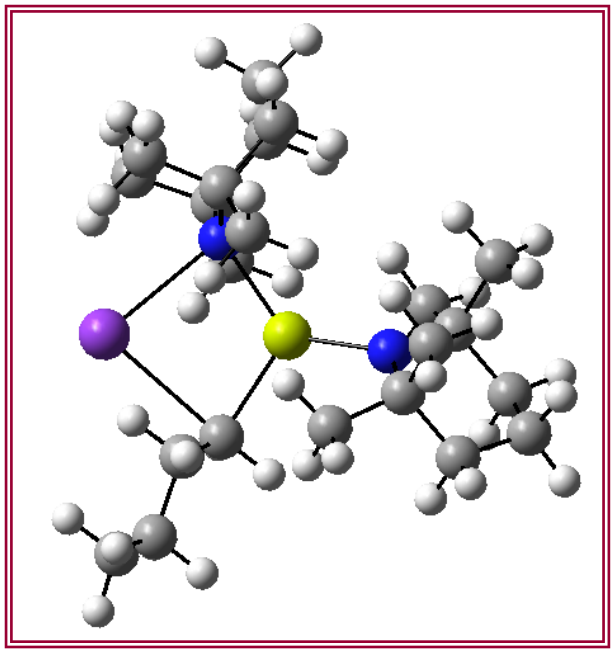

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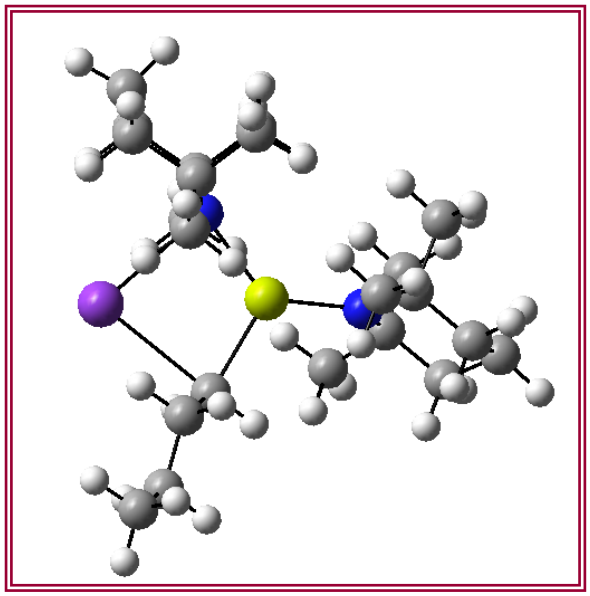
2	6	0	-3.962232	0.472483	-1.648278
3	6	0	2.089221	-0.027598	-2.059954
4	6	0	-3.266142	-1.937820	-1.251245
5	6	0	-2.783043	-0.455998	-1.247007
6	6	0	-4.949814	0.704388	-0.503215
7	6	0	1.906077	-2.511157	-1.867272
8	6	0	2.329311	-1.220280	-1.111623
9	6	0	3.878054	-1.264606	-0.906929
10	6	0	-4.196366	1.219361	0.725097
11	6	0	1.857851	-3.744479	-0.962283
12	6	0	-3.027187	0.286453	1.144406
13	6	0	-3.615172	-0.962497	1.870159
14	6	0	0.969799	-3.465614	0.253212

15	6	0	1.402910	-2.190457	1.024544
16	6	0	-2.212607	1.049420	2.210671
17	6	0	0.303776	-1.877059	2.054983
18	6	0	2.674832	-2.527674	1.865151
19	1	0	-2.159400	-0.610848	-3.348693
20	1	0	-4.478929	0.063127	-2.528382
21	1	0	-1.335802	0.665909	-2.443112
22	1	0	-3.529530	-2.267115	-2.265988
23	1	0	-0.906405	-1.056766	-2.192790
24	1	0	2.641470	-0.158589	-2.998209
25	1	0	-3.543751	1.444935	-1.946542
26	1	0	1.032171	0.073453	-2.328939
27	1	0	2.417056	0.920811	-1.618136
28	1	0	-2.468372	-2.588275	-0.875146
29	1	0	-5.719987	1.426153	-0.807417
30	1	0	-4.146615	-2.098886	-0.625015
31	1	0	2.577363	-2.684617	-2.720117
32	1	0	0.903525	-2.348623	-2.284562
33	1	0	-5.483808	-0.225228	-0.263898
34	1	0	4.394223	-1.278920	-1.875210
35	1	0	4.240297	-0.369655	-0.376870
36	1	0	-3.775590	2.206631	0.485554
37	1	0	1.470441	-4.605302	-1.522405
38	1	0	4.221014	-2.136453	-0.348409
39	1	0	-4.344145	-1.503325	1.262999
40	1	0	-4.886244	1.360957	1.569564
41	1	0	2.870880	-4.025123	-0.641810
42	1	0	-0.062759	-3.317276	-0.091069
43	1	0	-1.811775	1.984439	1.808271

44	1	0	-2.817190	-1.666559	2.129069
45	1	0	-0.654878	-1.682825	1.561966
46	1	0	-1.377997	0.441180	2.586655
47	1	0	-4.123784	-0.671344	2.799557
48	1	0	0.958679	-4.332592	0.928663
49	1	0	0.565555	-0.996876	2.664640
50	1	0	3.512702	-2.896132	1.271230
51	1	0	-2.838010	1.296863	3.077394
52	1	0	3.027178	-1.645604	2.423171
53	1	0	0.157250	-2.711631	2.751097
54	1	0	2.446692	-3.298565	2.612111
55	12	0	-0.141740	0.328208	0.047364
56	7	0	-2.139599	-0.027742	0.007878
57	7	0	1.535387	-1.010790	0.129034
58	19	0	2.768986	1.029947	1.490297
59	1	0	1.262402	3.163386	-1.477183
60	6	0	1.487977	3.286641	-0.407023
61	6	0	0.499064	2.441103	0.422305
62	6	0	1.509146	4.793967	-0.089798
63	1	0	2.537530	2.928586	-0.318601
64	1	0	0.648522	2.693337	1.497561
65	1	0	-0.497742	2.869359	0.226868
66	6	0	2.490177	5.598416	-0.950111
67	1	0	0.492650	5.189994	-0.218384
68	1	0	1.751708	4.933115	0.975390
69	1	0	2.476324	6.663918	-0.692604
70	1	0	3.520841	5.240580	-0.821060
71	1	0	2.244523	5.511111	-2.015784

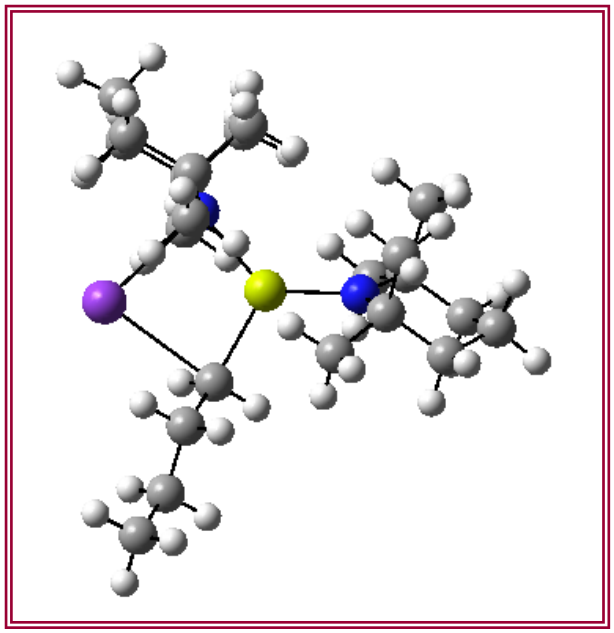


Model 5 E = -1774.990077 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.430201	5.742250	0.785193
2	1	0	1.244519	6.962208	0.295768
3	1	0	0.892546	5.877118	1.649382
4	6	0	1.355966	5.932982	0.656514
5	6	0	0.721814	4.922102	-0.305681
6	1	0	1.176712	5.025864	-1.303399
7	1	0	2.716064	0.307906	3.009526
8	1	0	1.928003	3.267117	0.329671
9	1	0	-0.343652	5.154635	-0.437818
10	1	0	0.402292	3.373460	1.157285
11	6	0	0.847024	3.457289	0.153505
12	1	0	2.837331	1.124135	1.457605
13	6	0	2.259387	0.374362	2.015368
14	1	0	1.248474	0.776435	2.151175
15	1	0	4.184371	-1.612661	2.151010

16	1	0	1.980744	-1.864258	3.331692
17	1	0	4.304786	-0.616843	0.705519
18	6	0	3.734136	-1.445538	1.163033
19	1	0	-1.802551	1.398958	2.105763
20	1	0	-2.230231	0.223744	3.367025
21	6	0	2.250837	-1.005511	1.320415
22	6	0	1.559736	-1.978144	2.324007
23	1	0	-0.835039	-0.083551	2.346428
24	1	0	0.573374	2.583977	-1.811124
25	6	0	0.207004	2.402893	-0.774305
26	19	0	2.811390	1.289859	-1.205070
27	6	0	-1.854630	0.328755	2.341612
28	1	0	0.486458	-1.776788	2.380552
29	1	0	4.958503	-2.914901	0.135105
30	1	0	-0.857525	2.674710	-0.856759
31	1	0	1.678199	-3.026736	2.045894
32	6	0	3.894710	-2.686722	0.282989
33	1	0	3.464737	-3.562327	0.784773
34	7	0	1.576954	-0.867641	0.002659
35	12	0	-0.216380	0.298763	-0.164728
36	1	0	-4.079774	1.295773	1.469404
37	1	0	-3.075300	-2.001914	2.822399
38	1	0	3.758873	-1.679013	-1.611824
39	6	0	-2.749925	-0.408636	1.323603
40	1	0	-4.603287	-0.087388	2.435334
41	6	0	3.205929	-2.464069	-1.064310
42	6	0	-4.171885	0.199973	1.466034
43	7	0	-2.172308	-0.190435	-0.013449
44	6	0	-2.790901	-1.901651	1.765415

45	1	0	-1.804667	-2.359873	1.631754
46	6	0	1.723072	-2.020695	-0.923736
47	1	0	1.220405	-3.805597	0.299346
48	1	0	3.270320	-3.368380	-1.684675
49	1	0	1.835040	-0.728076	-2.716177
50	1	0	-2.295025	1.390364	-2.188406
51	6	0	0.850497	-3.262344	-0.572217
52	1	0	-3.505458	-2.487983	1.181541
53	1	0	-0.176220	-2.948653	-0.359833
54	6	0	1.254950	-1.578568	-2.327039
55	1	0	-4.359406	1.294661	-1.029822
56	6	0	-5.100144	-0.198410	0.318961
57	1	0	-6.075205	0.295460	0.428691
58	1	0	0.196259	-1.296023	-2.330525
59	6	0	-3.032686	-0.409149	-1.188792
60	6	0	-2.403883	0.320902	-2.394506
61	6	0	-4.450319	0.199088	-1.006389
62	1	0	-1.411608	-0.082947	-2.641745
63	1	0	0.827082	-3.974822	-1.407493
64	1	0	-5.301211	-1.278076	0.342098
65	1	0	1.366904	-2.391388	-3.053761
66	1	0	-2.180231	-2.358515	-1.710675
67	1	0	-3.020216	0.203349	-3.294569
68	6	0	-3.171953	-1.905380	-1.599207
69	1	0	-3.716344	-2.493378	-0.855652
70	1	0	-5.088521	-0.086931	-1.854452
71	1	0	-3.705500	-2.012221	-2.554286

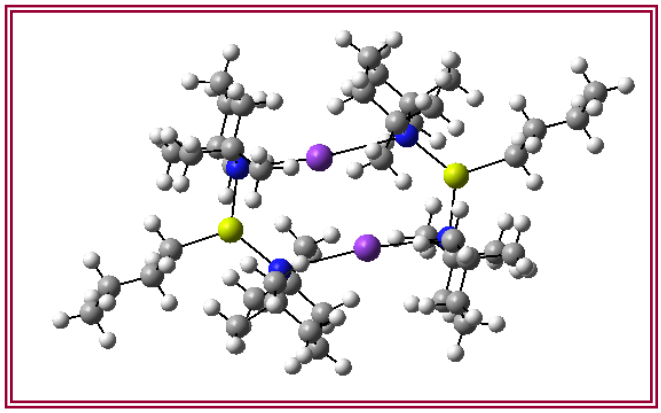


Model 6 E = -1774.9902278 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.032025	6.149270	0.165802
2	6	0	-0.041723	4.946823	-0.784852
3	6	0	0.072733	3.585508	-0.073153
4	19	0	2.752170	1.854884	-0.151851
5	6	0	1.483143	-0.099937	2.405029
6	6	0	-2.400289	1.193444	1.703443
7	6	0	0.053764	2.341177	-0.987480
8	6	0	3.528502	-1.302781	1.648211
9	6	0	1.999445	-1.159928	1.407630
10	6	0	-2.922853	-0.129957	1.108843
11	12	0	-0.208308	0.238366	-0.290520
12	6	0	-2.865204	-1.186709	2.252068
13	7	0	1.700287	-0.688851	0.030840
14	6	0	-4.408707	0.122863	0.730038
15	6	0	4.230234	-2.125445	0.565983

16	6	0	1.292711	-2.485039	1.820437
17	7	0	-2.092255	-0.465421	-0.060015
18	6	0	3.903336	-1.561087	-0.818003
19	6	0	2.374104	-1.424859	-1.069381
20	6	0	2.202400	-0.623103	-2.380206
21	6	0	-4.993348	-0.983178	-0.147299
22	6	0	-2.630473	-1.419834	-1.044192
23	6	0	-4.119213	-1.143620	-1.390341
24	6	0	1.804321	-2.845407	-1.365969
25	6	0	-1.835854	-1.235875	-2.353796
26	6	0	-2.473779	-2.914311	-0.634065
27	1	0	-0.118718	7.097425	-0.377597
28	1	0	0.896660	6.188000	0.751650
29	1	0	-0.865360	6.096595	0.877321
30	1	0	-0.966677	4.950606	-1.377513
31	1	0	0.779805	5.043853	-1.512233
32	1	0	-0.744791	3.509382	0.657602
33	1	0	0.985736	3.633644	0.562234
34	1	0	-0.903077	2.384191	-1.535718
35	1	0	0.797833	2.497293	-1.801145
36	1	0	0.230445	-2.436395	1.561820
37	1	0	1.375198	-2.652823	2.902603
38	1	0	1.715493	-3.363295	1.329042
39	1	0	2.182580	-3.228734	-2.322901
40	1	0	0.712885	-2.818396	-1.417666
41	1	0	2.074986	-3.576050	-0.601694
42	1	0	2.656239	-1.155190	-3.223981
43	1	0	1.148353	-0.458743	-2.631560
44	1	0	2.685750	0.363516	-2.340226

45	1	0	-2.739459	-3.589467	-1.459723
46	1	0	-3.105711	-3.180550	0.217398
47	1	0	-1.435857	-3.116651	-0.347475
48	1	0	-1.912063	-0.200852	-2.709359
49	1	0	-0.774703	-1.485274	-2.212475
50	1	0	-2.201459	-1.897316	-3.149061
51	1	0	-1.823094	-1.394880	2.520874
52	1	0	-3.323926	-2.137190	1.966547
53	1	0	-3.384808	-0.832204	3.153485
54	1	0	-6.024058	-0.735690	-0.435617
55	1	0	-5.051779	-1.928334	0.409339
56	1	0	-4.465512	1.068987	0.172618
57	1	0	-5.007669	0.253671	1.642384
58	1	0	-4.171283	-0.210766	-1.970426
59	1	0	-4.503884	-1.944342	-2.037841
60	1	0	4.371771	-0.563369	-0.907431
61	1	0	4.360812	-2.177817	-1.603656
62	1	0	5.315804	-2.126503	0.730790
63	1	0	3.914900	-3.174235	0.628495
64	1	0	3.979918	-0.293587	1.667122
65	1	0	3.715330	-1.733762	2.641265
66	1	0	1.932887	0.890930	2.241947
67	1	0	1.716036	-0.384259	3.437678
68	1	0	0.394052	0.011262	2.347490
69	1	0	-1.357956	1.103446	2.043355
70	1	0	-2.987976	1.499401	2.578095
71	1	0	-2.448765	1.993094	0.957307



Model 7 E = -3549.983362 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.524035	-4.980385	-0.354463
2	1	0	-2.401338	-5.080196	1.403200
3	1	0	-0.096442	-4.956882	-0.382056
4	6	0	-2.477324	-4.384019	0.566453
5	1	0	-0.104355	-5.554785	2.027104
6	1	0	-3.438388	-3.865122	0.671790
7	1	0	-7.005525	-0.049018	-0.026953
8	1	0	-1.511889	-3.237971	-1.664101
9	1	0	1.538786	-5.214341	1.518966
10	1	0	-5.521032	-0.637067	-1.726027
11	6	0	0.030877	-4.165622	0.368890
12	6	0	0.556181	-4.751818	1.678781
13	1	0	-1.743646	-4.838802	3.282232
14	1	0	-6.129403	-0.861729	1.284867
15	1	0	-2.411959	-2.005468	-0.777770
16	1	0	-4.583190	-1.629250	-0.611733
17	6	0	-1.295607	-3.370726	0.519662
18	6	0	-6.221088	0.076158	0.731177

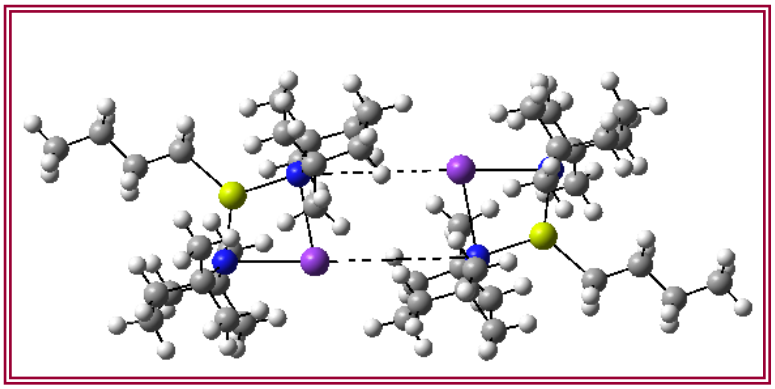
19	6	0	-1.479496	-2.577129	-0.789590
20	1	0	0.799645	-3.493936	-0.042899
21	1	0	-2.621204	-3.425808	3.867190
22	1	0	-5.955677	1.811281	-1.257861
23	6	0	-4.667457	-0.621231	-1.038648
24	1	0	-6.571894	0.836419	1.430331
25	6	0	-1.627722	-3.858783	3.749481
26	1	0	-3.773557	-0.437674	-1.651184
27	1	0	-0.643251	-1.880007	-0.944769
28	1	0	0.967064	-4.077532	3.701323
29	6	0	-4.866019	0.445707	0.057039
30	6	0	0.644892	-3.654701	2.740706
31	1	0	-1.208899	-4.030239	4.750165
32	6	0	-5.031631	1.812580	-0.663836
33	7	0	-1.265546	-2.391067	1.642833
34	6	0	-0.702645	-2.906140	2.932419
35	1	0	-4.207772	1.940167	-1.389451
36	1	0	-5.914341	2.980878	0.931694
37	1	0	1.441762	-2.944955	2.457855
38	1	0	-5.594001	1.780226	2.834596
39	6	0	-5.017295	2.999934	0.300640
40	1	0	-5.058427	3.944588	-0.257127
41	7	0	-3.670676	0.440284	0.952528
42	12	0	-3.180237	-1.403029	1.928962
43	1	0	-4.554913	0.581456	3.596945
44	6	0	-4.561732	1.562351	3.113236
45	6	0	-0.449657	-1.692973	3.849355
46	1	0	0.049592	-1.994925	4.777777
47	1	0	-1.391138	-1.208365	4.137633

48	6	0	-3.582075	1.592522	1.899274
49	1	0	-4.323172	-2.204851	4.310359
50	6	0	-3.759120	2.951903	1.169464
51	1	0	0.174630	-0.928865	3.364894
52	1	0	-4.268062	2.313380	3.858514
53	6	0	-4.704221	-2.174667	3.271958
54	1	0	-5.503253	-1.416150	3.308837
55	1	0	-3.765971	3.770852	1.901847
56	1	0	-2.884522	3.131865	0.523857
57	1	0	-2.007365	0.678142	3.132562
58	6	0	-2.173254	1.577529	2.526190
59	1	0	-1.379229	1.613605	1.770644
60	1	0	-4.612443	-4.333636	2.943404
61	6	0	-5.369007	-3.533551	2.976534
62	1	0	-2.024330	2.438052	3.188742
63	1	0	-5.819890	-3.521783	1.968939
64	1	0	-6.021959	-3.988849	4.985431
65	1	0	-7.236577	-3.180586	4.009285
66	6	0	-6.459634	-3.958165	3.976720
67	6	0	-7.101978	-5.312745	3.655167
68	1	0	-6.352969	-6.115321	3.650102
69	1	0	-7.575697	-5.301628	2.664941
70	1	0	-7.872256	-5.583223	4.387833
71	19	0	-1.484759	0.878922	-0.844117
72	1	0	2.524035	4.980385	0.354463
73	1	0	2.401338	5.080196	-1.403200
74	1	0	0.096442	4.956882	0.382056
75	6	0	2.477324	4.384019	-0.566453
76	1	0	0.104355	5.554785	-2.027104

77	1	0	3.438388	3.865122	-0.671790
78	1	0	7.005525	0.049018	0.026953
79	1	0	1.511889	3.237971	1.664101
80	1	0	-1.538786	5.214341	-1.518966
81	1	0	5.521032	0.637067	1.726027
82	6	0	-0.030877	4.165622	-0.368890
83	6	0	-0.556181	4.751818	-1.678781
84	1	0	1.743646	4.838802	-3.282232
85	1	0	6.129403	0.861729	-1.284867
86	1	0	2.411959	2.005468	0.777770
87	1	0	4.583190	1.629250	0.611733
88	6	0	1.295607	3.370726	-0.519662
89	6	0	6.221088	-0.076158	-0.731177
90	6	0	1.479496	2.577129	0.789590
91	1	0	-0.799645	3.493936	0.042899
92	1	0	2.621204	3.425808	-3.867190
93	1	0	5.955677	-1.811281	1.257861
94	6	0	4.667457	0.621231	1.038648
95	1	0	6.571894	-0.836419	-1.430331
96	6	0	1.627722	3.858783	-3.749481
97	1	0	3.773557	0.437674	1.651184
98	1	0	0.643251	1.880007	0.944769
99	1	0	-0.967064	4.077532	-3.701323
100	6	0	4.866019	-0.445707	-0.057039
101	6	0	-0.644892	3.654701	-2.740706
102	1	0	1.208899	4.030239	-4.750165
103	6	0	5.031631	-1.812580	0.663836
104	7	0	1.265546	2.391067	-1.642833
105	6	0	0.702645	2.906140	-2.932419

106	1	0	4.207772	-1.940167	1.389451
107	1	0	5.914341	-2.980878	-0.931694
108	1	0	-1.441762	2.944955	-2.457855
109	1	0	5.594001	-1.780226	-2.834596
110	6	0	5.017295	-2.999934	-0.300640
111	1	0	5.058427	-3.944588	0.257127
112	7	0	3.670676	-0.440284	-0.952528
113	12	0	3.180237	1.403029	-1.928962
114	1	0	4.554913	-0.581456	-3.596945
115	6	0	4.561732	-1.562351	-3.113236
116	6	0	0.449657	1.692973	-3.849355
117	1	0	-0.049592	1.994925	-4.777777
118	1	0	1.391138	1.208365	-4.137633
119	6	0	3.582075	-1.592522	-1.899274
120	1	0	4.323172	2.204851	-4.310359
121	6	0	3.759120	-2.951903	-1.169464
122	1	0	-0.174630	0.928865	-3.364894
123	1	0	4.268062	-2.313380	-3.858514
124	6	0	4.704221	2.174667	-3.271958
125	1	0	5.503253	1.416150	-3.308837
126	1	0	3.765971	-3.770852	-1.901847
127	1	0	2.884522	-3.131865	-0.523857
128	1	0	2.007365	-0.678142	-3.132562
129	6	0	2.173254	-1.577529	-2.526190
130	1	0	1.379229	-1.613605	-1.770644
131	1	0	4.612443	4.333636	-2.943404
132	6	0	5.369007	3.533551	-2.976534
133	1	0	2.024330	-2.438052	-3.188742
134	1	0	5.819890	3.521783	-1.968939

135	1	0	6.021959	3.988849	-4.985431
136	1	0	7.236577	3.180586	-4.009285
137	6	0	6.459634	3.958165	-3.976720
138	6	0	7.101978	5.312745	-3.655167
139	1	0	6.352969	6.115321	-3.650102
140	1	0	7.575697	5.301628	-2.664941
141	1	0	7.872256	5.583223	-4.387833
142	19	0	1.484759	-0.878922	0.844117



Model 8 E = -3549.9934285 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.804163	1.638234	-1.949577
2	6	0	-1.054017	2.729152	-0.573996
3	6	0	-5.011555	-1.222651	-2.257595
4	6	0	-3.412587	3.586251	-0.552937
5	6	0	-2.543658	2.291047	-0.579923
6	6	0	-0.618062	3.251279	0.793467
7	6	0	-6.884120	-2.561042	-1.342656
8	6	0	-5.390663	-2.194103	-1.125174
9	6	0	-4.553050	-3.490892	-1.374926
10	6	0	-0.871967	2.167258	1.836462
11	6	0	-7.456051	-3.370379	-0.181943
12	6	0	-2.331858	1.616878	1.841720
13	6	0	-3.243431	2.602308	2.630335
14	6	0	-7.277504	-2.565748	1.102230
15	6	0	-5.809793	-2.124037	1.369545
16	6	0	-2.254471	0.330267	2.696497
17	6	0	-5.908831	-1.057918	2.481891
18	6	0	-5.023515	-3.318670	1.986093
19	1	0	-2.540638	2.319440	-2.767425

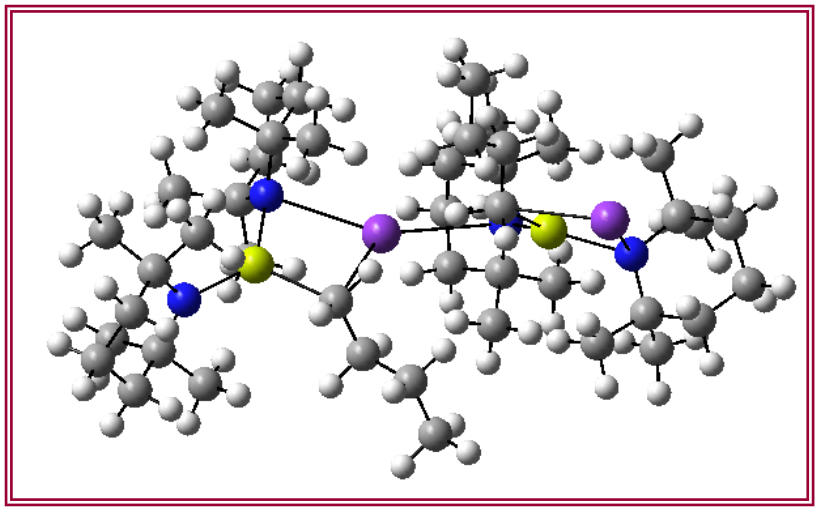
20	1	0	-0.886003	3.483309	-1.354865
21	1	0	-2.208794	0.723834	-2.075301
22	1	0	-3.248620	4.175939	-1.464777
23	1	0	-3.861596	1.383941	-2.083730
24	1	0	-5.201181	-1.668569	-3.241402
25	1	0	-0.448076	1.845168	-0.844156
26	1	0	-5.602416	-0.299576	-2.199167
27	1	0	-3.947247	-0.953223	-2.234434
28	1	0	-4.474724	3.340901	-0.496031
29	1	0	0.442567	3.553758	0.794385
30	1	0	-3.180842	4.237593	0.292265
31	1	0	-6.997041	-3.102684	-2.291943
32	1	0	-7.457416	-1.628653	-1.435685
33	1	0	-1.169309	4.165021	1.043228
34	1	0	-4.771395	-3.910849	-2.365265
35	1	0	-3.470528	-3.293811	-1.362358
36	1	0	-0.199679	1.317499	1.622527
37	1	0	-8.519930	-3.581329	-0.350202
38	1	0	-4.748670	-4.272800	-0.639171
39	1	0	-3.309785	3.582297	2.155086
40	1	0	-0.609805	2.521263	2.842314
41	1	0	-6.959516	-4.347673	-0.106795
42	1	0	-7.895148	-1.661176	1.022147
43	1	0	-1.446051	-0.334739	2.359112
44	1	0	-4.264802	2.208055	2.693968
45	1	0	-6.467892	-0.177014	2.141133
46	1	0	-3.194281	-0.226296	2.682017
47	1	0	-2.880110	2.754151	3.655558
48	1	0	-7.650656	-3.127035	1.969954

49	1	0	-4.924655	-0.739654	2.840968
50	1	0	-4.983729	-4.188572	1.325641
51	1	0	-2.036649	0.565537	3.744589
52	1	0	-3.988872	-3.020867	2.210025
53	1	0	-6.442830	-1.452838	3.354205
54	1	0	-5.475524	-3.649340	2.930778
55	12	0	-4.919970	0.576382	0.279389
56	7	0	-2.840860	1.280043	0.480374
57	7	0	-5.134805	-1.526358	0.180524
58	19	0	-2.287086	-1.481679	0.119130
59	6	0	-6.556748	1.957297	0.031062
60	6	0	-8.002321	1.441455	0.157736
61	1	0	-6.463488	2.434911	-0.962751
62	1	0	-6.428410	2.795361	0.740631
63	6	0	-9.094013	2.505089	-0.058934
64	1	0	-8.177219	0.622179	-0.559017
65	1	0	-8.164151	0.992408	1.152117
66	6	0	-10.522623	1.964695	0.075281
67	1	0	-8.941120	3.322915	0.660464
68	1	0	-8.961681	2.952155	-1.055181
69	1	0	-11.272410	2.749176	-0.085255
70	1	0	-10.715213	1.167704	-0.654568
71	1	0	-10.694095	1.541784	1.073705
72	6	0	2.804163	-1.638234	1.949577
73	6	0	1.054017	-2.729152	0.573996
74	6	0	5.011555	1.222651	2.257595
75	6	0	3.412587	-3.586251	0.552937
76	6	0	2.543658	-2.291047	0.579923
77	6	0	0.618062	-3.251279	-0.793467

78	6	0	6.884120	2.561042	1.342656
79	6	0	5.390663	2.194103	1.125174
80	6	0	4.553050	3.490892	1.374926
81	6	0	0.871967	-2.167258	-1.836462
82	6	0	7.456051	3.370379	0.181943
83	6	0	2.331858	-1.616878	-1.841720
84	6	0	3.243431	-2.602308	-2.630335
85	6	0	7.277504	2.565748	-1.102230
86	6	0	5.809793	2.124037	-1.369545
87	6	0	2.254471	-0.330267	-2.696497
88	6	0	5.908831	1.057918	-2.481891
89	6	0	5.023515	3.318670	-1.986093
90	1	0	2.540638	-2.319440	2.767425
91	1	0	0.886003	-3.483309	1.354865
92	1	0	2.208794	-0.723834	2.075301
93	1	0	3.248620	-4.175939	1.464777
94	1	0	3.861596	-1.383941	2.083730
95	1	0	5.201181	1.668569	3.241402
96	1	0	0.448076	-1.845168	0.844156
97	1	0	5.602416	0.299576	2.199167
98	1	0	3.947247	0.953223	2.234434
99	1	0	4.474724	-3.340901	0.496031
100	1	0	-0.442567	-3.553758	-0.794385
101	1	0	3.180842	-4.237593	-0.292265
102	1	0	6.997041	3.102684	2.291943
103	1	0	7.457416	1.628653	1.435685
104	1	0	1.169309	-4.165021	-1.043228
105	1	0	4.771395	3.910849	2.365265
106	1	0	3.470528	3.293811	1.362358

107	1	0	0.199679	-1.317499	-1.622527
108	1	0	8.519930	3.581329	0.350202
109	1	0	4.748670	4.272800	0.639171
110	1	0	3.309785	-3.582297	-2.155086
111	1	0	0.609805	-2.521263	-2.842314
112	1	0	6.959516	4.347673	0.106795
113	1	0	7.895148	1.661176	-1.022147
114	1	0	1.446051	0.334739	-2.359112
115	1	0	4.264802	-2.208055	-2.693968
116	1	0	6.467892	0.177014	-2.141133
117	1	0	3.194281	0.226296	-2.682017
118	1	0	2.880110	-2.754151	-3.655558
119	1	0	7.650656	3.127035	-1.969954
120	1	0	4.924655	0.739654	-2.840968
121	1	0	4.983729	4.188572	-1.325641
122	1	0	2.036649	-0.565537	-3.744589
123	1	0	3.988872	3.020867	-2.210025
124	1	0	6.442830	1.452838	-3.354205
125	1	0	5.475524	3.649340	-2.930778
126	12	0	4.919970	-0.576382	-0.279389
127	7	0	2.840860	-1.280043	-0.480374
128	7	0	5.134805	1.526358	-0.180524
129	19	0	2.287086	1.481679	-0.119130
130	6	0	6.556748	-1.957297	-0.031062
131	6	0	8.002321	-1.441455	-0.157736
132	1	0	6.463488	-2.434911	0.962751
133	1	0	6.428410	-2.795361	-0.740631
134	6	0	9.094013	-2.505089	0.058934
135	1	0	8.177219	-0.622179	0.559017

136	1	0	8.164151	-0.992408	-1.152117
137	6	0	10.522623	-1.964695	-0.075281
138	1	0	8.941120	-3.322915	-0.660464
139	1	0	8.961681	-2.952155	1.055181
140	1	0	11.272410	-2.749176	0.085255
141	1	0	10.715213	-1.167704	0.654568
142	1	0	10.694095	-1.541784	-1.073705



Model 9 E = -3549.9983491 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.189345	2.007893	3.873289
2	1	0	-4.971980	2.854692	2.543573
3	1	0	-2.226583	3.416998	3.229606
4	6	0	-4.399605	1.960146	2.796137
5	1	0	0.992199	-0.040844	5.613898
6	1	0	0.629158	-1.706976	6.087025
7	1	0	-3.817705	4.605918	1.730934
8	1	0	-5.047524	1.098494	2.615479
9	1	0	-7.845898	-0.939641	2.303258
10	1	0	2.309435	-1.194574	5.862578
11	6	0	1.288870	-1.086852	5.469856
12	1	0	-2.163986	0.902031	3.734523
13	1	0	-2.191239	5.197471	1.444929
14	1	0	-5.892832	-2.253752	2.966217
15	6	0	-2.270141	3.150284	2.164049
16	6	0	-2.833794	4.312515	1.343583
17	1	0	-5.519725	3.408908	0.725147

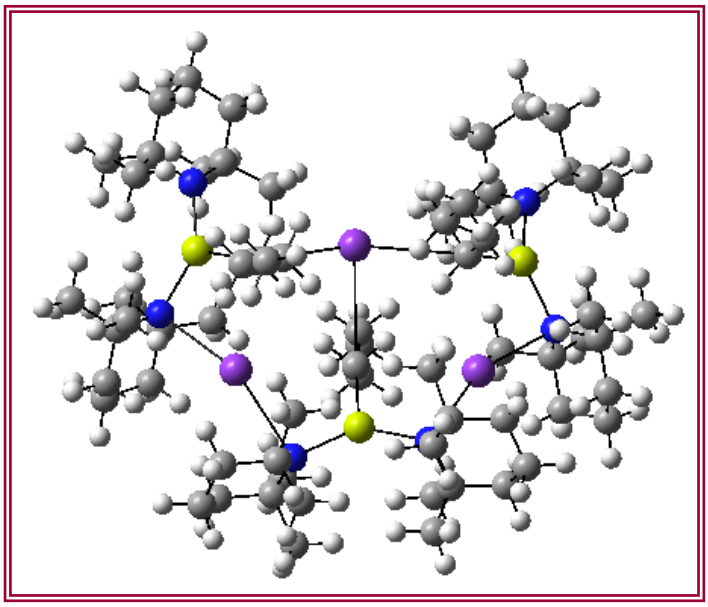
18	1	0	-6.915707	0.292461	1.421798
19	1	0	-2.757490	-0.269711	2.554941
20	1	0	-4.862862	-1.003635	2.287944
21	6	0	-3.078443	1.835097	1.977185
22	6	0	-7.401854	-0.684668	1.330284
23	6	0	-2.271748	0.707657	2.660645
24	1	0	-1.227684	2.975055	1.848443
25	1	0	-5.839227	1.958253	-0.230141
26	1	0	-7.753726	-3.298478	1.561274
27	6	0	-5.379046	-1.943660	2.047500
28	1	0	-8.224887	-0.574453	0.618817
29	6	0	-5.267296	2.890836	-0.202630
30	6	0	1.212464	-1.480341	3.990474
31	1	0	0.178813	-1.383944	3.633366
32	1	0	2.260342	3.652775	1.930629
33	1	0	-4.628134	-2.703724	1.800525
34	1	0	-1.256448	0.614451	2.254067
35	1	0	-3.404097	4.712279	-0.715005
36	6	0	-6.365608	-1.756339	0.875510
37	1	0	1.886196	0.415455	3.219920
38	6	0	-2.947554	3.904326	-0.126030
39	1	0	1.461242	-2.549534	3.879662
40	1	0	-5.610539	3.529104	-1.028396
41	6	0	-7.097383	-3.115202	0.698328
42	7	0	-3.245648	1.492744	0.542580
43	6	0	-3.744664	2.586286	-0.330510
44	1	0	3.161039	-0.723940	3.479876
45	1	0	-6.343612	-3.916020	0.693940
46	6	0	2.128767	-0.646494	3.075218

47	1	0	1.349232	2.197044	1.500959
48	6	0	2.301844	2.719556	1.356894
49	1	0	-8.712887	-2.470042	-0.603938
50	1	0	3.086542	2.100786	1.814561
51	1	0	-1.930291	3.767764	-0.529700
52	1	0	1.595781	4.945567	-0.152119
53	1	0	-8.057341	-0.371347	-1.419093
54	1	0	3.956971	4.581961	0.545668
55	1	0	0.499501	3.586815	-0.320257
56	6	0	-7.884989	-3.192211	-0.608840
57	1	0	-8.345968	-4.183476	-0.719758
58	7	0	-5.581027	-1.373364	-0.310128
59	12	0	-3.759092	-0.499360	-0.037090
60	6	0	1.482984	3.967194	-0.638557
61	1	0	5.607976	-0.087887	2.509151
62	1	0	6.875411	1.083208	2.149141
63	1	0	-6.661853	0.559898	-1.961996
64	6	0	2.586006	2.997452	-0.133064
65	6	0	-7.164907	-0.409436	-2.049706
66	6	0	3.950716	3.748880	-0.169669
67	1	0	5.264269	1.317147	1.485173
68	6	0	-3.531636	2.160062	-1.798867
69	1	0	1.033748	-0.721460	1.253486
70	6	0	2.060894	-0.975391	1.564660
71	19	0	-0.553488	0.849009	-0.317362
72	1	0	-3.838681	2.954628	-2.489567
73	6	0	6.018582	0.554083	1.716874
74	1	0	-4.127351	1.275686	-2.054098
75	6	0	-6.193233	-1.555329	-1.636424

76	1	0	4.770066	3.072178	0.095607
77	1	0	-1.163189	-1.671879	0.419341
78	1	0	0.630094	4.748952	-2.472855
79	1	0	2.035422	-2.080403	1.444368
80	6	0	-6.935405	-2.914637	-1.773034
81	1	0	-2.478119	1.934786	-2.016850
82	1	0	4.180364	4.168318	-1.150995
83	1	0	-7.504048	-0.523747	-3.089285
84	19	0	4.459423	-2.535987	2.131354
85	6	0	1.477932	4.125820	-2.160417
86	6	0	-1.979691	-1.791248	-0.324274
87	1	0	-2.471625	-2.724006	0.006749
88	1	0	-7.472822	-2.948970	-2.731475
89	1	0	-6.183325	-3.716437	-1.800576
90	1	0	2.380646	4.656785	-2.488641
91	7	0	2.558536	1.702342	-0.859565
92	12	0	3.365893	0.036019	0.069561
93	1	0	7.243982	-1.760443	1.798248
94	1	0	-4.498693	-0.636657	-2.698681
95	1	0	7.775989	1.439492	-0.005116
96	1	0	0.412148	2.313637	-2.623724
97	6	0	-5.064751	-1.579024	-2.687139
98	6	0	6.431379	-0.240528	0.458392
99	1	0	8.460573	-0.666834	1.162280
100	1	0	-4.364998	-2.393750	-2.475703
101	6	0	1.401496	2.753625	-2.832325
102	6	0	7.557889	-1.225920	0.882071
103	7	0	5.233192	-0.961093	-0.045767
104	1	0	-0.811600	-1.225631	-2.112200

105	6	0	7.034307	0.812353	-0.516850
106	1	0	6.245795	1.465398	-0.902260
107	6	0	-1.344269	-2.104680	-1.693302
108	6	0	2.504049	1.775946	-2.340686
109	1	0	-5.463269	-1.716946	-3.700430
110	1	0	4.113073	3.208711	-2.888871
111	1	0	1.456940	2.856775	-3.924460
112	1	0	-2.136611	-2.308183	-2.428083
113	1	0	0.461590	-3.087308	-1.009188
114	1	0	1.198456	0.006168	-2.446866
115	1	0	3.883458	-3.351377	-0.314459
116	6	0	3.845649	2.159807	-3.032827
117	1	0	-0.873790	-4.178349	-1.338342
118	1	0	7.536316	0.358898	-1.373281
119	6	0	-0.356206	-3.286846	-1.719835
120	1	0	4.664483	1.552712	-2.634606
121	6	0	2.141126	0.374543	-2.869415
122	1	0	6.249237	-3.608770	0.198749
123	6	0	7.882238	-2.260214	-0.198286
124	1	0	8.621149	-2.981757	0.173519
125	1	0	2.923271	-0.358247	-2.632698
126	6	0	5.477021	-2.007371	-1.073591
127	6	0	4.187490	-2.842432	-1.239439
128	6	0	6.608178	-2.983964	-0.640664
129	1	0	3.336587	-2.231209	-1.563865
130	1	0	3.791051	1.988753	-4.116243
131	1	0	8.349447	-1.767042	-1.059311
132	1	0	2.033196	0.373834	-3.960396
133	1	0	5.103412	-0.710214	-2.804923

134	1	0	4.321100	-3.624247	-1.995205
135	6	0	0.226183	-3.584793	-3.106807
136	1	0	0.774347	-2.719783	-3.503787
137	6	0	5.817292	-1.479367	-2.499068
138	1	0	6.815331	-1.042663	-2.563130
139	1	0	6.828882	-3.687153	-1.454493
140	1	0	-0.568380	-3.824572	-3.824359
141	1	0	0.919416	-4.435019	-3.085189
142	1	0	5.775854	-2.291951	-3.235814



Model 10 E = -5325.0254799 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.365043	5.039280	-3.350216
2	1	0	-5.513925	2.394857	-4.088123
3	1	0	5.972935	5.062791	-2.623380
4	1	0	3.672279	6.513445	-1.509997
5	1	0	-5.364050	-0.102310	-4.376662
6	1	0	-7.002233	1.979606	-3.247250
7	6	0	5.019634	4.528826	-2.629784
8	6	0	-5.935243	2.158450	-3.101791
9	1	0	6.115945	6.736197	-0.996398
10	1	0	5.215828	3.518389	-3.004627
11	1	0	-7.657688	-0.210865	-3.429015
12	1	0	-5.828461	3.041599	-2.464749
13	1	0	-0.140569	0.618941	-4.414648
14	1	0	0.781106	2.059165	-3.949327

15	1	0	-3.420518	1.386860	-3.666147
16	1	0	6.814377	0.675665	-3.933914
17	1	0	1.599213	0.498311	-4.111062
18	1	0	-2.828742	5.956036	-1.928927
19	1	0	2.379905	4.401326	-2.135905
20	6	0	0.674035	0.982511	-3.776580
21	1	0	-7.025362	-1.837160	-3.604711
22	1	0	-1.274962	4.773031	-0.462232
23	1	0	5.163244	7.578587	0.213922
24	1	0	4.514370	0.144032	-3.917442
25	6	0	4.125546	5.912812	-0.708785
26	6	0	-5.496410	-0.325128	-3.308904
27	6	0	5.394935	6.580928	-0.182520
28	6	0	-6.891301	-0.898990	-3.050530
29	1	0	-8.258563	1.327099	-1.869047
30	1	0	7.515266	4.914790	-1.298530
31	1	0	6.859211	1.680688	-2.471057
32	1	0	3.036270	2.803614	-1.776666
33	1	0	-3.852391	4.523851	-2.167081
34	1	0	4.313263	1.322772	-2.626657
35	6	0	-5.200138	0.943151	-2.462499
36	6	0	4.370980	4.463146	-1.214376
37	6	0	6.924520	0.653045	-2.841388
38	6	0	-3.694740	1.248447	-2.613664
39	6	0	2.972588	3.836135	-1.405262
40	1	0	3.394593	5.871854	0.112629
41	1	0	-4.749525	-1.099473	-3.064206
42	6	0	-3.682899	5.394729	-1.524475
43	1	0	7.796137	3.245465	-0.800919

44	1	0	-3.422274	2.177722	-2.095981
45	1	0	6.188782	-1.758634	-3.698492
46	6	0	4.492003	0.259894	-2.827275
47	1	0	7.930753	0.286415	-2.630697
48	1	0	-2.164824	3.253826	-0.671562
49	6	0	-2.094310	4.164719	-0.057008
50	1	0	-2.487350	6.882659	0.300708
51	6	0	7.586677	4.254823	-0.429979
52	1	0	-4.563192	6.036678	-1.608858
53	1	0	-3.064838	0.439375	-2.219788
54	6	0	-8.013801	1.096783	-0.830652
55	1	0	-2.420368	-3.966994	-3.693111
56	1	0	-1.860230	3.888744	0.979236
57	1	0	3.622392	-0.304557	-2.463488
58	1	0	-7.808669	2.044964	-0.325764
59	6	0	0.391825	0.672618	-2.301999
60	1	0	2.431103	3.827430	-0.451594
61	1	0	-8.914047	0.659705	-0.378427
62	1	0	6.923033	6.147237	1.305249
63	6	0	5.811753	-0.219826	-2.189231
64	6	0	5.999547	5.700865	0.910659
65	6	0	-7.090099	-1.135995	-1.551632
66	1	0	-8.108518	-1.496804	-1.352105
67	1	0	-0.523313	-1.229613	-2.682115
68	1	0	8.451773	4.587644	0.160410
69	6	0	6.013630	-1.700394	-2.615334
70	6	0	-3.430813	4.942830	-0.055638
71	1	0	-0.534806	1.190819	-2.004014
72	1	0	1.204963	1.089931	-1.686100

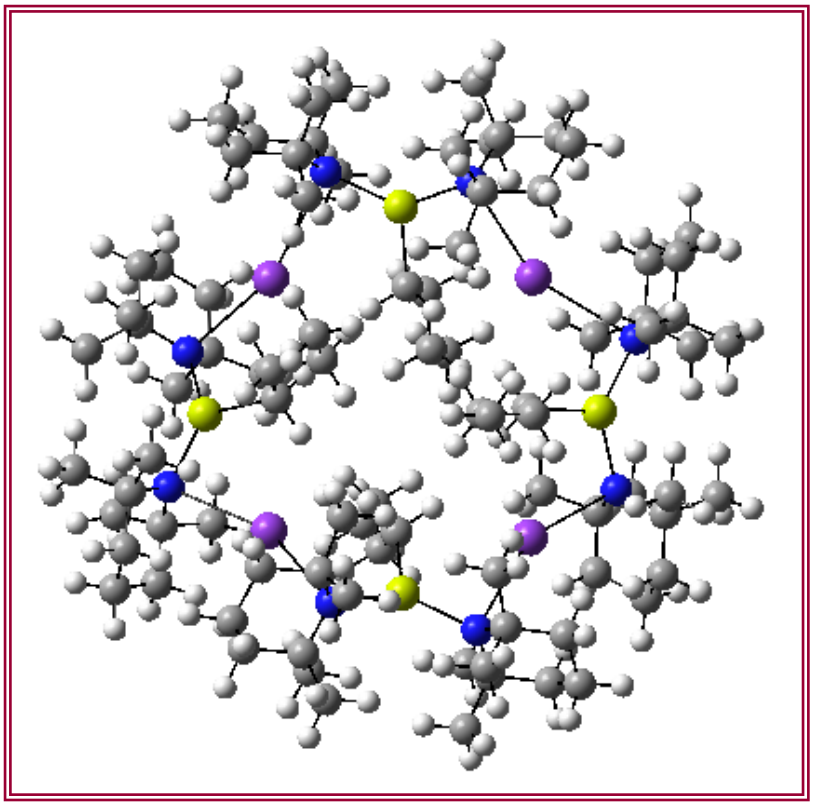
73	7	0	5.118875	3.643947	-0.246972
74	7	0	-5.475843	0.719953	-1.019511
75	1	0	1.167710	-1.336147	-2.297171
76	1	0	-2.467613	-2.643256	-2.524097
77	6	0	-3.175910	6.202508	0.821345
78	6	0	6.283077	4.254227	0.422493
79	6	0	-6.800214	0.128484	-0.694761
80	1	0	5.076310	-2.254279	-2.430281
81	6	0	0.234322	-0.829460	-1.993318
82	6	0	-2.111615	-3.667946	-2.684728
83	1	0	8.111652	-1.967284	-2.145453
84	1	0	-4.470100	-5.133257	-2.744852
85	1	0	-6.413588	-1.947372	-1.233757
86	1	0	5.286373	5.649909	1.746588
87	1	0	-1.013857	-3.636674	-2.684659
88	1	0	-4.952722	7.352023	0.326742
89	1	0	-2.672995	5.884450	1.747066
90	1	0	8.671688	-0.199733	-0.866885
91	1	0	-4.583150	-3.644584	-1.825351
92	6	0	7.144330	-2.394199	-1.852822
93	1	0	7.188783	-3.457505	-2.123307
94	7	0	5.685570	-0.087319	-0.714917
95	1	0	-2.299324	-6.251703	-3.089534
96	12	0	4.787179	1.659545	0.061033
97	6	0	-4.463468	6.925277	1.212632
98	12	0	-4.502091	2.021030	0.324208
99	6	0	-4.203024	-4.678524	-1.781390
100	7	0	-4.468440	4.059348	0.493653
101	1	0	-6.408754	5.887565	-0.674425

102	1	0	-4.236632	7.771831	1.873968
103	1	0	-6.952303	4.210092	-0.683173
104	1	0	8.035716	1.011912	0.239470
105	6	0	-2.656667	-4.647494	-1.625891
106	1	0	2.376323	-3.724737	-1.900854
107	6	0	8.137267	-0.064667	0.075324
108	19	0	-3.621450	-1.433504	-0.234892
109	1	0	-1.018746	-6.089518	-1.876368
110	1	0	2.461321	-5.418710	-2.404248
111	6	0	6.582407	3.418631	1.684950
112	6	0	-6.787058	-0.316483	0.783086
113	6	0	-2.101508	-6.046099	-2.029189
114	6	0	-6.745831	5.067512	-0.034489
115	6	0	-0.135279	-1.210341	-0.544864
116	1	0	7.432263	3.823408	2.248164
117	1	0	0.906293	-4.711430	-1.990791
118	1	0	-1.049834	-0.644930	-0.275101
119	1	0	6.854736	2.384176	1.427101
120	1	0	-7.752339	-0.749932	1.069677
121	1	0	-6.597132	0.522114	1.464393
122	6	0	6.741182	-0.759295	0.088067
123	6	0	1.969312	-4.726495	-1.711098
124	1	0	-2.307587	0.326129	1.397109
125	1	0	-5.993819	-5.331313	-0.744278
126	1	0	2.540946	2.286370	1.194747
127	6	0	-5.689419	4.683833	1.041916
128	1	0	0.633697	-0.807624	0.145584
129	6	0	6.935963	-2.239250	-0.344381
130	1	0	5.710199	3.397887	2.349391

131	1	0	-6.025074	-1.080121	0.983773
132	1	0	8.780188	-0.469779	0.868081
133	19	0	3.262864	-1.649268	-0.102157
134	6	0	-4.904385	-5.409439	-0.634753
135	1	0	-2.583978	1.901289	2.146988
136	19	0	-0.127846	1.801949	0.975934
137	6	0	-5.387558	5.931330	1.914360
138	6	0	-3.109716	1.009057	1.754110
139	6	0	2.999753	1.290344	1.345842
140	1	0	2.242196	0.550645	1.009121
141	1	0	-7.692315	5.383660	0.425512
142	1	0	-2.545160	-6.862340	-1.456527
143	1	0	7.777834	-2.682445	0.205427
144	7	0	-2.242942	-4.161158	-0.282842
145	1	0	6.044314	-2.818123	-0.050849
146	1	0	-4.672241	-6.481094	-0.672880
147	1	0	-4.897474	5.598154	2.840982
148	12	0	-0.313651	-3.369366	-0.037509
149	1	0	-6.330109	6.413934	2.207330
150	1	0	-4.858753	-3.798261	0.792978
151	1	0	4.184740	-4.355703	-0.382323
152	1	0	6.189542	0.246635	1.970775
153	1	0	-6.667537	2.750822	1.418664
154	6	0	6.295479	-0.767852	1.565873
155	6	0	-4.463638	-4.825069	0.708786
156	6	0	-6.355510	3.649031	1.972776
157	6	0	2.165057	-5.163255	-0.243473
158	1	0	5.334204	-1.277304	1.708940
159	1	0	4.114727	-6.097945	-0.563593

160	1	0	1.934508	-7.235497	-0.951071
161	6	0	3.694542	-5.261332	0.010936
162	6	0	-3.770848	0.328899	2.971837
163	6	0	-2.918811	-4.795353	0.879058
164	1	0	-5.666404	3.349497	2.771577
165	1	0	3.966327	1.829107	3.210583
166	7	0	1.523390	-4.137435	0.618290
167	1	0	-4.301276	-0.588713	2.662405
168	6	0	3.226243	1.095389	2.856323
169	1	0	7.031231	-1.285591	2.192628
170	1	0	0.468639	-6.554403	-0.221758
171	1	0	-7.267189	4.045514	2.436171
172	6	0	1.559117	-6.594169	-0.142502
173	1	0	-2.791922	-6.981754	0.502790
174	1	0	-2.037427	-0.705949	3.753970
175	1	0	-4.917145	-5.385110	1.537728
176	1	0	-2.945411	-2.902000	2.015379
177	1	0	-4.561688	0.983171	3.370688
178	1	0	3.684995	0.111854	3.047627
179	1	0	1.531802	2.213650	3.607575
180	1	0	-2.320450	0.874545	4.475206
181	1	0	1.834812	-1.989580	2.263962
182	6	0	-2.828478	-0.039408	4.132419
183	6	0	-2.440781	-6.238125	1.221188
184	6	0	-2.613573	-3.942354	2.127667
185	1	0	1.230562	0.474355	3.438549
186	6	0	1.981650	1.217097	3.758355
187	1	0	-1.348423	-6.285453	1.236609
188	1	0	3.863580	-3.329732	2.039081

189	1	0	1.802755	-7.092263	0.798163
190	6	0	1.853976	-4.188279	2.065060
191	6	0	4.046461	-5.404547	1.493524
192	1	0	0.280202	-2.752606	2.617753
193	1	0	-3.111980	-4.344634	3.017290
194	6	0	1.367829	-2.874336	2.713315
195	1	0	5.135465	-5.378676	1.628107
196	1	0	-1.539873	-3.926756	2.351431
197	1	0	-2.808834	-6.548545	2.208103
198	6	0	3.387177	-4.287318	2.306266
199	1	0	3.719136	-6.383502	1.865754
200	1	0	0.097352	-5.357035	2.681250
201	6	0	-3.534452	-0.706737	5.318462
202	1	0	1.595775	-2.853993	3.785351
203	6	0	2.264905	1.022850	5.252492
204	1	0	-4.021765	-1.642064	5.014377
205	1	0	2.988789	1.763576	5.612667
206	6	0	1.173959	-5.335727	2.869827
207	1	0	3.587126	-4.424895	3.377512
208	1	0	-2.832070	-0.945466	6.125485
209	1	0	-4.309731	-0.051667	5.734570
210	1	0	2.685546	0.028379	5.445771
211	1	0	1.568721	-6.321214	2.616037
212	1	0	1.354952	1.123464	5.855627
213	1	0	1.323953	-5.196903	3.948702



Model 11 E = -7100.0557033 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.258295	4.277132	5.269428
2	1	0	3.346535	-4.279077	5.281188
3	1	0	-4.290466	5.463379	4.477765
4	1	0	-1.430156	5.750128	4.492231
5	1	0	1.490898	-5.731277	4.546056
6	1	0	4.359977	-5.458473	4.454835
7	6	0	-3.757304	4.523650	4.322723
8	1	0	1.986086	2.093590	4.700028
9	6	0	3.821497	-4.518592	4.320410
10	1	0	1.737948	0.340687	4.726016
11	1	0	-3.206555	7.356707	3.850148
12	1	0	-4.506383	3.751277	4.127428

13	1	0	3.241673	-7.347689	3.859193
14	1	0	4.563907	-3.743418	4.111264
15	1	0	-1.830212	-2.082619	4.659854
16	1	0	-1.615011	-0.325301	4.676682
17	1	0	1.500868	-3.185230	4.297815
18	1	0	-7.329266	2.235162	4.004001
19	1	0	3.318298	1.006545	4.286808
20	1	0	-3.197424	-1.021519	4.295506
21	6	0	2.235463	1.155681	4.187176
22	1	0	7.411704	-2.256617	3.926331
23	1	0	-1.427916	3.205687	4.240927
24	6	0	-2.116256	-1.150004	4.156522
25	1	0	1.677281	-7.930351	3.323616
26	1	0	5.765791	-0.575572	3.877687
27	1	0	-1.659244	7.948718	3.276324
28	1	0	-5.674587	0.554172	3.917103
29	6	0	-1.766703	5.787625	3.447098
30	6	0	1.801985	-5.769840	3.493165
31	6	0	-2.397584	7.147975	3.138862
32	6	0	2.416664	-7.133808	3.168263
33	1	0	5.245147	-6.550194	3.056074
34	1	0	-5.225351	6.534029	3.098525
35	1	0	-6.500309	3.486696	3.059466
36	1	0	-2.514768	2.406907	3.107926
37	1	0	6.532432	-3.498636	3.015349
38	1	0	-4.573777	1.722572	3.198568
39	6	0	2.760579	-4.585848	3.180679
40	6	0	-2.725205	4.598151	3.157074
41	6	0	-7.144485	2.606058	2.986889

42	6	0	1.941384	-3.283546	3.298846
43	6	0	-1.894810	3.300944	3.253701
44	1	0	-0.854042	5.677345	2.837947
45	1	0	0.875239	-5.653192	2.906399
46	6	0	7.191975	-2.631835	2.917807
47	1	0	-5.957971	5.443809	1.922138
48	1	0	2.563277	-2.393713	3.136979
49	1	0	-7.952871	0.091841	2.862146
50	6	0	-5.311720	0.947073	2.959977
51	1	0	-8.107269	2.933167	2.588992
52	1	0	4.625653	-1.704644	3.158015
53	6	0	5.382335	-0.946798	2.919919
54	1	0	8.028664	-0.125942	2.768167
55	6	0	-5.286123	6.299860	2.033759
56	1	0	8.136701	-2.981971	2.497097
57	1	0	1.119151	-3.233235	2.575432
58	6	0	1.809234	1.203178	2.715442
59	6	0	5.282313	-6.304910	1.992668
60	1	0	0.719193	1.329136	2.654126
61	1	0	2.600521	6.755425	2.448528
62	1	0	-2.671418	-6.787789	2.427044
63	1	0	4.871661	-0.107305	2.431057
64	1	0	-4.781966	0.129333	2.454662
65	1	0	5.954923	-5.450471	1.874410
66	6	0	-1.744082	-1.189910	2.669977
67	1	0	-1.090953	3.256268	2.509778
68	1	0	5.733188	-7.166230	1.481523
69	1	0	-3.446555	8.121377	1.504185
70	6	0	-6.468443	1.509796	2.109958

71	1	0	2.317605	3.274373	2.451316
72	6	0	-2.939123	7.168274	1.707456
73	6	0	2.922438	-7.156149	1.723741
74	1	0	3.419044	-8.112051	1.507353
75	1	0	2.019073	0.235897	2.234336
76	1	0	-2.219165	-3.272236	2.421216
77	1	0	-5.752385	7.164304	1.541952
78	6	0	-7.487503	0.355649	1.902590
79	6	0	6.514498	-1.529319	2.050054
80	1	0	-0.654773	-1.293102	2.567257
81	1	0	-1.991727	-0.227482	2.197326
82	7	0	-3.305481	4.679366	1.792602
83	7	0	3.306920	-4.669356	1.802514
84	1	0	-3.518465	-2.207011	1.986013
85	1	0	-1.568489	-5.533119	1.851652
86	6	0	7.543692	-0.389251	1.818206
87	6	0	-3.897433	5.984148	1.404006
88	6	0	3.880417	-5.977440	1.398114
89	1	0	3.575543	2.184121	1.959390
90	1	0	-6.945336	-0.548277	1.575258
91	6	0	2.478810	2.330940	1.907787
92	1	0	1.524435	5.496584	1.829018
93	6	0	-2.421941	-2.330485	1.887654
94	6	0	2.425336	6.079250	1.603315
95	6	0	-2.468757	-6.103896	1.594298
96	1	0	-9.218373	1.477796	1.238973
97	1	0	-1.456418	-8.661093	1.204624
98	1	0	2.054134	-7.109754	1.046337
99	1	0	3.268368	5.376684	1.577191

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102	1	0	-3.303487	-5.391987	1.554971
103	1	0	9.245517	-1.540423	1.125017
104	1	0	7.007326	0.518286	1.492167
105	1	0	-8.400329	3.575564	0.737829
106	1	0	-0.292740	-7.378073	0.923109
107	1	0	3.863355	8.198828	1.055254
108	1	0	0.267342	7.371941	0.909515
109	6	0	-8.558200	0.686930	0.860883
110	1	0	-9.200631	-0.185668	0.684301
111	7	0	-5.898417	1.983696	0.823712
112	1	0	-3.881737	-8.231528	0.999486
113	12	0	-4.033370	2.964256	0.820925
114	6	0	8.590616	-0.739504	0.758916
115	12	0	4.035278	-2.956748	0.823809
116	6	0	-1.153972	-7.898383	0.474122
117	7	0	5.912550	-2.001306	0.777551
118	1	0	8.385884	-3.625826	0.644225
119	6	0	1.139090	7.892617	0.481789
120	1	0	9.242871	0.122834	0.568560
121	1	0	6.958568	-4.477562	0.059738
122	1	0	5.725946	3.134231	0.690043
123	1	0	6.890447	4.457218	0.538542
124	1	0	-6.992754	4.446523	0.133834
125	6	0	-2.307630	-6.877122	0.269723
126	6	0	2.289608	6.866740	0.284718
127	1	0	-5.774493	-3.184145	0.665959
128	6	0	-7.673698	3.615995	-0.075940

129	19	0	0.617649	-4.651047	0.284135
130	1	0	-4.464863	-6.991131	-0.123575
131	6	0	3.624433	7.655738	0.130999
132	1	0	5.168367	4.800556	0.451838
133	1	0	-6.919075	-4.519972	0.483580
134	6	0	-4.122990	5.960860	-0.122800
135	1	0	0.905563	2.578937	0.488215
136	6	0	2.007529	2.486992	0.444321
137	6	0	4.068293	-5.950714	-0.133677
138	6	0	-3.634852	-7.672405	0.086994
139	6	0	7.646683	-3.655221	-0.158590
140	6	0	-2.013075	-2.470369	0.404331
141	19	0	-0.670217	4.649959	0.195522
142	1	0	-4.524542	6.916043	-0.481477
143	1	0	-5.191345	-4.839683	0.414640
144	6	0	5.936728	4.071619	0.159115
145	1	0	-0.908120	-2.529079	0.389174
146	1	0	-4.848987	5.189212	-0.413555
147	1	0	4.456241	-6.906288	-0.505967
148	1	0	4.790475	-5.181229	-0.439371
149	6	0	-6.878261	2.287722	-0.251855
150	1	0	4.452556	6.972065	-0.079610
151	6	0	-5.965647	-4.117893	0.120887
152	1	0	1.491251	-2.162914	0.109928
153	1	0	0.173743	-9.200333	-0.643933
154	1	0	-1.507283	2.116906	0.039497
155	6	0	6.866055	-2.316379	-0.318568
156	1	0	-0.159677	9.217563	-0.643816
157	1	0	2.103425	1.505502	-0.060490

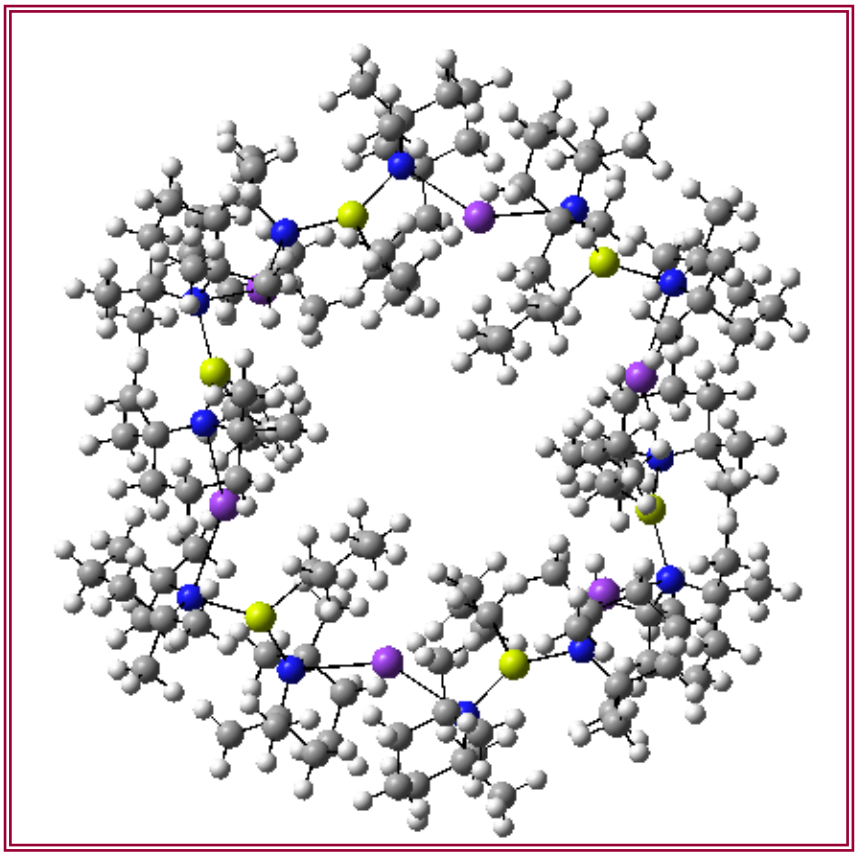
158	1	0	-2.158850	-1.490233	-0.091150
159	6	0	-7.900000	1.133041	-0.446465
160	1	0	-3.193183	5.767820	-0.673792
161	1	0	3.125934	-5.750807	-0.660208
162	1	0	3.596021	8.392496	-0.674096
163	1	0	-8.229606	3.859740	-0.991246
164	19	0	-4.680237	-0.665473	-0.223952
165	6	0	-0.697550	-8.558432	-0.828626
166	1	0	2.496267	-0.889521	-0.379831
167	19	0	4.613729	0.613085	-0.253746
168	6	0	7.898206	-1.174822	-0.534047
169	6	0	2.462947	-1.995378	-0.394265
170	6	0	0.710193	8.571492	-0.820644
171	6	0	-2.494919	2.021433	-0.453782
172	1	0	-2.592769	0.919409	-0.485664
173	1	0	8.185727	-3.903906	-1.082617
174	1	0	-3.590864	-8.396131	-0.729125
175	1	0	-8.664099	1.430737	-1.177478
176	7	0	-1.997028	-5.900021	-0.806110
177	1	0	-7.380913	0.268839	-0.891199
178	1	0	-1.485114	-9.219316	-1.212402
179	1	0	1.509027	9.230942	-1.182936
180	7	0	1.990276	5.902702	-0.806477
181	12	0	2.960097	4.031749	-0.815278
182	1	0	7.379628	-0.302744	-0.963478
183	12	0	-2.967861	-4.030870	-0.832153
184	1	0	8.641335	-1.481428	-1.282843
185	1	0	7.099871	2.046775	-0.994665
186	1	0	0.541175	-6.943533	-1.532290

187	1	0	-7.138997	-2.092943	-1.022678
188	1	0	-5.409095	3.287642	-1.551350
189	1	0	7.173427	5.722646	-1.454421
190	1	0	5.344939	-3.281838	-1.586415
191	1	0	-0.527819	6.974758	-1.562020
192	6	0	-6.107705	2.441269	-1.578722
193	6	0	5.979159	3.873381	-1.370920
194	1	0	8.113593	3.405315	-1.451055
195	6	0	-0.357759	-7.488379	-1.868208
196	6	0	6.068154	-2.457131	-1.630433
197	6	0	-5.991322	-3.901788	-1.407223
198	1	0	-5.522260	1.546593	-1.821645
199	6	0	0.380841	7.515662	-1.877927
200	6	0	7.158850	2.910526	-1.676660
201	1	0	-8.130045	-3.457818	-1.508523
202	1	0	-7.164334	-5.762393	-1.530279
203	6	0	-7.178644	-2.948927	-1.715987
204	6	0	2.317058	-2.408041	-1.876284
205	7	0	4.674607	3.299861	-1.786628
206	6	0	-1.511565	-6.471956	-2.087267
207	1	0	5.508252	-1.545573	-1.871149
208	1	0	-2.211325	3.576355	-1.987021
209	7	0	-4.688428	-3.308368	-1.799973
210	6	0	6.315832	5.270767	-1.970961
211	1	0	5.462043	5.946398	-1.864812
212	1	0	2.201977	-3.505626	-1.969594
213	6	0	-2.352319	2.479279	-1.922795
214	6	0	1.530755	6.492631	-2.088832
215	1	0	-6.794663	2.622167	-2.413969

216	1	0	-5.444564	-5.962717	-1.916820
217	1	0	6.735461	-2.663067	-2.475734
218	6	0	-6.303963	-5.295240	-2.028302
219	1	0	2.968906	8.128293	-2.533896
220	1	0	-2.928306	-8.113824	-2.576092
221	1	0	0.208810	-1.994601	-2.175631
222	1	0	-0.084188	-7.954170	-2.824834
223	1	0	-0.134917	-4.780396	-2.420688
224	1	0	3.253311	-2.198184	-2.416334
225	1	0	0.126422	7.993600	-2.833864
226	1	0	-3.299002	2.308666	-2.457924
227	1	0	-0.257252	2.027142	-2.258201
228	1	0	1.262484	-0.650087	-2.553025
229	1	0	0.133720	4.828624	-2.471996
230	1	0	-3.270745	-1.095682	-2.530710
231	6	0	1.166897	-1.740409	-2.653246
232	1	0	3.245504	1.109622	-2.564401
233	6	0	-2.599763	-7.150717	-2.972115
234	6	0	2.638725	7.173219	-2.947476
235	6	0	-0.943518	-5.315814	-2.934626
236	1	0	-1.346335	0.717997	-2.659667
237	1	0	6.570780	5.226666	-3.031805
238	6	0	-1.226402	1.808009	-2.731669
239	1	0	3.515760	6.524330	-3.021617
240	1	0	-3.481037	-6.508192	-3.052019
241	6	0	0.967822	5.350552	-2.958298
242	1	0	-5.695255	-0.866659	-2.860042
243	1	0	5.665353	0.861160	-2.868263
244	6	0	7.152681	2.397421	-3.118676

245	1	0	-6.543191	-5.241111	-3.092316
246	1	0	7.948693	1.654777	-3.260558
247	1	0	1.737541	4.604125	-3.189098
248	6	0	4.605426	2.747108	-3.162713
249	6	0	-4.609854	-2.736312	-3.168230
250	6	0	-7.160923	-2.416672	-3.150939
251	1	0	-2.419188	-2.519004	-3.125969
252	1	0	-0.537121	-5.680552	-3.885352
253	6	0	-3.315472	-1.902417	-3.271573
254	1	0	-7.964196	-1.681912	-3.292866
255	1	0	-1.719457	-4.582428	-3.186838
256	6	0	3.303512	1.928563	-3.290933
257	6	0	5.791123	1.785034	-3.457328
258	1	0	2.412406	2.551666	-3.141198
259	1	0	-2.220732	-7.335750	-3.986178
260	6	0	-5.802668	-1.783441	-3.463698
261	1	0	2.277473	7.374373	-3.964935
262	1	0	7.377777	3.218434	-3.810864
263	1	0	0.596415	5.726048	-3.919145
264	1	0	-7.367270	-3.230830	-3.856902
265	1	0	-3.755626	-4.519364	-4.127600
266	1	0	3.780436	4.550604	-4.109764
267	6	0	1.122685	-2.115131	-4.139067
268	1	0	-3.224585	-1.439296	-4.260986
269	1	0	3.215316	1.483141	-4.288690
270	6	0	-1.189350	2.221816	-4.207242
271	1	0	1.001329	-3.197386	-4.275845
272	1	0	-1.045905	3.304479	-4.316766
273	6	0	4.552501	3.802242	-4.308741

274	1	0	5.496575	4.334454	-4.439271
275	6	0	-4.532456	-3.775909	-4.326909
276	1	0	5.764409	1.469922	-4.509424
277	1	0	-5.766541	-1.453061	-4.510802
278	1	0	0.292079	-1.620479	-4.656215
279	1	0	2.050898	-1.823252	-4.647148
280	1	0	-2.128913	1.963541	-4.712601
281	1	0	-5.469629	-4.315179	-4.476192
282	1	0	-0.374972	1.723659	-4.746358
283	1	0	-4.290210	-3.282314	-5.277524
284	1	0	4.317665	3.323270	-5.268712



Model 12 E = -10650.083603 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.298074	2.525482	5.028745
2	6	0	-6.281963	6.465709	3.862581
3	6	0	-9.080893	3.420651	3.540903
4	6	0	-8.521457	0.370688	4.339472
5	6	0	-7.004653	0.268133	4.171547
6	6	0	-9.142819	0.944976	3.065424
7	6	0	-6.354621	1.618178	3.762712
8	6	0	-8.506718	2.294506	2.631363
9	6	0	-5.297371	6.363679	2.659537
10	6	0	-8.219451	6.650569	1.207998
11	6	0	-4.754161	7.786844	2.354529

12	6	0	-4.113094	5.515658	3.164704
13	6	0	-5.761944	8.654602	1.597889
14	7	0	-7.024588	2.216480	2.577079
15	6	0	-4.884426	1.326524	3.397475
16	6	0	-3.699192	-2.539533	3.894538
17	6	0	-9.014325	2.604220	1.207074
18	7	0	-5.837371	5.704564	1.443330
19	6	0	-2.483198	-8.615882	3.853776
20	6	0	-0.368665	4.578660	3.931760
21	6	0	-6.783129	6.503728	0.623999
22	6	0	-6.233738	7.927920	0.336509
23	12	0	-5.946134	3.609248	1.436033
24	6	0	-4.383959	-7.934589	2.344996
25	6	0	0.958774	-6.705117	5.006270
26	6	0	5.333150	4.246045	5.018316
27	6	0	-2.711961	-6.262557	3.134626
28	6	0	-4.654058	-9.246939	1.606611
29	6	0	-8.491555	-3.142209	0.754981
30	6	0	-2.875592	-7.714721	2.644727
31	6	0	4.558000	7.233510	4.257627
32	6	0	3.722502	5.959573	4.119931
33	6	0	-3.510354	-2.353514	2.384815
34	6	0	-6.954223	5.792977	-0.735153
35	6	0	-10.015673	-1.466760	-0.290096
36	6	0	-0.306002	4.294085	2.426884
37	6	0	-4.700152	-2.841058	1.536083
38	6	0	4.575657	4.718369	3.741053
39	19	0	-6.591081	-0.019435	0.408439
40	6	0	3.596979	3.578439	3.392711

41	6	0	1.772138	-6.298193	3.740582
42	6	0	-9.042798	-2.638447	-0.595429
43	6	0	1.546268	-9.559885	3.508262
44	6	0	1.297955	-4.875135	3.381455
45	6	0	4.190749	-1.972010	3.963373
46	6	0	-9.879050	-3.816695	-1.178222
47	6	0	3.268695	-6.200720	4.146757
48	6	0	-0.118892	5.550520	1.554958
49	7	0	-2.040678	-7.877264	1.427910
50	6	0	-3.791313	-9.321652	0.344711
51	6	0	-4.565993	2.630515	0.007739
52	6	0	3.928840	-7.571382	4.305972
53	6	0	7.490712	6.194839	3.501859
54	6	0	8.766688	2.236064	3.875165
55	6	0	5.371954	7.458124	2.982297
56	6	0	-1.707522	-10.420890	1.232527
57	6	0	-10.435768	-0.693627	-1.542237
58	19	0	-3.297047	5.683700	-0.366556
59	6	0	6.856642	0.819364	3.205223
60	6	0	-2.279099	-9.104201	0.626957
61	6	0	-4.585716	-2.599731	0.015909
62	7	0	1.578831	-7.170670	2.552415
63	7	0	5.430025	4.979481	2.552393
64	6	0	-6.714928	-6.458988	-1.210561
65	6	0	6.232382	6.228013	2.583629
66	6	0	-2.222105	9.077907	-1.234183
67	7	0	-7.893086	-2.197177	-1.425921
68	6	0	2.239564	-8.499515	2.601414
69	12	0	-0.165184	-6.934578	1.403442

70	6	0	1.578289	8.973890	0.658712
71	6	0	3.904362	-1.878473	2.460368
72	6	0	3.728979	-8.391923	3.030240
73	6	0	8.180098	1.416786	2.687692
74	6	0	-4.816584	2.596881	-1.514765
75	19	0	-3.241045	-5.667577	-0.438014
76	6	0	-9.196367	-0.236376	-2.314333
77	12	0	-6.109214	-3.302299	-1.431813
78	6	0	0.036174	5.300233	0.039727
79	6	0	9.138919	0.231719	2.391009
80	6	0	-3.743034	8.320480	-3.058239
81	6	0	-8.224234	-1.403703	-2.636435
82	12	0	6.107148	3.333198	1.440453
83	6	0	-1.576995	-8.929018	-0.735730
84	6	0	2.216454	-9.085756	1.174123
85	6	0	-2.251244	8.457081	-2.646524
86	19	0	3.267211	5.722900	0.369006
87	6	0	0.008301	-5.278690	-0.057152
88	6	0	6.758786	6.481718	1.155651
89	6	0	-6.197893	-6.172821	-2.635822
90	7	0	7.873062	2.199144	1.463644
91	6	0	4.880996	-2.683642	1.582010
92	6	0	2.276205	9.141778	-0.707107
93	12	0	0.186125	6.939766	-1.443470
94	6	0	1.690189	10.446687	-1.324756
95	6	0	10.393769	0.663189	1.628854
96	6	0	-3.791634	1.803070	-2.347241
97	7	0	-5.412167	-4.914248	-2.584741
98	7	0	-1.573212	7.138455	-2.571805

99	6	0	-7.461989	-6.140049	-3.546055
100	6	0	3.786564	9.377968	-0.430233
101	6	0	-8.809983	-2.217010	-3.828230
102	6	0	9.881482	3.789014	1.216100
103	6	0	-5.323219	-7.382865	-3.063932
104	6	0	-3.946544	7.462382	-4.308292
105	6	0	-6.916206	-0.777611	-3.159308
106	6	0	4.581861	2.627959	-0.003540
107	6	0	-1.578534	9.502375	-3.585173
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299	1	0	-8.195691	-3.100500	-4.023142
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390	1	0	-3.794560	5.556662	-3.320344
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425	1	0	2.733618	-8.439320	0.453394
426	1	0	-3.942398	-10.281209	-0.168468

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