

Supporting Information

TEMPO-Mediated Homocoupling of Aryl Grignard Reagents: Mechanistic Studies

Sandip Murarka, Juri Möbus, Gerhard Erker, Christian Mück-Lichtenfeld * and
Armido Studer *

Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Corrensstraße 40,
48149 Münster, Germany.

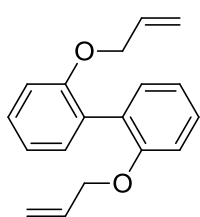
studer@uni-muenster.de; cml@uni-muenster.de

Experimental Section:

General: All reactions involving air- or moisture-sensitive reagents or intermediates were carried out in flame dried glassware under an argon atmosphere. THF was freshly distilled from Na under argon. All other solvents and reagents were purified according to standard procedures or were used as received from Aldrich, Fluka, Acros or Lancaster. ^1H NMR and ^{13}C NMR spectra were recorded on a *Bruker DPX 300* at 300 K and a *Varian UNITYplus 600* at 299 K. All resonances are reported relative to TMS. Spectra were calibrated relative to solvent's residual proton and carbon chemical shift: CHCl_3 ($\delta = 7.26$ for ^1H NMR and $\delta = 77.00$ for ^{13}C NMR), C_6D_6 ($\delta = 7.36$ for ^1H NMR and $\delta = 128.37$ for ^{13}C NMR). TLC was performed using Merck silica gel 60 F-254 plates, detection of compounds with UV light or dipping into a solution of KMnO_4 (1.5 g in 400 mL H_2O , 5 g NaHCO_3), followed by heating. Flash column chromatography (FC) was performed using Merck or Fluka silica gel 60 (40-63 μm) applying a pressure of about 0.4 bar. Mass spectra were recorded on a *Finnigan MAT 4200S*, a *Bruker Daltonics Micro Tof*, a *Waters-Micromass Quatro LCZ* (ESI); peaks are given in m/z (% of basis peak). GC analyses were carried out on a *Hewlett Packard HP 6890 Series* GC system equipped with a HP 5 column (30 m x 0.32 mm, film thickness 0.25 μm) or a HP 1 column (25 m x 0.32 mm, film thickness 0.25 μm) using hydrogen as carrier gas.

General Procedure for the stoichiometric oxidative homocoupling of aryl Grignard reagent with TEMPO:¹ *i*-PrMgCl in THF (1.76 M, 0.215 mL, 0.378 mmol, 1.05 equiv) was added drop wise to the corresponding aryl iodide (0.36 mmol) in dry THF (1.0 ml) at 0 °C and was then stirred at room temperature for 2 h. The completion of the I-Mg exchange reaction was checked by GC-analysis of a reaction aliquot. Then TEMPO (0.061 g, 0.389 mmol, 1.08 equiv) was added and the resulting reaction mixture was refluxed for 1 h. The reaction was then quenched with a saturated aqueous NH_4Cl solution (5 mL) and MTBE (5 mL) was added. The aqueous layer was extracted twice with MTBE (2 x 5 mL); the combined organic phases were washed with saturated brine (10 mL), dried over MgSO_4 , filtered and concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel using 2% MTBE/pentane as an eluent.

2,2'-Bis(allyloxy)-1,1'-biphenyl (4):



The title compound was obtained in 88% yield (0.042 g, 0.158 mmol) starting from 1-(allyloxy)-2-iodobenzene (0.093 g, 0.357 mmol, 100% magnesiation).

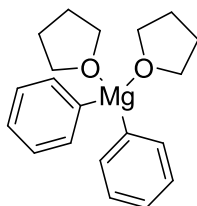
FTIR (neat): 2864, 1647, 1593, 1502, 1479, 1441, 1423, 1262, 1217, 1161, 1116, 1049, 994, 922, 825, 747 cm^{-1} .

^1H NMR (300 MHz, CDCl_3) δ 7.37 – 7.28 (m, 4H, H_{Aryl}), 7.08 – 7.00 (m, 2H, H_{Aryl}), 7.00 – 6.94 (m, 2H, H_{Aryl}), 5.95 (ddt, $^3J = 17.3$ Hz, $^3J = 10.6$ Hz, $^3J = 4.8$ Hz, 2H, $-\text{CH}=\text{CH}_2$), 5.25 (ddt, $^3J = 17.3$ Hz, $^2J = 3.3$ Hz, $^4J = 1.7$ Hz, 2H, $-\text{CH}=\text{CH}^{\text{Z}}\text{H}^{\text{E}}$), 5.16 (ddt, $^3J = 10.6$ Hz, $^2J = 3.3$ Hz, $^4J = 1.6$ Hz, 2H, $-\text{CH}=\text{CH}^{\text{Z}}\text{H}^{\text{E}}$), 4.53 (ddd, $^3J = 4.8$ Hz, $^4J = 1.7$ Hz, $^4J = 1.6$ Hz, 4H, $-\text{O}-\text{CH}_2-\text{CH}=\text{CH}_2$).

^{13}C NMR (75 MHz, CDCl_3) δ 156.1, 133.6, 131.5, 128.4, 128.3, 120.5, 116.3, 112.4, 68.9.

HRMS (ESI) Exact mass calculated for $\text{C}_{18}\text{H}_{18}\text{O}_2$ Na ($[\text{M} + \text{Na}]^+$): 289.1199. Found: 289.1202. The spectral data of the compound are in complete agreement with the literature data.²

Preparation of diphenylmagnesium



Diphenylmagnesium was prepared according to a modified literature procedure.³ Magnesium turnings (3.09 g, 127 mmol, 2 eq) were suspended in THF (70 mL) and activated with iodine at 50 °C. Then phenyl bromide (10.0 g, 64 mmol, 1 eq) was added drop wise to the stirred suspension at 50 °C and the reaction mixture was stirred for 2 h at 50 °C. After cooling to room temperature degassed 1,4-dioxane (6.0 mL, 6.2 g, 70 mmol, 1.1 eq) was added and slowly a colorless precipitate formed. The resulting suspension was stirred overnight at room temperature and subsequently the volatiles were evaporated *in vacuo*. The grey solid residue and the unconsumed magnesium was taken up in Et_2O (50 mL), the insolubles were removed by cannula filtration at 40 °C and washed with Et_2O (30 mL) twice at 40 °C. The combined

filtrates were concentrated *in vacuo* to ca. 20 mL at 40 °C and then cooled to -40 °C for precipitation. The yellowish supernatant solution was removed by cannula filtration and the precipitate washed with Et₂O (10 mL) twice at -40 °C. The precipitate was dried *in vacuo* and yielded Ph₂Mg(thf)₂ (6.63 g, 20.5 mmol, 66%) as colorless solid, which was stored and handled in a glovebox.

Anal. Calc. for C₂₀H₂₆MgO₂: C, 74.43; H, 8.12. Found C, 73.00; H, 8.37.

¹H NMR (600 MHz, 299 K, C₆D₆): δ 8.03 (m, 2H, o-Ph), 7.41 (m, 2H, m-Ph), 7.30 (m, 1H, p-Ph), 3.53 (m, 4H, O-CH₂), 1.25 (m, 4H, CH₂).

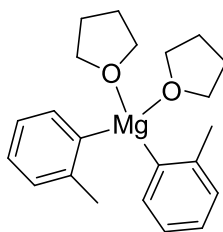
¹³C{¹H} NMR (151 MHz, 299 K, C₆D₆): δ 167.5 (i-Ph), 141.3 (o-Ph), 126.5 (m-Ph), 125.1 (p-Ph), 69.5 (O-CH₂), 25.2 (CH₂).

¹H,¹H GCOSY (600 MHz / 600 MHz, 299 K, C₆D₆)[selected traces]: δ¹H / δ¹H: 8.03 / 7.41 (o-Ph / m-Ph), 7.41 / 8.03, 7.30 (m-Ph / o-Ph, p-Ph), 3.53 / 1.25 (O-CH₂ / CH₂).

¹H,¹³C GHSQC (600 MHz / 151 MHz, 299 K, C₆D₆): δ¹H / δ¹³C: 8.03 / 141.3 (o-Ph), 7.41 / 126.5 (m-Ph), 7.30 / 125.1 (p-Ph), 3.53 / 69.5 (O-CH₂), 1.25 / 25.2 (CH₂).

¹H,¹³C GHMBC (600 MHz / 151 MHz, 299 K, C₆D₆)[selected traces]: δ¹H / δ¹³C: 8.03 / 167.5, 141.3, 126.5, 125.1 (o-Ph / i-Ph, o-Ph, m-Ph, p-Ph), 7.41 / 167.5, 126.5, 125.1 (m-Ph / i-Ph, m-Ph, p-Ph), 3.53 / 69.5, 25.2 (O-CH₂ / O-CH₂, CH₂).

Preparation of di(ortho-tolyl)magnesium⁴



Di(ortho-tolyl)magnesium was prepared according to a modified literature procedure.^{3b-d} Magnesium turnings (3.0 g, 116 mmol, 2 eq) were suspended in THF (80 mL) and activated with iodine at 50 °C. Then 2-bromotoluene (10.0 g, 58 mmol, 1 eq) was added drop wise to the stirred suspension at 50 °C and the reaction mixture was stirred for 2 h at 50 °C. After cooling to room temperature degassed 1,4-dioxane (5.5 mL, 5.7 g, 64 mmol, 1.1 eq) was added and slowly a colorless precipitate formed. The resulting suspension was stirred overnight at room temperature and subsequently the volatiles were evaporated *in vacuo*. The grey solid residue and the unconsumed magnesium was taken up in Et₂O (100 mL), the

insolubles were removed by cannula filtration at 40 °C and washed with Et₂O (30 mL) twice at 40 °C. The combined filtrates were concentrated *in vacuo* to ca. 30 mL at 40 °C and then cooled to -40 °C for precipitation. The yellowish supernatant solution was removed by cannula filtration and the precipitate washed with Et₂O (10 mL) twice at -40 °C. The precipitate was dried *in vacuo* and yielded (o-tol)₂Mg(thf)₂ (7.38 g, 21.0 mmol, 73%) as colorless solid, which was stored and handled in a glovebox.

Anal. Calc. for C₂₂H₃₀MgO₂: C, 75.33; H, 8.62. Found C, 74.71; H, 8.74.

¹H NMR (600 MHz, 299 K, C₆D₆) δ 7.88 (m, 2H, o'-Tol), 7.42 (m, 2H, m-Tol), 7.38 (m, 2H, p-Tol), 7.37 (m, 2H, m'-Tol), 3.50 (m, 8H, O-CH₂), 2.69 (s, 6H, o-Me), 1.16 (m, 8H, CH₂).

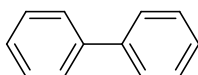
¹³C{¹H} NMR (151 MHz, 299 K, C₆D₆) δ 168.0 (i-Tol), 147.8 (o-Tol), 140.6 (o'-Tol), 126.9 (m-Tol), 125.5 (p-Tol), 123.6 (m'-Tol), 69.2 (O-CH₂), 28.5 (o-Me), 25.2 (CH₂).

¹H, ¹H GCOSY (600 MHz / 600 MHz, 299 K, C₆D₆)[selected trace]: δ¹H / δ¹H: 3.50 / 1.16 (O-CH₂ / CH₂).

¹H, ¹³C GHSQC (600 MHz / 151 MHz, 299 K, C₆D₆): δ¹H / δ¹³C: 7.88 / 140.6 (o'-Tol), 7.42 / 126.9 (m-Tol), 7.38 / 125.5 (p-Tol), 7.37 / 123.6 (m'-Tol), 3.50 / 69.2 (O-CH₂), 2.69 / 28.5 (o-Me), 1.16 / 25.2 (CH₂).

¹H, ¹³C GHMBC (600 MHz / 151 MHz, 299 K, C₆D₆)[selected traces]: δ¹H / δ¹³C: 7.88 / 168.0, 147.8, 125.5, 123.6 (o'-Tol / i-Tol, o-Tol, p-Tol, m'-Tol), 7.42 / 123.6 (m-Tol / m'-Tol), 3.50 / 69.2, 25.2 (O-CH₂ / O-CH₂, CH₂), 2.69 / 168.0, 147.8, 126.9 (o-Me / i-Tol, o-Tol, m-Tol).

Attempted homocoupling of diphenylmagnesium



Bromide-free, room temperature:

Diphenylmagnesium (100 mg, 0.3 mmol, 1 eq) was dissolved in THF (2 mL) in a glovebox at room temperature and TEMPO (97 mg, 0.6 mmol, 2 eq) was added in portions at room temperature. The reaction mixture was stirred for a total of 18 h at room temperature monitoring the reaction progress by GC and GC-MS. The coupling product biphenyl could

only be detected in traces (~1%) along with various side products and the composition of the reaction mixture did not change after the first sample (2 h). Heating of the reaction mixture to 80 °C for 3 h also did not result in an increase of the coupling product.

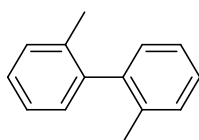
Bromide-free, reflux:

Diphenylmagnesium (100 mg, 0.3 mmol, 1 eq) was dissolved in THF (2 mL) in a glovebox at room temperature and TEMPO (97 mg, 0.6 mmol, 2 eq) was added in portions at room temperature. The reaction mixture was stirred for 3 h at 80 °C. The GC and GC-MS analysis of an aliquot of the mixture showed no improvement compared to the room temperature experiment. The coupling product biphenyl could only be detected in traces (~1%) along with various side products.

With one equivalent of MgBr₂:

Diphenylmagnesium (323 mg, 1 mmol, 1 eq) was dissolved in THF (2 mL) in a glovebox at room temperature, anhydrous magnesium bromide (185 mg, 1 mmol, 1 eq) was added and the grey solution stirred for 15 min at room temperature for equilibration. Then, TEMPO (315 mg, 2 mmol, 2 eq) was added in portions at room temperature and the reaction mixture stirred overnight at room temperature. Full conversion was confirmed by GC analysis. The reaction mixture was poured onto a silica gel on a frit and the filter pad washed with Et₂O (50 ml). The low boiling components were evaporated from the filtrate by rotary evaporation and the product biphenyl was obtained by column chromatography (silica gel, eluent pentane/Et₂O 10:1, R_f = 0.60) as a pale yellow solid (109 mg, 0.71 mmol, 71%).

Attempted homocoupling of di(ortho-tolyl)magnesium:



Bromide-free:

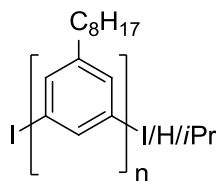
Di(ortho-tolyl)magnesium (100 mg, 0.28 mmol, 1 eq) was dissolved in THF (2 mL) in a glovebox at room temperature and TEMPO (90 mg, 0.57 mmol, 2 eq) was added in portions at room temperature. The reaction mixture was stirred for 2 h at 80 °C and an aliquot of the

reaction mixture analyzed by GC and GC-MS. The coupling product, 2,2'-dimethyl-biphenyl, could not be detected.

With one equivalent of MgBr_2 :

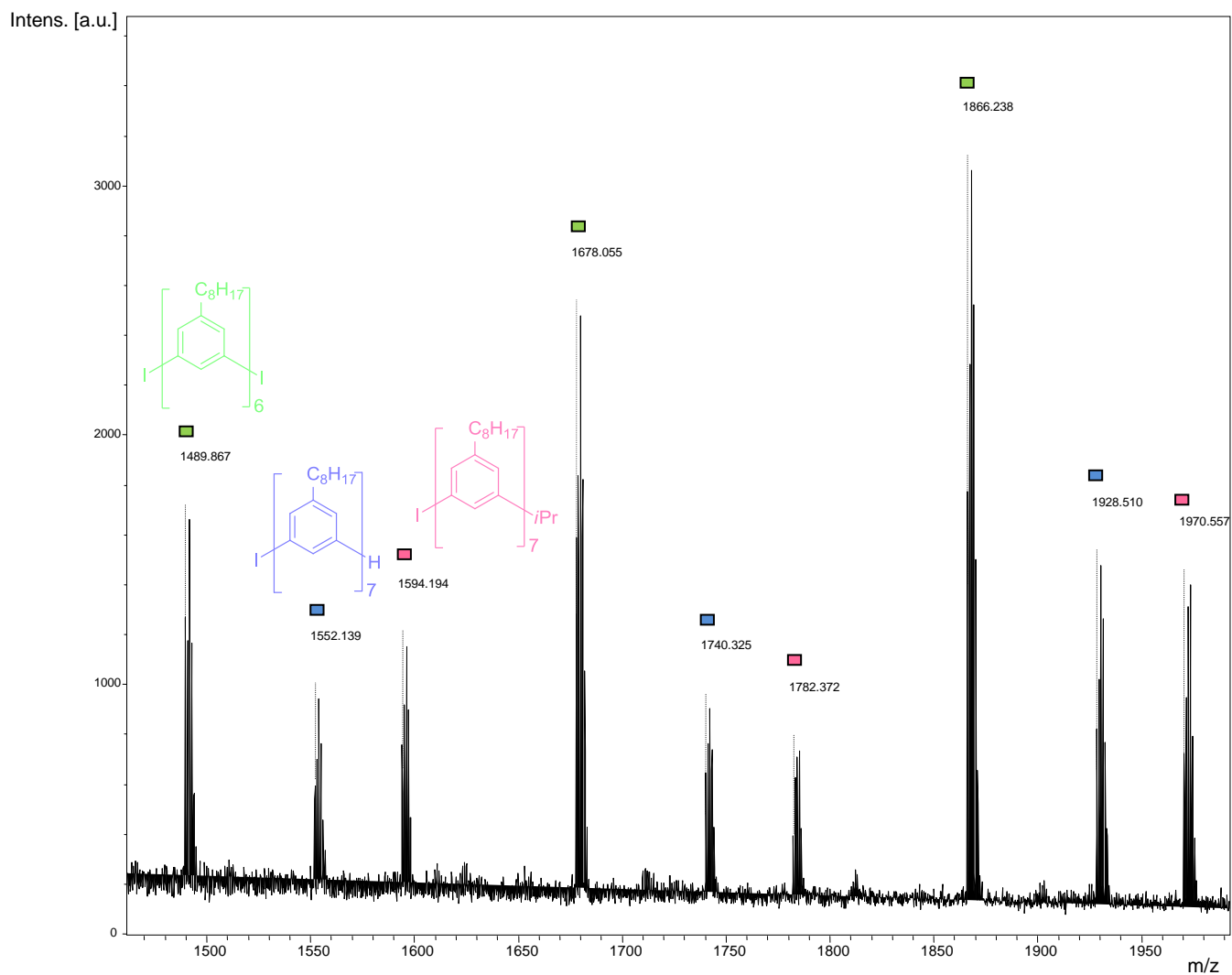
Diphenylmagnesium (350 mg, 1 mmol, 1 eq) was dissolved in THF (2 mL) in a glovebox at room temperature, anhydrous magnesium bromide (185 mg, 1 mmol, 1 eq) was added and the grey solution stirred for 15 min at room temperature for equilibration. Then, TEMPO (315 mg, 2 mmol, 2 eq) was added in portions at room temperature in the glovebox and the reaction mixture was refluxed for 3 h. GC and GC-MS analysis of an aliquot of the reaction mixture revealed a ratio toluene : coupling product 1:2.

A representative procedure for the synthesis of poly-*meta*-phenylene **8**⁵



A solution of 1,3-diiodo-5-octylbenzene (0.221g, 0.50 mmol) in THF (1 mL) was cooled to $-40\text{ }^\circ\text{C}$ and a 1.95 M solution of *i*-PrMgCl in THF (0.261 mL, 0.51 mmol, 1.02 equiv) was added very slowly. Then the resulting solution was stirred for additional 1.5 h. After which a small aliquot was withdrawn, quenched with sat. NH_4Cl , extracted with MTBE and submitted to GC analysis, which shows clean monomagnesiation with no trace of bismagnesiation. Then TEMPO (7.85 mg, 0.05 mmol, 10 mol%) was added and the resulting reaction mixture was allowed to warm to room temperature and stirred for 24 h. After completion, the reaction was quenched with saturated NH_4Cl (2 mL), and then CH_2Cl_2 (5 mL) was added. The aqueous layer was extracted with CH_2Cl_2 (2 x 5 mL); the combined organic layers were dried over MgSO_4 , filtered and concentrated *in vacuo*. The resulting crude material was dissolved in a minimum amount of dichloromethane (2 mL) and reprecipitated by addition of MeOH (10 mL). The solid particles obtained were allowed to settle down and then MeOH was decanted. The precipitation procedure was repeated two times. The analytically pure poly-(5-octylarene) **2a** hence obtained was dried under high vacuum to give white solid (70%) which was used for further analytical measurements. GPC (THF, against polystyrene standard): $M_n = 13700$, PDI = 1.74. Please see reference no. 3 for the complete characterization data.

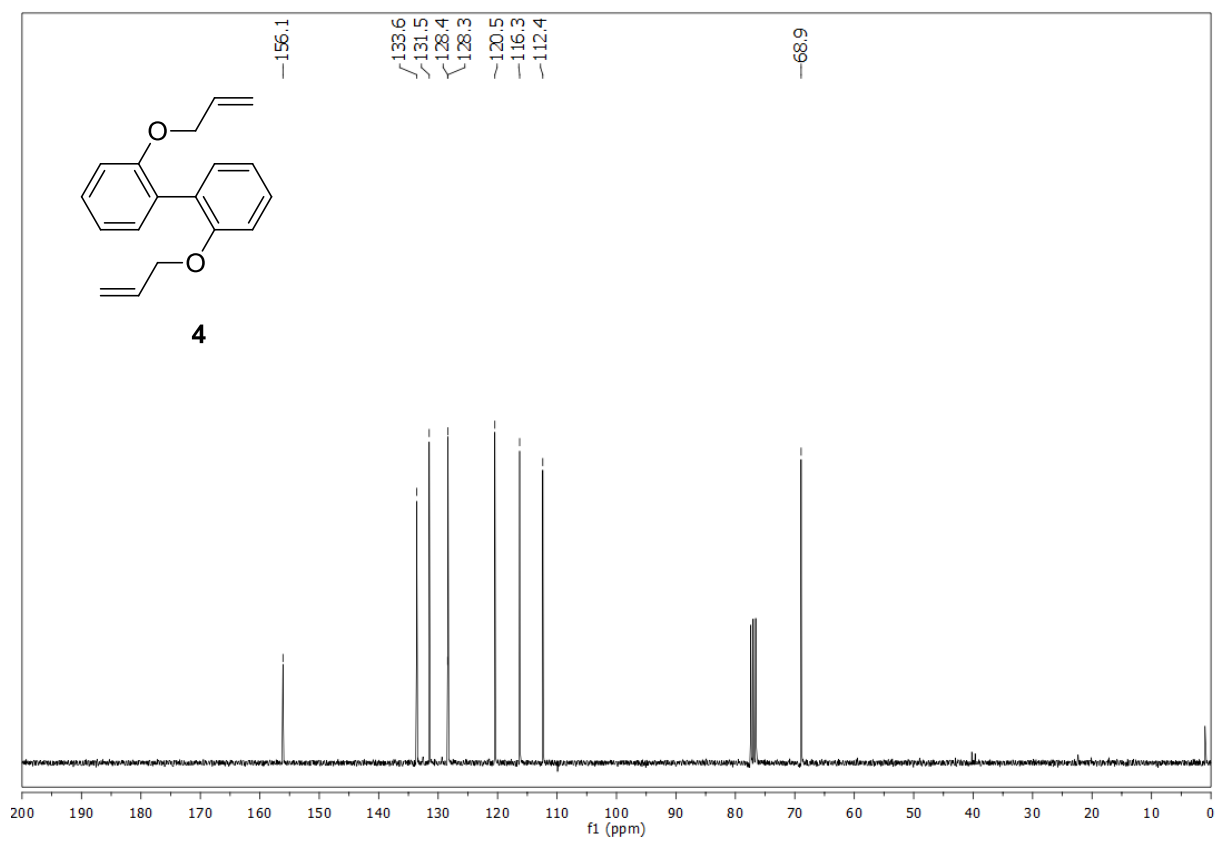
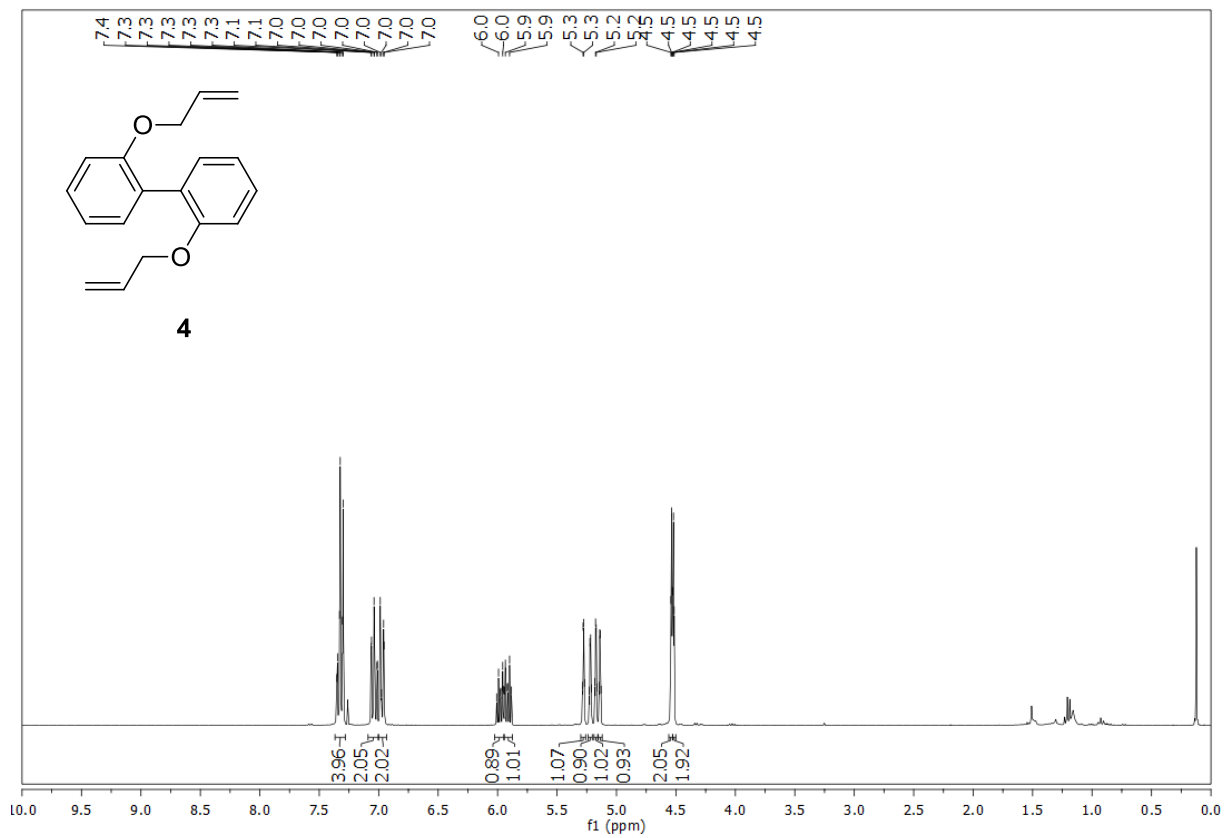
End group analysis of polymer 8 by mass spectrometric analysis (MALDI-MS)



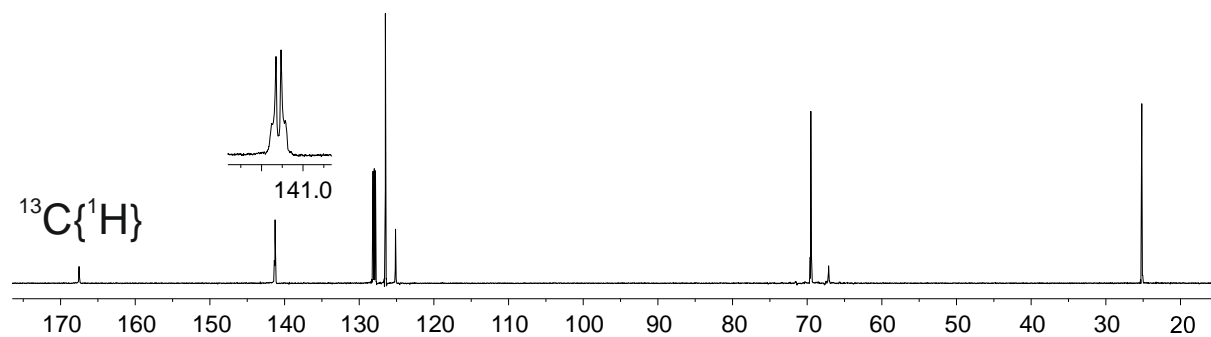
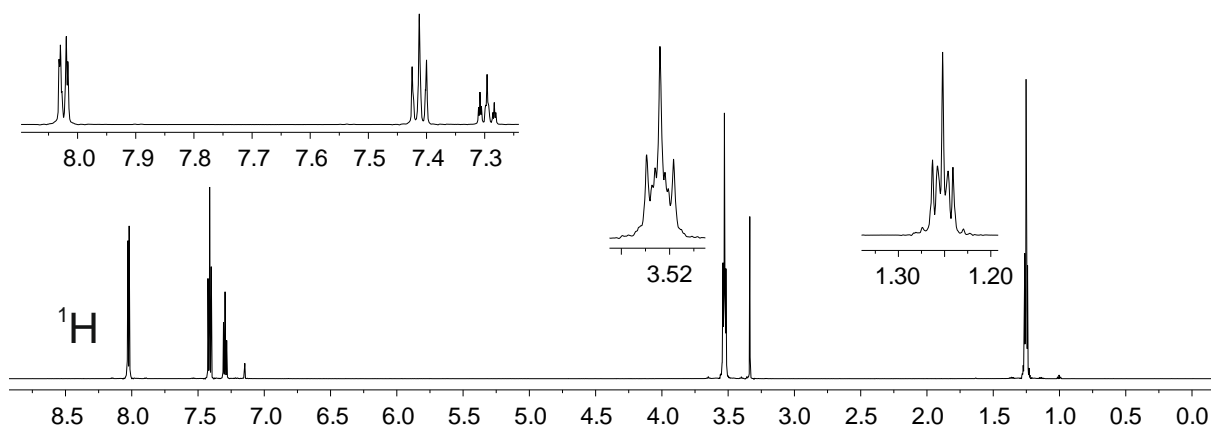
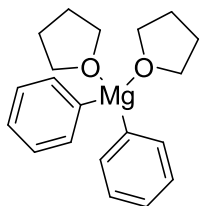
The corresponding data file is attached at the end of this SI.

References:

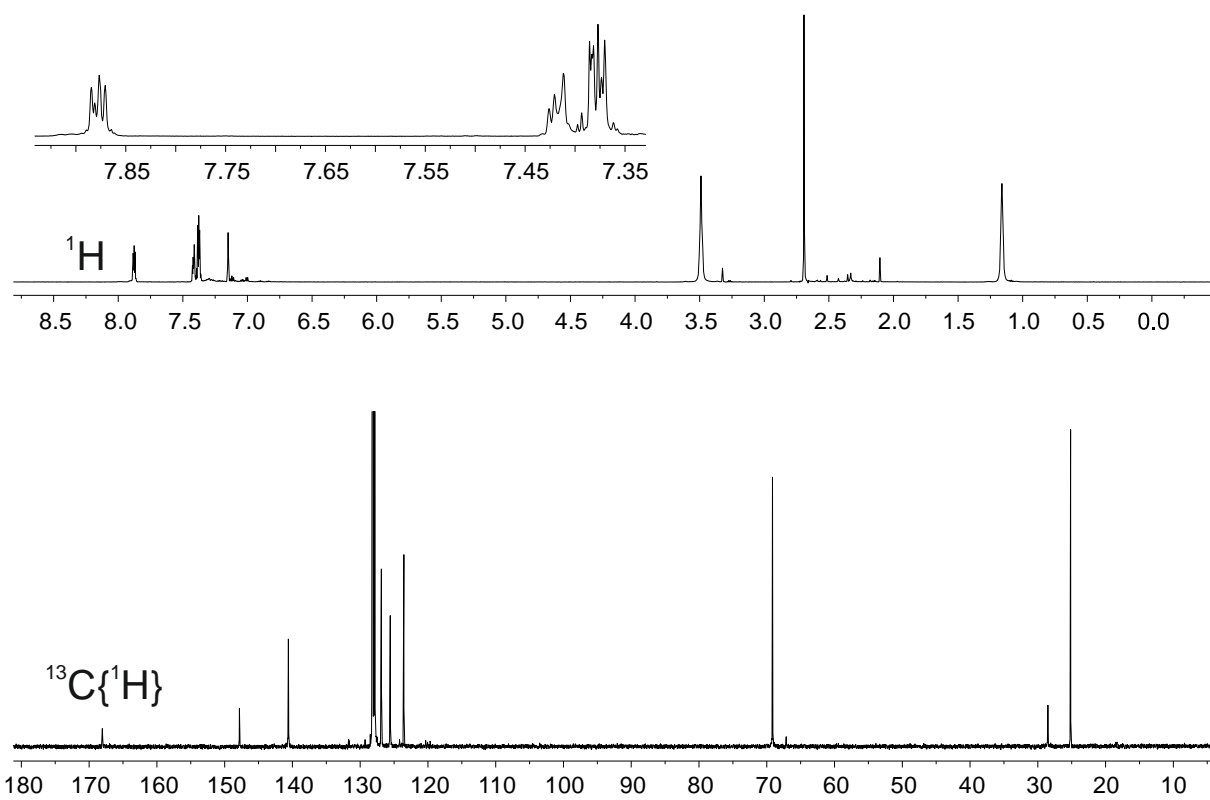
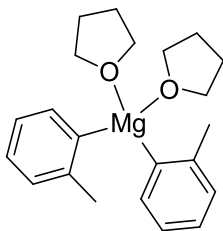
- (1) Maji, M. S.; Pfeifer, T.; Studer, A. *Angew. Chem., Int. Ed.* **2008**, *47*, 9547.
- (2) Su, X.; Fox, D. J.; Blackwell, D. T.; Tanaka, K.; Spring, D. R. *Chem. Commun.* **2006**, 3883.
- (3) (a) Markies, P. R.; Schat, G.; Akkerman, O. S.; Bickelhaupt, F.; Smeets, W. J. J.; van der Sluis, P.; Spek, S. L. *J. Organomet. Chem.* **1990**, *393*, 315-331. (b) Seidel, W.; Bürger, I. Z. *Anorg. Allg. Chem.* **1978**, *447*, 195-198. (c) Waggoner, K. M.; Power, P. P. *Organometallics* **1992**, *11*, 3209-3214. (d) Kerr, W. J.; Watson, A. J. B.; Hayes, D. *Org. Biomol. Chem.* **2008**, *6*, 1238-1243.
- (4) Screttas, C. G.; Maria-Screttas, M. *J. Organomet. Chem.* **1985**, *292*, 325-333.
- (5) Murarka, S.; Studer, A. *Angew. Chem. Int. Ed.* **2012**, *51*, 12362.



^1H NMR (600 MHz, C_6D_6) and $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, C_6D_6) spectra of diphenylmagnesium.



^1H NMR (600 MHz, C_6D_6) and $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, C_6D_6) spectra of di(ortho-tolyl)magnesium.



DFT Calculations: All calculations were performed with the TURBOMOLE 6.5 program. The structures were optimized without any geometry constraints using the B3LYP functional together with an atom-pairwise dispersion correction (D3). A flexible triple zeta basis set (def2-TZVP) was used in all calculations. The nature of transition structures (NIMAG=1) was proven by calculation of harmonic vibrational frequencies. Solution energies for THF were obtained in single point calculations with the COSMO model as implemented in Turbomole with $\epsilon = 7.58$.

Electronic energies of the intermediates and transition structures discussed in this work:

Structure	E(B3LYP-D3/def2-TZVP) [E _h]	E(B3LYP-D3/def2-TZVP) +COSMO($\epsilon=7.58$) [E _h]
THF	-232.4118506	-232.4165999
TEMPO	-483.6367556	-483.6437655
MgPh ₂ (THF) ₂	-1128.1419114	-1128.1588178
9-Cpx1	-1379.3659590	-1379.3842254
9-Int1	-1379.3458692	-1379.3588734
9-TS1	-1379.3403698	-1379.3545975
9-Pr1	-1379.3915842	-1379.4001860
(MgBrPh) ₂ (THF) ₂	-6476.5290708	-6476.5467151
10-Cpx1	-6727.7564295	-6727.7738721
10-Cpx2	-6727.7507343	-6727.7723078
10-Cpx3	-6727.7444976	-6727.7667175
10-Cpx4	-6727.7457547	-6727.7696737
10-Int1	-6727.7267368	-6727.7423383
10-Int2	-6727.7468151	-6727.7648905
10-TS1	-6727.7182913	-6727.7382905
10-TS2	-6727.7392718	-6727.7579805
10-Pr1	-6727.7764201	-6727.7946723
10-Pr2	-6727.7869920	-6727.8046269

Cartesian coordinates in Å of all structures discussed in this work:

Structure: **MgPh₂(THF)₂**

C	-2.4509282	1.3547968	-1.6581486
C	-3.4813592	1.7871794	-2.4908558
C	-3.8521872	1.0166140	-3.5872327
C	-3.1832722	-0.1776788	-3.8319198
C	-2.1559028	-0.5886336	-2.9848983
C	-1.7439100	0.1557783	-1.8648970
Mg	-0.1721513	-0.4395938	-0.5588249
C	2.1141212	-2.5875100	-0.7366034
C	2.9009694	-3.6645965	-0.3344367
C	2.5900237	-4.3539789	0.8326949
C	1.4872283	-3.9557275	1.5793890
C	0.7170234	-2.8742993	1.1554642
C	0.9942679	-2.1403267	-0.0121505
O	1.2618341	1.0753008	-0.6658647
C	2.6783845	0.9465597	-0.3835542
C	3.1531182	2.3685128	-0.1313527
C	2.2564392	3.1787798	-1.0736780
C	0.9218066	2.4556486	-0.9588011
O	-0.8770631	0.2443502	1.2978546
C	0.0033563	0.3974998	2.4388181
C	-0.8339755	0.0132718	3.6514037
C	-2.2533793	0.3783872	3.2032852
C	-2.2372907	-0.0140093	1.7348213
H	-2.1955909	1.9914665	-0.8113639
H	-3.9955413	2.7208423	-2.2870744
H	-4.6524907	1.3420215	-4.2414058

H	-3.4645246	-0.7886688	-4.6830221
H	-1.6634307	-1.5308525	-3.2131385
H	2.3933062	-2.0828620	-1.6597442
H	3.7541058	-3.9703349	-0.9308179
H	3.1958425	-5.1934903	1.1527282
H	1.2277308	-4.4897374	2.4875359
H	-0.1410380	-2.6045007	1.7694098
H	3.1639142	0.5020365	-1.2551431
H	2.7911496	0.2667880	0.4578150
H	2.9708291	2.6525494	0.9078745
H	4.2160653	2.4906983	-0.3362418
H	2.6327297	3.1221832	-2.0971122
H	2.1785678	4.2299484	-0.7984974
H	0.3180218	2.4676130	-1.8637685
H	0.3195728	2.8349263	-0.1292411
H	0.3242779	1.4418994	2.4750239
H	0.8685388	-0.2460707	2.2850738
H	-0.7568118	-1.0600222	3.8346334
H	-0.5175406	0.5365272	4.5530149
H	-2.4254736	1.4519506	3.3090753
H	-3.0277512	-0.1473011	3.7606771
H	-2.9020212	0.5633653	1.0967167
H	-2.4495912	-1.0772998	1.5964799

Structure: **(MgBrPh) 2 (THF) 2**

C	-2.8858248	1.4025501	-1.4145059
C	-3.8507253	1.3247471	-2.4165909
C	-4.6161456	0.1717857	-2.5540812
C	-4.4076231	-0.8914269	-1.6817977
C	-3.4375541	-0.7936064	-0.6864463
C	-2.6393667	0.3509678	-0.5145498
Mg	-1.0840412	0.4414136	0.8869641
Br	1.0445666	1.7250134	0.3144120
C	4.6154653	-2.1933198	-0.3164251
C	5.9984826	-2.3565037	-0.2994418
C	6.8159278	-1.3051292	0.1004315
C	6.2374130	-0.0991552	0.4795193
C	4.8520604	0.0454475	0.4562601
C	3.9903007	-0.9917245	0.0593035
Mg	1.9216798	-0.7246959	0.0013800
Br	0.0881828	-1.7781809	1.4907010
O	1.0647383	-1.0570752	-1.8256469
C	1.4165515	-0.1485654	-2.9000452
C	0.0728396	0.3142778	-3.4247566
C	-0.7799675	-0.9620508	-3.3497885
C	-0.1489505	-1.7718490	-2.2093817
O	-1.5446005	1.1458370	2.7224716
C	-0.5775781	1.2907712	3.8057190
C	-1.4190794	1.3431312	5.0704915
C	-2.7175389	1.9943503	4.5812169
C	-2.8988151	1.3699664	3.2071383
H	-2.3003829	2.3163722	-1.3471355
H	-4.0040949	2.1591827	-3.0919923
H	-5.3664580	0.1021776	-3.3324713
H	-4.9981418	-1.7955354	-1.7809632
H	-3.2959385	-1.6509493	-0.0327569
H	4.0123196	-3.0405260	-0.6343348
H	6.4395023	-3.3019414	-0.5959051
H	7.8927746	-1.4247425	0.1163391
H	6.8661288	0.7274082	0.7922313
H	4.4367081	1.0036882	0.7577265
H	1.9953274	-0.6996602	-3.6462747
H	2.0346473	0.6402379	-2.4752483
H	-0.3334979	1.0803181	-2.7647592
H	0.1372073	0.7212676	-4.4332554
H	-0.7239916	-1.5183319	-4.2862760
H	-1.8239960	-0.7387161	-3.1436351
H	0.1385014	-2.7789241	-2.5140809
H	-0.7784938	-1.8285781	-1.3272159
H	-0.0231824	2.2134922	3.6305034

H	0.1041727	0.4439629	3.7546475
H	-1.6137293	0.3347613	5.4409325
H	-0.9283924	1.9081873	5.8616382
H	-2.5948463	3.0758346	4.4955072
H	-3.5678214	1.7974931	5.2326127
H	-3.4094862	2.0026421	2.4839014
H	-3.4052339	0.4039031	3.2577137

Structure: **TEMPO**

N	-0.9390391	-0.1354696	0.0000000
C	-0.2434160	-0.0417677	1.3223680
C	1.1436481	-0.6923148	1.2390152
C	1.9302141	-0.2891630	0.0000000
C	1.1436481	-0.6923148	-1.2390152
C	-0.2434160	-0.0417677	-1.3223680
O	-2.1799236	0.1637341	0.0000000
C	-0.1452547	1.4352987	1.7349634
C	-1.0983476	-0.7963239	2.3421694
C	-0.1452547	1.4352987	-1.7349634
C	-1.0983476	-0.7963239	-2.3421694
H	1.6879099	-0.4406691	2.1522195
H	1.0201180	-1.7797870	1.2350103
H	2.9041874	-0.7839050	0.0000000
H	2.1314625	0.7850829	0.0000000
H	1.6879099	-0.4406691	-2.1522195
H	1.0201180	-1.7797870	-1.2350103
H	0.5489754	1.9932226	1.1080005
H	-1.1274416	1.9013602	1.6636574
H	0.2007980	1.5066274	2.7677311
H	-1.2444070	-1.8308714	2.0282152
H	-0.5914231	-0.7947984	3.3088540
H	-2.0746101	-0.3301164	2.4524647
H	0.5489754	1.9932226	-1.1080005
H	0.2007980	1.5066274	-2.7677311
H	-1.1274416	1.9013602	-1.6636574
H	-1.2444070	-1.8308714	-2.0282152
H	-2.0746101	-0.3301164	-2.4524647
H	-0.5914231	-0.7947984	-3.3088540

Structure: **THF**

O	0.0000000	0.0000000	-1.4863279
C	-1.1316266	-0.3097321	-0.6654297
C	-0.7578358	0.1104368	0.7547116
C	0.7578358	-0.1104368	0.7547116
C	1.1316266	0.3097321	-0.6654297
H	-2.0020230	0.2212021	-1.0563589
H	-1.3321972	-1.3866999	-0.7185253
H	-1.2808796	-0.4682311	1.5162049
H	-0.9864763	1.1671658	0.9125613
H	1.2808796	0.4682311	1.5162049
H	0.9864763	-1.1671658	0.9125613
H	2.0020230	-0.2212021	-1.0563589
H	1.3321972	1.3866999	-0.7185253

Structure: **9-Cpx1**

C	2.3496027	-2.8256267	-0.1592643
C	2.7776107	-4.1489836	-0.0761820
C	2.9982121	-4.7285900	1.1681681
C	2.7959513	-3.9654007	2.3126633
C	2.3700250	-2.6431317	2.2016243
C	2.1191074	-2.0156362	0.9683511
Mg	1.4221394	-0.0112225	0.7201213
C	2.6843317	2.6318207	-0.3855171
C	3.1402672	3.9485052	-0.3759344
C	3.1286923	4.6785178	0.8078572
C	2.6652600	4.0726840	1.9703686
C	2.2154946	2.7537614	1.9338420
C	2.1984185	1.9779508	0.7608966
N	-0.9121463	-0.0609325	-1.4989442
C	-1.5832251	-1.4020881	-1.5362710

C	-3.0539381	-1.2336208	-1.9379748
C	-3.2617639	-0.2955834	-3.1178765
C	-2.7312251	1.0819090	-2.7493816
C	-1.2387985	1.0971192	-2.3951099
O	0.2603052	-0.0334555	-0.9942115
C	-0.8262315	-2.2945998	-2.5311654
C	-1.4994073	-2.0133314	-0.1370717
C	-0.3576828	0.9959014	-3.6494570
C	-0.9045016	2.3813652	-1.6346790
O	-0.1808312	0.1794845	2.0660204
C	-1.0495373	1.3365450	2.1027400
C	-1.5970801	1.3693004	3.5196782
C	-1.6799170	-0.1215115	3.8646875
C	-0.4231236	-0.6778579	3.2102984
H	2.1975540	-2.4126951	-1.1546219
H	2.9423595	-4.7274569	-0.9792871
H	3.3303483	-5.7572642	1.2448020
H	2.9755481	-4.4002525	3.2903810
H	2.2395366	-2.0861860	3.1270707
H	2.7134412	2.0989439	-1.3343111
H	3.5065037	4.4062455	-1.2890137
H	3.4810870	5.7031845	0.8251514
H	2.6583343	4.6274392	2.9029457
H	1.8671822	2.3197785	2.8705642
H	-3.4519512	-2.2286963	-2.1461303
H	-3.6109843	-0.8460420	-1.0790124
H	-4.3249024	-0.2313851	-3.3589839
H	-2.7662821	-0.6792224	-4.0129981
H	-2.8835506	1.7972574	-3.5600407
H	-3.2979636	1.4561050	-1.8912015
H	-0.9331316	-1.9501621	-3.5586118
H	-1.2192469	-3.3101366	-2.4692395
H	0.2309956	-2.3227771	-2.2757188
H	-1.9398120	-1.3424502	0.6011631
H	-0.4725938	-2.2299146	0.1503745
H	-2.0613572	-2.9482651	-0.1310455
H	-0.6234885	0.1429005	-4.2720145
H	0.6885404	0.9057063	-3.3609408
H	-0.4763402	1.9021782	-4.2445124
H	-1.4909802	2.4494946	-0.7176820
H	-1.1567391	3.2370804	-2.2624897
H	0.1490928	2.4384267	-1.3735195
H	-0.4552443	2.2039296	1.8236228
H	-1.8452459	1.1881930	1.3660983
H	-2.5571759	1.8805267	3.5809035
H	-0.8942970	1.8787052	4.1824253
H	-1.7044803	-0.3167491	4.9360563
H	-2.5723796	-0.5657339	3.4178238
H	0.4431785	-0.6124923	3.8714746
H	-0.5115639	-1.7015060	2.8522417

Structure: **9-Int1**

C	2.5162974	2.3468530	-1.2304388
C	3.4224041	2.9392949	-2.1087165
C	3.8827013	2.2337884	-3.2143024
C	3.4398164	0.9335404	-3.4359234
C	2.5344408	0.3438761	-2.5578826
C	2.0390416	1.0608476	-1.4748281
Mg	0.2471370	0.5544137	-0.2238991
C	3.0173186	-0.0462409	1.3449330
C	3.8815573	-0.8920059	2.0354873
C	3.7695868	-2.2713273	1.8904360
C	2.7933614	-2.7987009	1.0521080
C	1.9252708	-1.9486799	0.3695854
C	2.0097570	-0.5672643	0.5384043
O	0.2515553	2.2186723	1.0523278
C	0.6746252	2.3172086	2.4296991
C	-0.4087692	3.1360650	3.1106672
C	-0.8166870	4.1136790	2.0031042
C	-0.7207734	3.2612540	0.7427384

H	2.1799450	2.9062847	-0.3650487
H	3.7716407	3.9490544	-1.9243098
H	4.5938951	2.6889103	-3.8923478
H	3.8088852	0.3723832	-4.2866243
H	2.2266331	-0.6796036	-2.7315565
H	3.1493038	1.0259581	1.4331135
H	4.6532953	-0.4747640	2.6723157
H	4.4486412	-2.9306753	2.4167277
H	2.7065986	-3.8720670	0.9270529
H	1.1662143	-2.3806641	-0.2724111
H	0.7892977	1.3074508	2.8175201
H	1.6453602	2.8202383	2.4627234
H	-0.0474310	3.6331772	4.0102483
H	-1.2482169	2.4948028	3.3857199
H	-1.8173394	4.5211897	2.1410790
H	-0.1144398	4.9488105	1.9596880
H	-1.6519892	2.7583909	0.4828443
H	-0.3550672	3.8084972	-0.1261459
N	-1.5054946	-0.7472210	-0.4422292
C	-1.8390174	-1.4633382	-1.7165165
C	-1.7798039	-2.9781439	-1.4664303
C	-2.6136800	-3.4287547	-0.2763465
C	-2.1786798	-2.6573053	0.9609564
C	-2.2701980	-1.1341258	0.7873999
O	-1.6178036	0.6790338	-0.6542551
C	-3.1905446	-1.0437164	-2.3150900
C	-0.7439680	-1.1087985	-2.7242964
C	-3.7283327	-0.6485957	0.7838255
C	-1.5668691	-0.4834598	1.9834847
H	-2.4857437	-4.5019705	-0.1133667
H	-3.6776057	-3.2738432	-0.4719529
H	-2.7775934	-2.9391704	1.8310034
H	-1.1402853	-2.9149514	1.1923389
H	-4.0377201	-1.5067685	-1.8148541
H	-3.2294549	-1.3360726	-3.3660052
H	-3.2916160	0.0382671	-2.2496143
H	0.2370243	-1.3782530	-2.3295656
H	-0.7511953	-0.0456676	-2.9586549
H	-0.8904958	-1.6666378	-3.6506556
H	-4.3806507	-1.2709880	0.1767369
H	-3.7664130	0.3711250	0.4036949
H	-4.1198566	-0.6588182	1.8030212
H	-0.5080053	-0.7554463	2.0080158
H	-2.0165405	-0.8306266	2.9151122
H	-1.6644294	0.5994320	1.9423262
H	-2.0919949	-3.4872748	-2.3819691
H	-0.7369003	-3.2605578	-1.2902020

Structure: **9-TS1**

C	2.3915649	2.3307190	-1.3210063
C	3.3473274	2.8508737	-2.1776828
C	3.8588781	2.0813971	-3.2226908
C	3.3878500	0.7771227	-3.3945041
C	2.4314579	0.2551769	-2.5438301
C	1.8725018	1.0146764	-1.4816753
Mg	0.0421842	0.6962477	-0.3966356
C	3.0881762	0.4585275	1.1683177
C	3.7271047	-0.3441307	2.1089419
C	3.5193661	-1.7210894	2.1065896
C	2.6818650	-2.2916050	1.1534817
C	2.0468552	-1.4833665	0.2137879
C	2.2235456	-0.1033178	0.2379882
O	0.0080209	2.3222011	0.9033864
C	0.5644669	2.4901301	2.2270716
C	-0.5192707	3.2054517	3.0145695
C	-1.1412574	4.1162233	1.9511327
C	-1.1019839	3.2494413	0.6984508
H	2.0181677	2.9608818	-0.5205301
H	3.6944145	3.8691395	-2.0387296
H	4.6108322	2.4864275	-3.8874682

H	3.7745405	0.1672264	-4.2034013
H	2.1120742	-0.7693911	-2.6974316
H	3.2832499	1.5253015	1.1505105
H	4.3972759	0.1004895	2.8361085
H	4.0214810	-2.3475044	2.8332883
H	2.5257734	-3.3641807	1.1393229
H	1.4027180	-1.9420546	-0.5285319
H	0.8258394	1.5061456	2.6087692
H	1.4748297	3.0903668	2.1485057
H	-0.1170722	3.7521067	3.8667884
H	-1.2547332	2.4873110	3.3827334
H	-2.1559873	4.4274906	2.1955433
H	-0.5335298	5.0139081	1.8201731
H	-1.9978502	2.6449654	0.5595186
H	-0.8999912	3.8112446	-0.2133524
N	-1.4841389	-0.8231828	-0.4430015
C	-1.8950028	-1.5417700	-1.6952836
C	-1.5054406	-3.0207813	-1.5550575
C	-2.0383360	-3.6663532	-0.2835166
C	-1.5753770	-2.8678597	0.9270018
C	-1.9670879	-1.3839950	0.8626017
O	-1.8654715	0.5698298	-0.5439602
C	-3.3859979	-1.3787929	-2.0304771
C	-1.0925425	-0.9383447	-2.8503635
C	-3.4707796	-1.1785266	1.1028018
C	-1.2184470	-0.6481304	1.9800010
H	-1.6822487	-4.6970320	-0.2087442
H	-3.1292776	-3.7222339	-0.3117589
H	-1.9797850	-3.2882317	1.8516112
H	-0.4857850	-2.9329848	1.0005816
H	-4.0298461	-2.0252983	-1.4398296
H	-3.5488149	-1.6251884	-3.0810855
H	-3.6802933	-0.3434277	-1.8671504
H	-0.0209109	-0.9862505	-2.6555515
H	-1.3699378	0.1009734	-3.0186898
H	-1.2859292	-1.4984440	-3.7667344
H	-4.0877396	-1.8967272	0.5696580
H	-3.7512604	-0.1743798	0.7886922
H	-3.6876031	-1.2865183	2.1672494
H	-0.1355191	-0.7222588	1.8450294
H	-1.4525608	-1.1003136	2.9448760
H	-1.5141868	0.3986724	2.0144703
H	-1.8575238	-3.5533852	-2.4422069
H	-0.4128415	-3.0936181	-1.5586733

Structure: **9-Pr1**

Mg	-0.1927639	0.5036146	-1.1188939
N	-2.0452122	-0.6687180	-0.6824248
C	-3.0794684	-0.1376435	0.2618305
C	-4.3977850	0.0484310	-0.5037694
C	-4.8414116	-1.1994270	-1.2530514
C	-3.7311028	-1.6340373	-2.1986077
C	-2.3909419	-1.8790537	-1.4887342
O	-0.8141287	-0.9007715	0.0339480
C	-3.2691331	-1.0159756	1.5096564
C	-2.6036877	1.2420973	0.7267406
C	-2.4168871	-3.1769999	-0.6646581
C	-1.3102486	-2.0318963	-2.5647577
O	1.6906975	-0.3875833	-1.4823767
C	2.8501206	0.2703074	-2.0692109
C	4.0282469	-0.6726867	-1.8291977
C	3.5609038	-1.5272247	-0.6459697
C	2.0758354	-1.6685384	-0.9225501
H	-5.1622283	0.3744807	0.2064766
H	-4.2642484	0.8621767	-1.2238590
H	-5.7555869	-0.9951379	-1.8165469
H	-5.0865448	-2.0022445	-0.5531557
H	-4.0049738	-2.5456748	-2.7365001
H	-3.5836612	-0.8518329	-2.9504874
H	-3.8734557	-1.8997391	1.3187371

H	-3.7667639	-0.4379501	2.2908951
H	-2.2931705	-1.3291156	1.8756639
H	-2.4133211	1.8947478	-0.1299184
H	-1.6969920	1.1653117	1.3227212
H	-3.3730445	1.7127891	1.3427164
H	-3.3285061	-3.2900187	-0.0830138
H	-1.5654813	-3.1850374	0.0142285
H	-2.3425890	-4.0380960	-1.3321340
H	-1.1870852	-1.0991417	-3.1247052
H	-1.5968543	-2.8096617	-3.2750343
H	-0.3562639	-2.3110249	-2.1229824
H	2.6461957	0.4458515	-3.1252402
H	2.9726471	1.2262477	-1.5655106
H	4.9427871	-0.1201486	-1.6190871
H	4.2025978	-1.3027796	-2.7036366
H	4.0660495	-2.4913751	-0.5891881
H	3.7232184	-0.9952504	0.2918708
H	1.8828153	-2.4475118	-1.6663053
H	1.4401998	-1.8421176	-0.0583322
C	3.9313676	1.6122872	1.2961230
C	4.9644471	2.0612891	0.4834627
C	4.7461912	3.1037852	-0.4109919
C	3.4872603	3.6893283	-0.4872169
C	2.4535846	3.2362699	0.3230269
C	2.6617176	2.1935079	1.2316744
C	1.3530901	0.3555579	2.3117619
C	1.5686326	1.7203155	2.1069885
C	0.7290209	2.6315303	2.7557655
C	-0.2817631	2.1885024	3.5967483
C	-0.4833172	0.8262797	3.7919672
C	0.3322346	-0.0888798	3.1396229
H	4.1140536	0.8219110	2.0131445
H	5.9442391	1.6059969	0.5587225
H	5.5510091	3.4579496	-1.0426436
H	3.3038470	4.4920269	-1.1903349
H	1.4678384	3.6734258	0.2345934
H	1.9706204	-0.3641831	1.7917920
H	0.8897414	3.6930641	2.6170134
H	-0.9169693	2.9081296	4.0979342
H	-1.2843363	0.4807560	4.4325662
H	0.1587171	-1.1504920	3.2526346

Structure: **10-Cpx1**

C	-3.7483886	2.2117080	1.2461078
C	-5.0474416	2.6723517	1.4499467
C	-6.0575486	1.7755343	1.7791958
C	-5.7533219	0.4241654	1.9038161
C	-4.4491366	-0.0173040	1.6938437
C	-3.3996301	0.8541385	1.3549376
Mg	-1.4461876	0.2192211	0.9462257
Br	0.3557952	2.1135004	0.9880021
C	3.6003357	-2.0109423	0.6082967
C	4.5509819	-2.5950577	-0.2260213
C	5.3186581	-1.7970105	-1.0668774
C	5.1293808	-0.4189595	-1.0570179
C	4.1762518	0.1456408	-0.2128371
C	3.3739407	-0.6241065	0.6464093
Mg	1.8212917	0.1881507	1.7935245
Br	-0.0955827	-1.4395803	2.3935937
N	-0.9424051	-0.5169134	-2.0991358
C	0.3904212	-0.8480166	-2.7048354
C	0.2115823	-1.1567426	-4.1962220
C	-0.6782391	-0.1573461	-4.9209394
C	-2.0587823	-0.1671310	-4.2816184
C	-2.0620175	0.1992047	-2.7895993
O	-0.9829466	-0.5640017	-0.8227220
C	1.3292824	0.3480743	-2.4887430
C	0.9405130	-2.0765585	-1.9807984
C	-1.8760881	1.7098281	-2.5789689
C	-3.3815334	-0.2550209	-2.1625261

O	2.2821763	0.7636254	3.6930506
C	3.1730603	-0.0984724	4.4529135
C	2.3502379	-0.5160755	5.6561650
C	1.5697096	0.7667828	5.9662552
C	1.2712679	1.3375871	4.5820415
H	-2.9846772	2.9449016	0.9973035
H	-5.2720641	3.7291683	1.3545032
H	-7.0702719	2.1258707	1.9399440
H	-6.5325763	-0.2835797	2.1649526
H	-4.2534382	-1.0816503	1.7993310
H	3.0036523	-2.6702842	1.2343288
H	4.6895343	-3.6707561	-0.2257258
H	6.0579142	-2.2434185	-1.7214341
H	5.7245142	0.2130813	-1.7073053
H	4.0517608	1.2253299	-0.2430174
H	1.2076055	-1.1973273	-4.6412430
H	-0.2221284	-2.1561219	-4.2996227
H	-0.7586572	-0.4282124	-5.9758262
H	-0.2426041	0.8441513	-4.8932012
H	-2.7354907	0.5246988	-4.7872007
H	-2.4898295	-1.1665862	-4.3932799
H	1.0609504	1.1999057	-3.1120483
H	2.3480914	0.0468729	-2.7312716
H	1.3154346	0.6635170	-1.4485546
H	0.2367848	-2.9081461	-2.0405776
H	1.1515954	-1.8685663	-0.9365159
H	1.8751776	-2.3724607	-2.4574394
H	-1.0003315	2.0937693	-3.0990269
H	-1.7757331	1.9457919	-1.5206294
H	-2.7573723	2.2297350	-2.9559981
H	-3.4582435	-1.3431292	-2.1704991
H	-4.2019498	0.1506938	-2.7562280
H	-3.5016580	0.0992555	-1.1413308
H	3.4808002	-0.9139927	3.7998119
H	4.0543861	0.4828170	4.7347274
H	2.9703710	-0.8497236	6.4872553
H	1.6692634	-1.3226466	5.3798748
H	0.6553092	0.5814740	6.5276483
H	2.1883428	1.4570221	6.5429374
H	0.2970004	1.0271895	4.2076327
H	1.3529001	2.4210821	4.5222620

Structure: **10-Cpx2**

C	-4.1617616	1.7583005	0.3905649
C	-5.5482479	1.7950286	0.2622436
C	-6.3309510	0.8509369	0.9181737
C	-5.7141528	-0.1155411	1.7050306
C	-4.3259984	-0.1373495	1.8187809
C	-3.4985056	0.7903956	1.1626497
Mg	-1.4102995	0.6186598	1.2185907
Br	0.1676469	2.6554091	1.1263865
C	3.4259329	3.1143143	4.0650995
C	4.5424096	3.5616205	4.7678458
C	5.5759269	2.6805392	5.0663585
C	5.4800338	1.3553141	4.6568269
C	4.3551576	0.9277471	3.9548680
C	3.2876867	1.7846518	3.6329863
Mg	1.6830998	1.0769890	2.4920465
Br	-0.1515629	-0.6258506	3.0818449
N	-1.0071604	-0.8516782	-1.5552224
C	-0.6651397	0.1269351	-2.6349958
C	-0.5536704	-0.6097092	-3.9783177
C	-1.6628617	-1.6210825	-4.2280096
C	-1.6585153	-2.6550912	-3.1106826
C	-1.8951720	-2.0479075	-1.7215173
O	-0.7806612	-0.4741426	-0.3545913
C	-1.7480917	1.2154156	-2.6671661
C	0.6867931	0.7543335	-2.2917896
C	-3.3593048	-1.6188059	-1.5405703
C	-1.5180645	-3.0588078	-0.6382090

O	2.5556735	0.0168715	0.9627806
C	2.4389517	-1.3853886	0.6167192
C	3.8032496	-1.7530105	0.0602613
C	4.2241773	-0.4636534	-0.6535472
C	3.6791034	0.6266935	0.2613730
H	-3.5874902	2.5200528	-0.1312489
H	-6.0193736	2.5607344	-0.3444592
H	-7.4100971	0.8731076	0.8235970
H	-6.3153360	-0.8489600	2.2311590
H	-3.8817503	-0.9091089	2.4428177
H	2.6406132	3.8336681	3.8492420
H	4.6077273	4.5970519	5.0837512
H	6.4461194	3.0226170	5.6138750
H	6.2781936	0.6580882	4.8880252
H	4.3171825	-0.1184342	3.6550300
H	-0.5226461	0.1461105	-4.7656380
H	0.4076049	-1.1322932	-4.0062479
H	-1.5018199	-2.1125457	-5.1896493
H	-2.6341817	-1.1260971	-4.2949215
H	-2.4259988	-3.4144189	-3.2722537
H	-0.6942188	-3.1733955	-3.1106223
H	-2.7111026	0.8322880	-2.9975701
H	-1.4378101	2.0049211	-3.3525672
H	-1.8788561	1.6558453	-1.6800417
H	1.4464721	-0.0195076	-2.1749560
H	0.6429935	1.3441792	-1.3800026
H	0.9861707	1.4054809	-3.1139637
H	-3.7143992	-1.0027455	-2.3640633
H	-3.4960621	-1.0622333	-0.6155853
H	-3.9811909	-2.5140957	-1.4973861
H	-0.4546838	-3.2991638	-0.6806368
H	-2.0854335	-3.9747528	-0.8057600
H	-1.7482314	-2.6868942	0.3571921
H	2.1535315	-1.9260518	1.5155300
H	1.6418755	-1.4883020	-0.1218375
H	3.7585114	-2.6153463	-0.6042130
H	4.4937738	-1.9821551	0.8742172
H	5.3021680	-0.3795236	-0.7831472
H	3.7597278	-0.4064961	-1.6396895
H	4.3977757	0.9458592	1.0160633
H	3.3045200	1.5003804	-0.2708515

Structure: **10-Cpx3**

C	1.7513056	0.7128622	4.3450092
C	1.2890690	1.0667535	5.6113538
C	0.9254278	2.3833159	5.8757300
C	1.0301822	3.3302478	4.8622994
C	1.4905085	2.9536165	3.6015563
C	1.8682115	1.6356154	3.2900567
Mg	-0.7436736	0.7224314	0.2314559
Br	0.6312118	2.7376228	-0.0680626
C	3.9349287	-0.9502719	-0.4906239
C	4.5563769	-1.4157756	-1.6473472
C	4.9006148	-0.5240620	-2.6580341
C	4.6219195	0.8282646	-2.4911712
C	3.9974227	1.2722724	-1.3272476
C	3.6246003	0.4054614	-0.2857709
Mg	2.3903526	1.0363138	1.3165046
Br	0.5566160	-1.1467309	1.1772242
N	-1.2999087	-1.0803612	-1.9588255
C	-0.2080561	-1.0832653	-2.9921488
C	0.3686693	-2.5022943	-3.0917616
C	-0.6894872	-3.5930034	-3.1742516
C	-1.5801246	-3.5306827	-1.9413006
C	-2.2933291	-2.1827490	-1.7612681
O	-1.5956867	0.0525318	-1.4178744
C	-0.8057351	-0.6030745	-4.3256853
C	0.8938678	-0.1218395	-2.5598415
C	-3.4400563	-1.9962541	-2.7692381
C	-2.8534001	-2.0900722	-0.3411887

O	-2.0826372	1.2776203	1.6220728
C	-1.7963122	0.9501962	3.0369728
C	-2.3427277	2.1200798	3.8410349
C	-2.3032289	3.2772731	2.8387450
C	-2.7037582	2.5954539	1.5464389
H	2.0122457	-0.3289828	4.1782784
H	1.2156273	0.3183045	6.3931759
H	0.5685841	2.6676291	6.8588989
H	0.7526826	4.3615192	5.0550200
H	1.5433807	3.7207028	2.8337745
H	3.6649075	-1.6835662	0.2647721
H	4.7739102	-2.4727685	-1.7613876
H	5.3837661	-0.8779020	-3.5615204
H	4.8876665	1.5354711	-3.2699456
H	3.7774362	2.3336205	-1.2486160
H	1.0290866	-2.5236290	-3.9604448
H	0.9975124	-2.6740019	-2.2144432
H	-0.2052516	-4.5701874	-3.2246610
H	-1.2810935	-3.4977578	-4.0885863
H	-2.3481443	-4.3066547	-1.9673459
H	-0.9689294	-3.7131834	-1.0534988
H	-1.4900053	-1.3239739	-4.7676526
H	0.0118456	-0.4371738	-5.0277323
H	-1.3310039	0.3415168	-4.1846292
H	1.2898671	-0.3782779	-1.5795035
H	0.5630573	0.9135837	-2.5556750
H	1.7242685	-0.2082528	-3.2602556
H	-3.1357494	-2.2051325	-3.7919200
H	-3.8240259	-0.9773514	-2.7192864
H	-4.2479246	-2.6815684	-2.5101053
H	-2.0529581	-2.1176758	0.3974400
H	-3.5007523	-2.9517526	-0.1749521
H	-3.4432048	-1.1868715	-0.1969097
H	-2.2747142	-0.0037803	3.2484883
H	-0.7186083	0.8522944	3.1420990
H	-1.7234837	2.3056680	4.7159111
H	-3.3678981	1.9283293	4.1655911
H	-2.9758072	4.0936854	3.0997193
H	-1.2883550	3.6670338	2.7531410
H	-3.7841497	2.4532419	1.4654152
H	-2.3269483	3.0903481	0.6525337

Structure: **10-Cpx4**

C	1.1254009	0.6299473	3.8190140
C	1.1002296	1.7838182	4.5993607
C	1.7651841	2.9272977	4.1698860
C	2.4653553	2.8941031	2.9688308
C	2.4823938	1.7275538	2.2069261
C	1.8038120	0.5570897	2.5899106
Mg	-1.8541141	-1.9573234	0.3311620
Br	-4.2394855	-2.2610860	0.5176120
C	2.9937878	-3.3896452	-0.3830444
C	3.5300016	-3.9945249	-1.5166663
C	3.9218485	-3.2148137	-2.6003249
C	3.7924502	-1.8327609	-2.5237313
C	3.2646286	-1.2465683	-1.3746235
C	2.8283745	-1.9968474	-0.2693005
Mg	1.8068839	-1.1874243	1.3957656
Br	-0.1548402	-2.8185437	1.9733806
N	-1.2201065	1.1140500	0.3273807
C	-2.1679553	1.5669835	1.3964880
C	-1.6398295	2.8858105	1.9788238
C	-1.2561970	3.9102081	0.9207748
C	-0.1587676	3.3335434	0.0393049
C	-0.5443528	2.0204567	-0.6550362
O	-1.2243513	-0.1239231	-0.0062014
C	-3.5708461	1.7214017	0.7862209
C	-2.2117348	0.5079501	2.4974183
C	-1.5002488	2.2488003	-1.8377921
C	0.7206306	1.3227401	-1.1516237

O	-1.3553571	-2.7335903	-1.4554267
C	-0.0113165	-3.1636941	-1.8465672
C	-0.0834170	-3.3557098	-3.3500220
C	-1.5456405	-3.7576729	-3.5681269
C	-2.2806209	-2.8769228	-2.5725786
H	0.5923841	-0.2415929	4.1897604
H	0.5616972	1.7923840	5.5405371
H	1.7479188	3.8294825	4.7695626
H	3.0015943	3.7741293	2.6305088
H	3.0539005	1.7419802	1.2816337
H	2.6716751	-4.0370895	0.4284521
H	3.6400536	-5.0728030	-1.5585959
H	4.3323714	-3.6784533	-3.4894531
H	4.1060790	-1.2133095	-3.3569953
H	3.1864158	-0.1631631	-1.3569332
H	-2.4134851	3.2772486	2.6423186
H	-0.7664211	2.6663144	2.5975359
H	-0.8901739	4.8163126	1.4073334
H	-2.1249486	4.2081860	0.3275869
H	0.1380645	4.0399854	-0.7387879
H	0.7201329	3.1469389	0.6593674
H	-3.6370363	2.5571635	0.0932763
H	-4.2789785	1.8976361	1.5969264
H	-3.8716548	0.8058356	0.2776078
H	-1.2114318	0.1885350	2.7759372
H	-2.8190854	-0.3523069	2.2189382
H	-2.6808238	0.9524244	3.3756884
H	-2.3545748	2.8658164	-1.5691561
H	-1.8649324	1.2942023	-2.2172544
H	-0.9560843	2.7527886	-2.6372624
H	1.3712852	1.0789272	-0.3136678
H	1.2598059	2.0078004	-1.8066479
H	0.5000599	0.4148514	-1.7066218
H	0.6969870	-2.4048683	-1.5302572
H	0.2062732	-4.0890955	-1.3145558
H	0.6307570	-4.1028510	-3.6910911
H	0.1393322	-2.4180412	-3.8634823
H	-1.8903578	-3.5921734	-4.5881827
H	-1.6945502	-4.8113518	-3.3233132
H	-2.4776364	-1.8804463	-2.9755827
H	-3.2064125	-3.2921002	-2.1823248

Structure: **10-Int1**

C	3.2991065	0.9934417	2.6449004
C	3.1595464	1.7539876	3.8040593
C	2.7521522	3.0822093	3.7190057
C	2.4928803	3.6527879	2.4768544
C	2.6292206	2.8917395	1.3165372
C	2.9956352	1.5531009	1.4099531
Mg	-0.8040480	-0.0358517	-0.7204407
Br	0.9803759	1.4721928	-1.9799521
C	5.4454065	-0.4984463	0.1564710
C	6.8059449	-0.5398903	-0.1372454
C	7.3689853	0.4304276	-0.9602273
C	6.5740468	1.4414739	-1.4906877
C	5.2132669	1.4828915	-1.1980931
C	4.6410029	0.4904058	-0.4052328
Mg	2.4841204	0.3244596	-0.3393296
Br	1.0560936	-1.6952815	0.1356953
O	-0.7066086	1.1315087	0.9587347
C	-0.4550940	0.8190014	2.3556845
C	-1.3570216	1.7650366	3.1265363
C	-1.3322678	3.0202636	2.2488455
C	-1.3263926	2.4483808	0.8380117
H	3.6280167	-0.0365769	2.7206256
H	3.3765275	1.3130112	4.7698120
H	2.6545557	3.6769786	4.6186800
H	2.1916295	4.6917548	2.4082174
H	2.4209049	3.3461872	0.3543239
H	5.0241181	-1.2537085	0.8116350

H	7.4260684	-1.3236669	0.2815913
H	8.4294070	0.4055173	-1.1781976
H	7.0140968	2.2028673	-2.1237992
H	4.6076606	2.2853439	-1.6051121
H	-0.6748990	-0.2346392	2.5049761
H	0.5987623	1.0010504	2.5616167
H	-0.9878851	1.9440402	4.1355829
H	-2.3687018	1.3594116	3.1929312
H	-2.1848131	3.6773787	2.4156582
H	-0.4177965	3.5851855	2.4331034
H	-2.3273600	2.2959620	0.4319556
H	-0.7336128	3.0258717	0.1306961
N	-2.4437052	-1.2289295	-1.3418296
C	-2.4557756	-1.7748552	-2.7403177
C	-2.3569909	-3.3055251	-2.6647354
C	-3.4098936	-3.9324887	-1.7628056
C	-3.3020857	-3.3252774	-0.3717317
C	-3.4291982	-1.7944534	-0.3650911
O	-2.5699745	0.2177615	-1.3812923
C	-3.6722281	-1.3188706	-3.5593550
C	-1.1969973	-1.2529195	-3.4396881
C	-4.8729241	-1.3389871	-0.6252510
C	-3.0235785	-1.2964678	1.0256235
H	-3.2639488	-5.0143906	-1.7110050
H	-4.4106252	-3.7782218	-2.1739550
H	-4.0639388	-3.7339693	0.2973645
H	-2.3284251	-3.5910564	0.0525326
H	-4.5769100	-1.8715880	-3.3186454
H	-3.4704314	-1.4651484	-4.6219888
H	-3.8488337	-0.2594492	-3.3806399
H	-0.2959448	-1.5173403	-2.8775969
H	-1.2355479	-0.1731938	-3.5714718
H	-1.1025296	-1.7114027	-4.4252883
H	-5.3469510	-1.8822866	-1.4385076
H	-4.8774957	-0.2766864	-0.8640821
H	-5.4739587	-1.5000945	0.2718040
H	-1.9904747	-1.5784852	1.2456141
H	-3.6565829	-1.7566562	1.7858579
H	-3.1300899	-0.2154548	1.0966043
H	-2.4221167	-3.7017546	-3.6812629
H	-1.3648745	-3.5676165	-2.2832367

Structure: **10-Int2**

C	2.6452994	2.2001956	-0.1201765
C	3.4519633	2.9258744	-0.9948241
C	3.8006132	2.3915562	-2.2301902
C	3.3584649	1.1192719	-2.5779558
C	2.5555019	0.3951314	-1.7003166
C	2.1504195	0.9500184	-0.4898538
Mg	0.4684343	0.2293041	0.8006505
C	3.0324360	-0.4415150	2.4249913
C	3.9468144	-1.2953576	3.0374964
C	4.1089771	-2.5952547	2.5693436
C	3.3571168	-3.0436390	1.4879289
C	2.4409424	-2.1908512	0.8775517
C	2.2526099	-0.9024235	1.3686491
O	-1.3322398	3.1749393	-0.5407168
C	-0.4019882	4.2994852	-0.5139800
C	0.1096908	4.4509033	-1.9486706
C	-0.2711507	3.1224369	-2.6156047
C	-1.5680813	2.7750847	-1.9119596
H	2.3964971	2.6284111	0.8427504
H	3.8156282	3.9046737	-0.7031477
H	4.4338339	2.9514278	-2.9072220
H	3.6492207	0.6832616	-3.5266367
H	2.2536395	-0.6048532	-1.9834020
H	2.9252020	0.5740441	2.7886638
H	4.5390187	-0.9418634	3.8734235
H	4.8286996	-3.2542163	3.0387433
H	3.4873682	-4.0534823	1.1163510

H	1.8693768	-2.5539784	0.0302368
H	-0.9412012	5.1755117	-0.1542346
H	0.3815743	4.0398584	0.1929356
H	1.1832264	4.6271347	-1.9707555
H	-0.3870264	5.2846880	-2.4471789
H	-0.3937094	3.2101276	-3.6945215
H	0.4838693	2.3629753	-2.4092935
H	-2.4183070	3.3419903	-2.3014795
H	-1.8113792	1.7159501	-1.8976625
N	-1.3336234	-1.0532994	0.4397249
C	-1.6287661	-1.6579545	-0.9022220
C	-1.4724543	-3.1825598	-0.7838122
C	-2.2686314	-3.7905217	0.3591561
C	-1.8827411	-3.0979063	1.6562923
C	-2.0960220	-1.5744710	1.6268487
O	-1.4461554	0.3806384	0.3130533
C	-3.0064143	-1.2730498	-1.4621027
C	-0.5516703	-1.1648861	-1.8684000
C	-3.5891382	-1.2209593	1.6386986
C	-1.4568780	-1.0028714	2.8946344
H	-2.0597332	-4.8604295	0.4299075
H	-3.3418493	-3.6999557	0.1764460
H	-2.4538785	-3.4947519	2.4982940
H	-0.8265040	-3.2932344	1.8657112
H	-3.8143471	-1.8603129	-1.0351459
H	-3.0159739	-1.4365802	-2.5407116
H	-3.2163204	-0.2216570	-1.2745369
H	0.4382462	-1.4195682	-1.4906050
H	-0.5969870	-0.0898292	-2.0249789
H	-0.6696626	-1.6545158	-2.8356788
H	-4.1738386	-1.8257010	0.9514764
H	-3.7616369	-0.1728176	1.4024733
H	-3.9828657	-1.3917166	2.6415757
H	-0.3726297	-1.1473061	2.8964131
H	-1.8519557	-1.5313620	3.7627686
H	-1.6708684	0.0531041	3.0392281
H	-1.7537477	-3.6232459	-1.7432695
H	-0.4128014	-3.4074664	-0.6293967
Br	0.1037808	2.2606770	2.4908569
Mg	-2.0031010	2.0872828	1.0434176
Br	-4.2321866	2.7104062	1.6539508

Structure: **10-TS1**

C	3.5382373	0.9431120	2.3974451
C	3.1308864	1.6746920	3.5095265
C	2.6433588	2.9699934	3.3515550
C	2.5644804	3.5314505	2.0815124
C	2.9774896	2.7983400	0.9699648
C	3.4546595	1.5005276	1.1271010
Mg	-0.9106614	0.0288444	-0.7647718
Br	0.7976053	1.6041593	-2.0663062
C	5.2137366	-0.5208582	0.1548516
C	6.5889403	-0.6259537	0.0682971
C	7.3446038	0.3829244	-0.5348571
C	6.6899033	1.4998051	-1.0641230
C	5.3161125	1.6153985	-0.9866918
C	4.5134545	0.6025431	-0.3814929
Mg	2.4515243	0.3651286	-0.6862188
Br	1.0327611	-1.5606153	0.0392239
O	-0.8410410	1.2069123	0.8903561
C	-0.3119131	0.9849751	2.2258933
C	-1.0310784	1.9962860	3.1017157
C	-1.2547047	3.1674778	2.1399633
C	-1.5693706	2.4670335	0.8275789
H	3.9354387	-0.0568194	2.5274294
H	3.2005670	1.2390209	4.4994312
H	2.3376373	3.5436456	4.2176274
H	2.1962721	4.5429558	1.9555039
H	2.9273553	3.2554415	-0.0129894
H	4.6594306	-1.3272439	0.6250697

H	7.0838846	-1.5058972	0.4634923
H	8.4217402	0.2995422	-0.5948270
H	7.2651506	2.2812294	-1.5475467
H	4.8431602	2.4974039	-1.4040081
H	-0.5030599	-0.0516406	2.4929940
H	0.7623972	1.1572949	2.2012038
H	-0.4357919	2.2679859	3.9721866
H	-1.9861980	1.5942412	3.4456289
H	-2.0614101	3.8298755	2.4512804
H	-0.3404067	3.7544642	2.0458639
H	-2.6279686	2.2310820	0.7105102
H	-1.2225564	3.0030734	-0.0543273
N	-2.5143447	-1.2363444	-1.3002588
C	-2.5372067	-1.8269750	-2.6799175
C	-2.3663793	-3.3483573	-2.5594613
C	-3.3657643	-3.9914993	-1.6096128
C	-3.2510376	-3.3349782	-0.2418809
C	-3.4480009	-1.8117672	-0.2797659
O	-2.7008003	0.2029500	-1.3822268
C	-3.7928989	-1.4521161	-3.4799470
C	-1.3207864	-1.2707186	-3.4267918
C	-4.9162115	-1.4295249	-0.5183264
C	-3.0329134	-1.2518287	1.0851991
H	-3.1686379	-5.0631952	-1.5271956
H	-4.3825524	-3.8960507	-1.9982154
H	-3.9764923	-3.7559942	0.4591018
H	-2.2560223	-3.5430167	0.1645393
H	-4.6651713	-2.0366246	-3.1985060
H	-3.6120638	-1.6233081	-4.5426663
H	-4.0126221	-0.3965045	-3.3292077
H	-0.3962443	-1.4770128	-2.8785356
H	-1.4127640	-0.1987421	-3.5915198
H	-1.2269820	-1.7565902	-4.3991076
H	-5.3851395	-2.0213764	-1.3000349
H	-4.9730547	-0.3776002	-0.7936140
H	-5.4884517	-1.5844613	0.3983990
H	-1.9809491	-1.4707511	1.2874520
H	-3.6211021	-1.7243739	1.8733505
H	-3.1954626	-0.1767691	1.1315759
H	-2.4406598	-3.7806310	-3.5604810
H	-1.3539112	-3.5536697	-2.1973912

Structure: **10-TS2**

C	3.1103309	1.9194954	-0.0090970
C	4.0876784	2.4686593	-0.8209404
C	4.4624355	1.8415344	-2.0105960
C	3.8348197	0.6469909	-2.3710367
C	2.8548592	0.0955699	-1.5657812
C	2.4318191	0.7179380	-0.3604046
Mg	0.6383077	0.3348343	0.7375054
C	3.1153332	-0.3123866	2.4370438
C	3.4619075	-1.2784370	3.3799948
C	3.3719106	-2.6289563	3.0577532
C	2.9440114	-3.0166471	1.7912523
C	2.5939658	-2.0495447	0.8527217
C	2.6646496	-0.7018148	1.1825884
O	-1.6893245	3.2956204	-0.1332602
C	-2.7976858	3.6919086	-0.9907425
C	-2.1852432	3.8189606	-2.3744195
C	-0.7712544	4.3184292	-2.0597878
C	-0.4152251	3.5389067	-0.8035801
H	2.8444238	2.4387940	0.9048588
H	4.5632313	3.3985276	-0.5290681
H	5.2314677	2.2700022	-2.6400393
H	4.1149057	0.1474952	-3.2918572
H	2.4057678	-0.8406639	-1.8788356
H	3.1894280	0.7384715	2.6916201
H	3.8020725	-0.9768548	4.3635923
H	3.6424021	-3.3789821	3.7902298
H	2.8838673	-4.0684603	1.5365435

H	2.2656372	-2.3570254	-0.1342755
H	-3.5751600	2.9357776	-0.9033928
H	-3.1874990	4.6409251	-0.6188222
H	-2.7496883	4.4985409	-3.0117342
H	-2.1458116	2.8428448	-2.8624866
H	-0.0591234	4.1315787	-2.8621297
H	-0.7832652	5.3908754	-1.8557106
H	0.0355809	2.5739316	-1.0403032
H	0.2322005	4.0674305	-0.1087245
N	-1.0650167	-0.9608008	0.2490895
C	-1.5358147	-1.2895366	-1.1371446
C	-1.1820802	-2.7605942	-1.3977229
C	-1.7093936	-3.7035320	-0.3246123
C	-1.2075498	-3.2602652	1.0427779
C	-1.5655057	-1.8051079	1.3890423
O	-1.3130895	0.4330615	0.4835786
C	-3.0299822	-1.0108102	-1.3630952
C	-0.7484326	-0.4141961	-2.1141597
C	-3.0591642	-1.6442533	1.7000766
C	-0.7736244	-1.4139580	2.6411944
H	-1.3746314	-4.7231996	-0.5289164
H	-2.8013449	-3.7321889	-0.3431279
H	-1.6084592	-3.8994536	1.8326491
H	-0.1190603	-3.3613382	1.0745592
H	-3.6769489	-1.7867945	-0.9654065
H	-3.2203288	-0.9421843	-2.4350581
H	-3.3115113	-0.0626425	-0.9074750
H	0.3253515	-0.4907255	-1.9521787
H	-1.0371041	0.6313589	-2.0225568
H	-0.9553367	-0.7358239	-3.1357053
H	-3.6978828	-2.1704470	0.9966464
H	-3.3574791	-0.5973796	1.7164452
H	-3.2582528	-2.0545310	2.6909226
H	0.3058460	-1.4888594	2.4784162
H	-1.0103330	-2.1068285	3.4486640
H	-1.0175689	-0.4137772	2.9951196
H	-1.5654860	-3.0335535	-2.3836514
H	-0.0919483	-2.8474931	-1.4451139
Br	0.3354730	2.2448719	2.5465208
Mg	-1.9374244	1.9958576	1.4090194
Br	-4.1596488	2.2508547	2.2725247

Structure: **10-Pr1**

Mg	-0.6773842	-0.1754320	-0.6409350
Br	1.4540382	1.3851471	-0.8080101
Mg	2.8437752	-0.7859723	-0.5384742
Br	0.7585314	-2.1578871	0.2397239
N	-1.9663015	-1.0730398	-2.0922836
C	-1.5154616	-1.2147205	-3.5156162
C	-1.3716132	-2.7108675	-3.8326859
C	-2.6192299	-3.5190440	-3.5089936
C	-2.9807044	-3.3143669	-2.0451871
C	-3.1833851	-1.8384331	-1.6699505
O	-2.1322674	0.3323636	-1.7693882
C	-2.4330965	-0.5009808	-4.5196796
C	-0.1266011	-0.5782002	-3.6164470
C	-4.4908022	-1.2758235	-2.2492251
C	-3.2776598	-1.7537514	-0.1425327
O	-1.3025707	0.6280876	1.1449554
C	-0.4126337	1.0067228	2.2228821
C	-0.4303665	2.5421483	2.2678847
C	-1.5285253	2.9474514	1.2623246
C	-2.3142402	1.6637962	1.0546887
H	-1.0984071	-2.8113591	-4.8863718
H	-0.5359170	-3.1058963	-3.2463030
H	-2.4406543	-4.5792931	-3.7058149
H	-3.4490208	-3.2234689	-4.1560720
H	-3.8908732	-3.8608083	-1.7840628
H	-2.1749752	-3.7173863	-1.4234966
H	-3.3408245	-1.0590596	-4.7349102

H	-1.9021143	-0.3606710	-5.4630414
H	-2.7061075	0.4764438	-4.1250291
H	0.5642809	-1.0445983	-2.9077963
H	-0.1641994	0.4929335	-3.4282945
H	0.2848335	-0.7367683	-4.6145048
H	-4.6573122	-1.5673700	-3.2830813
H	-4.4723087	-0.1885636	-2.1910225
H	-5.3363130	-1.6432823	-1.6644186
H	-2.3474200	-2.0790531	0.3301003
H	-4.0698854	-2.4149766	0.2124857
H	-3.5121818	-0.7427696	0.1827904
H	-0.7899302	0.5580521	3.1444048
H	0.5639866	0.5923511	1.9947614
H	0.5353146	2.9495353	1.9841105
H	-0.6567983	2.8913314	3.2743134
H	-2.1575729	3.7587684	1.6272748
H	-1.0815893	3.2583572	0.3180738
H	-3.0453276	1.4936404	1.8512710
H	-2.7878539	1.5592718	0.0815994
C	3.5246678	2.9388718	2.0562528
C	3.0245066	4.1622983	2.4804327
C	2.3927551	4.2707399	3.7142962
C	2.2505929	3.1429799	4.5139695
C	2.7463281	1.9184067	4.0872766
C	3.4020879	1.8010138	2.8581299
C	5.2687396	0.4625908	1.8733023
C	3.9909374	0.5095097	2.4445079
C	3.3148559	-0.6979197	2.6524085
C	3.9040950	-1.9129392	2.3174887
C	5.1829377	-1.9434218	1.7725561
C	5.8608944	-0.7497305	1.5481511
H	3.9923817	2.8572135	1.0842085
H	3.1210661	5.0307416	1.8413128
H	2.0069144	5.2260936	4.0463572
H	1.7603551	3.2178467	5.4765607
H	2.6590741	1.0497306	4.7275760
H	5.8110303	1.3855255	1.7150084
H	2.3149051	-0.6892811	3.0647664
H	3.3528363	-2.8314274	2.4681245
H	5.6405917	-2.8882581	1.5112374
H	6.8531165	-0.7631431	1.1160594

Structure: **10-Pr2**

C	4.2824283	1.3418446	-1.8047850
C	4.4172559	1.2266396	-3.1802805
C	4.2728188	-0.0109135	-3.7983968
C	3.9971487	-1.1336987	-3.0285386
C	3.8712116	-1.0194011	-1.6478931
C	4.0120470	0.2209372	-1.0164893
Mg	0.4928749	-1.0514155	-1.8869773
C	3.0366127	1.3481300	0.9866208
C	2.8202870	1.4242648	2.3561925
C	3.4161014	0.5020713	3.2085299
C	4.2288481	-0.4969956	2.6836152
C	4.4354567	-0.5796319	1.3138114
C	3.8397537	0.3399566	0.4459867
O	-2.5324227	2.0709409	-1.1895987
C	-3.4724710	2.9309057	-0.4968752
C	-3.4992025	4.2143684	-1.3260746
C	-3.0302649	3.7692434	-2.7358286
C	-2.8085870	2.2647064	-2.5979112
H	4.3910356	2.3080032	-1.3293976
H	4.6269468	2.1071956	-3.7741112
H	4.3683539	-0.0979957	-4.8730653
H	3.8697165	-2.0996139	-3.5003890
H	3.6559194	-1.8975655	-1.0517752
H	2.5478026	2.0548247	0.3285713
H	2.1653557	2.1920523	2.7450659
H	3.2447057	0.5596506	4.2760479
H	4.7028187	-1.2139315	3.3427124

H	5.0710727	-1.3568665	0.9083746
H	-4.4399706	2.4218364	-0.4874091
H	-3.1086260	3.0635209	0.5176252
H	-2.8105755	4.9448689	-0.9046236
H	-4.4955013	4.6545252	-1.3375115
H	-3.7615860	3.9916536	-3.5118888
H	-2.0959131	4.2615078	-3.0022259
H	-3.7070354	1.6912806	-2.8431664
H	-1.9607123	1.8798419	-3.1563828
N	-1.0035581	-1.5854127	0.2770021
C	-2.4852661	-1.5661222	0.2994765
C	-2.9401973	-2.9278858	0.8516108
C	-2.2966756	-3.2766563	2.1870645
C	-0.7812522	-3.2257413	2.0519513
C	-0.2583362	-1.8766867	1.5304358
O	-0.4986531	-0.3818089	-0.3243811
C	-3.1219329	-0.4236963	1.1191015
C	-2.9651434	-1.4603597	-1.1527532
C	-0.3425563	-0.7883614	2.6123410
C	1.2128241	-2.0538873	1.1513446
H	-2.6112366	-4.2746995	2.5017750
H	-2.6342041	-2.5914476	2.9685901
H	-0.2948666	-3.4315349	3.0084290
H	-0.4627282	-4.0064123	1.3547213
H	-3.1935481	-0.6609027	2.1775690
H	-4.1318327	-0.2277140	0.7550963
H	-2.5616563	0.5060212	1.0421972
H	-2.4547295	-2.1980901	-1.7748715
H	-2.7860070	-0.4699450	-1.5655766
H	-4.0386978	-1.6536848	-1.1990052
H	-1.3175487	-0.7374750	3.0902391
H	-0.1095927	0.1942877	2.2066072
H	0.3964168	-0.9975698	3.3876448
H	1.3107149	-2.7644755	0.3258162
H	1.7744305	-2.4419966	2.0014064
H	1.6686856	-1.1070619	0.8730706
H	-4.0303821	-2.9168157	0.9311170
H	-2.6783593	-3.6961686	0.1184083
Br	0.7464887	1.5557828	-2.4718229
Mg	-0.7110827	1.5388502	-0.3893301
Br	-0.4432212	3.1209296	1.4231666