Supporting Information

Zinc Chloride-Catalyzed Grignard Addition Reaction of Aromatic Nitriles

Manabu Hatano,*[a] Kisara Kuwano,[a] Riho Asukai,[a] Ayako Nagayoshi,[a] Haruka Hoshihara,[a] Tsubasa Hirata,[a] Miho Umezawa,[b] Sahori Tsubaki,[b] Takeshi Yoshikawa,*[b] Ken Sakata*[b]

[a] *Faculty of Pharmaceutical Sciences, Kobe Pharmaceutical University, 4-19-1, Motoyamakita-machi, Higashinada, Kobe 658-8558, Japan*

[b] *Faculty of Pharmaceutical Sciences, Toho University, Miyama, Funabashi, Chiba 274-8510, Japan*

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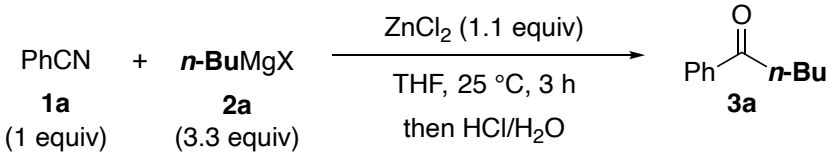
1. General information.

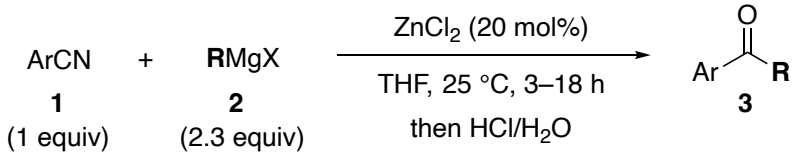
^{1}H NMR spectra were measured on a JEOL ECZ400 (400 MHz) spectrometer at ambient temperature. Data were recorded as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (s = singlet; d = doublet; t = triplet; q = quartet, m = multiplet, br = broad), coupling constant (Hz), integration, and assignment. ^{13}C NMR spectra were measured on a JEOL ECZ400 (100 MHz) spectrometer. Chemical shifts were recorded in ppm from the solvent resonance employed as the internal standard (deuterochloroform at 77.10 ppm). ^{19}F NMR spectra were measured on a JEOL ECS-400 (376 MHz) spectrometer. Chemical shifts were recorded in ppm from the solvent resonance employed as the external standard ($CFCl_3$ at 0 ppm). JEOL Delta (v6.1.0) was used as NMR processing software. Infrared (IR) spectra were recorded on a JASCO FT/IR-4600 spectrometer. Melting points were measured on Stanford Research Systems MPA100. High resolution mass spectral analyses were measured on Thermo Scientific Exactive Orbitrap ESI mass spectrometer. The products were purified using column chromatography on silica gel (Kanto Chemical Co., Inc. 37560). For thin-layer chromatography (TLC) analysis throughout this work, Merck precoated TLC plates (silica gel 60GF254 0.25 mm) were used. Visualization was accomplished by UV light (254 nm), anisaldehyde, $KMnO_4$, and phosphomolybdic acid. Dry solvents, such as tetrahydrofuran (THF), were purchased, and were used without any purification. Aromatic nitriles **1**, (*N,N,N',N'*-tetramethylethylenediamine)zinc(II) dichloride, *n*-butylmagnesium chloride (**2a**, 1.0 *M* in THF, and 2.0 *M* in THF), *n*-butylmagnesium bromide (**2a'**, 1.0 *M* in THF), methylmagnesium chloride (**2b**, 3.0 *M* in THF), ethylmagnesium chloride (**2c**, 1.0 *M* in THF), isobutylmagnesium chloride (**2d**, 2.0 *M* in THF), benzylmagnesium chloride (**2e**, 1.0 *M* in THF), phenethylmagnesium chloride (**2f**, 1.0 *M* in THF), *n*-octylmagnesium chloride (**2g**, 2.0 *M* in THF), cyclopentylmagnesium chloride (**2h**, 2.0 *M* in Et_2O), phenylmagnesium bromide (**2i**, 1.0 *M* in THF), isopropylmagnesium chloride (**2j**, 1.0 *M* in THF, and 2.0 *M* in THF) were commercially available and used without purification. Zinc chloride was commercially available and used without purification, and melt-dried (>300 °C) with a heat gun under reduced pressure (<5 Torr) for 5 min prior to use. The values of the yields for major products are based on isolation after silica gel column chromatography unless otherwise noted.

2. Representative procedure for the alkyl addition to aromatic nitriles 1 with Grignard reagents 2 and stoichiometric amount of $ZnCl_2$ (Table 1, entry 4).



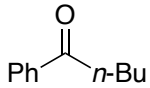
To a two-necked round flask, zinc chloride (300 mg, 2.2 mmol) was added and melt-dried (>300 °C) by a heat gun under reduced pressure (<5 Torr) for 5 min. Grignard reagent *n*-BuMgCl **2a** (1.0 *M* in THF, 6.6 mL, 6.6 mmol) was added, and the solution was stirred at 25 °C for 30 min. Benzonitrile **1a** (204 μL, 2.0 mmol) was added, and the mixture was stirred at 25 °C for 3 h. The reaction was monitored by TLC. The mixture was then cooled to 0 °C, and diethyl ether (30 mL) and 1 *M* HCl aqueous solution (50 mL) were added. The mixture was stirred at 25 °C for 1 h, and then extracted with diethyl ether (30 mL × 3). The combined organic phase was washed with brine (50 mL) and dried over $MgSO_4$. The solution was concentrated under reduced pressure, and the resultant residue was purified by silica gel column chromatography (eluent: *n*-hexane:EtOAc = 20:1 to 2:1) to give the desired product **3a** (250 mg, 77% yield).

3. General procedure for the $ZnCl_2$-catalyzed alkyl addition to aromatic nitriles 1 with Grignard reagents 2 (Schemes 2 and 3).

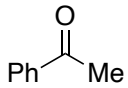


To a two-necked round flask, zinc chloride (54.5 mg, 0.40 mmol) was added and melt-dried (>300 °C) by a heat gun under reduced pressure (<5 Torr) for 5 min. Grignard reagent RMgX **2** (1.0–3.0 *M* in THF or Et_2O, 4.6 mmol) and THF were added, and the solution was stirred at 25 °C for 30 min (If a Grignard reagent is >1.0 *M*, the solution of the Grignard reagent is diluted with THF to 1.0 *M*.). Nitrile **1** (2.0 mmol) was added, and the mixture was stirred at 25 °C for 3–18 h. The reaction was monitored by TLC. The mixture was then cooled to 0 °C, and diethyl ether (20 mL) and 1 *M* HCl aqueous solution (20 mL) were added. The mixture was stirred at 25 °C for 1 h, and then extracted with diethyl ether (20 mL × 3). The combined organic phase was washed with brine (20 mL) and dried over $MgSO_4$. The solution was concentrated under reduced pressure, and the resultant residue was purified by silica gel column chromatography (eluent: *n*-hexane:EtOAc = 20:1 to 2:1) to give the desired product **3**.

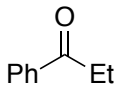
4. Products (Table 1 and Scheme 2).



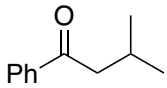
1-Phenylpentan-1-one (3aa):[1] 309 mg, 95% yield (6 h) (Table 1 and Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 2.96 (t, *J* = 7.2 Hz, 2H), 1.72 (quintet, *J* = 7.2 Hz, 2H), 1.41 (sextet, *J* = 7.2 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 137.1, 132.9, 128.5 (2C), 128.0 (2C), 38.3, 26.5, 22.5, 13.9. IR (film) 2958, 2871, 1685, 1596, 1448, 1265, 1207, 1012 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{15}O$ 163.1117; Found 163.1116.



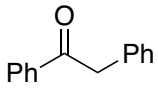
Acetophenone (3ab):[2] 217 mg, 90% yield (3 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 2.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 137.1, 133.1, 128.6 (2C), 128.4 (2C), 26.6. IR (film) 1679, 1597, 1448, 1357, 1262, 1179, 1024 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for C_8H_8NaO 143.0467; Found 143.0469.



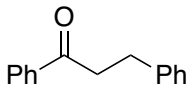
Propiophenone (3ac):[3] 269 mg, >99% yield (3 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.6 Hz, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 3.01 (q, *J* = 7.6 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.9, 136.9, 132.9, 128.6 (2C), 128.0 (2C), 31.8, 8.3. IR (film) 2978, 2938, 1686, 1596, 1449, 1352, 1220, 1078, 1014 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_9H_{11}O$ 135.0804; Found 135.0806.



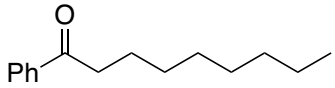
3-Methyl-1-phenylbutan-1-one (3ad):[4] 293 mg, 90% yield (6 h) (Scheme 2). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 6.8 Hz, 2H), 7.54 (t, *J* = 6.4 Hz, 1H), 7.45 (t, *J* = 6.4 Hz, 2H), 2.83 (d, *J* = 6.8 Hz, 2H), 2.30 (septet, *J* = 6.4 Hz, 1H), 1.00 (d, *J* = 6.4 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.3, 137.4, 132.9, 128.5 (2C), 128.1 (2C), 47.5, 25.2, 22.8 (2C). IR (film) 2957, 2870, 1685, 1597, 1580, 1467, 1448, 1365, 1284, 1213, 1005 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{15}O$ 163.1117; Found 163.1117.



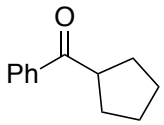
1,2-Diphenylethan-1-one (3ae):[5] 352 mg, 90% yield (3 h) (Scheme 2). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 2H), 7.30-7.22 (m, 3H), 4.28 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 136.6, 134.5, 133.2, 129.5 (2C), 128.5 (2C), 128.7 (2C), 128.6 (2C), 126.9, 45.5. IR (film) 3027, 1685, 1448, 1411, 1337, 1076 cm^{-1}. M.p. 56-57 °C. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{14}H_{13}O$ 197.0961; Found 197.0961.



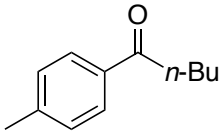
1,3-Diphenylpropan-1-one (3af):[6] 295 mg, 70% yield (3 h) (Scheme 2). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 6.9 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.28-7.23 (m, 2H), 7.20 (t, *J* = 6.9 Hz, 1H), 3.31 (d, *J* = 7.2 Hz, 2H), 3.07 (d, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 141.3, 136.8, 133.1, 128.7 (2C), 128.6 (2C), 128.4 (2C), 128.0 (2C), 126.1, 40.4, 30.1. IR (film) 3026, 2928, 1685, 1597, 1494, 1449, 1363, 1290, 1205 cm^{-1}. M.p. 71-74 °C. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{15}H_{14}NaO$ 233.0937; Found 233.0937.



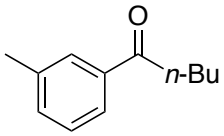
1-Phenylnonan-1-one (3ag):[7] 395 mg, 90% yield (3 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 6.9 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 2H), 2.96 (t, *J* = 7.6 Hz, 2H), 1.73 (m, 2H), 1.45-1.20 (m, 10H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 137.1, 132.9, 128.5 (2C), 128.0 (2C), 38.6, 31.8, 29.5, 29.4, 29.2, 24.4, 22.7, 14.1. IR (film) 2926, 2855, 1686, 1597, 1580, 1449, 1408, 1370, 1216, 1001 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{15}H_{22}NaO$ 241.1563; Found 241.1562.



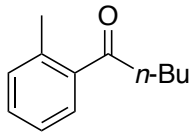
Cyclopentyl(phenyl)methanone (3ah):[8] 288 mg, 83% yield (6 h) (Scheme 2). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 2H), 3.71 (quintet, *J* = 7.6 Hz, 1H), 2.00-1.85 (m, 4H), 1.80-1.60 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.8, 136.9, 132.7, 128.5 (2C), 128.4 (2C), 16.3, 30.0 (2C), 26.3 (2C). IR (film) 2952, 2868, 1678, 1596, 1579, 1448, 1360, 1220, 1179, 1001 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{15}O$ 175.1117; Found 175.1117.



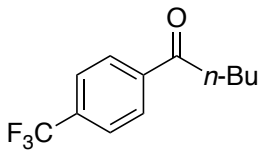
1-(*p*-Tolyl)pentan-1-one (3ba):[9] 308 mg, 87% yield (9 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 2.91 (t, *J* = 7.2 Hz, 2H), 2.38 (s, 3H), 1.70 (quintet, *J* = 7.2 Hz, 2H), 1.41 (sextet, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 143.4, 134.5, 128.9 (2C), 128.1 (2C), 38.1, 26.5, 22.4, 21.5, 13.9. IR (film) 2958, 1683, 1607, 1464, 1408, 1267, 1204, 1180, 1014 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{17}O$ 177.1274; Found 177.1275.



1-(*m*-Tolyl)pentan-1-one (3ca):[9] 303 mg, 86% yield (6 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.73 (m, 2H), 7.38-7.30 (m, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.40 (s, 3H), 1.72 (quintet, *J* = 7.2 Hz, 2H), 1.40 (sextet, *J* = 7.2 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 138.3, 137.1, 133.6, 128.5, 128.4, 125.3, 38.4, 26.5, 22.5, 21.4, 14.0. IR (film) 2958, 1684, 1603, 1582, 1464, 1260, 1162, 1041 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{17}O$ 177.1274; Found 177.1275.

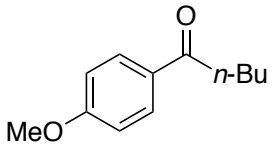


1-(*o*-Tolyl)pentan-1-one (3da):[9] 316 mg, 90% yield (6 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 2.88 (t, *J* = 7.6 Hz, 2H), 2.48 (s, 3H), 1.68 (quintet, *J* = 7.2 Hz, 2H), 1.39 (sextet, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.0, 138.4, 137.8, 131.9, 131.0, 128.3, 125.6, 41.4, 26.5, 22.5, 21.2, 14.0. IR (film) 2958, 1686, 1600, 1571, 1456, 1258, 1211, 1009 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{17}O$ 177.1274; Found 177.1275.

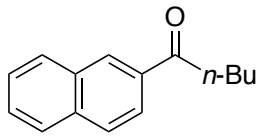


1-(4-(Trifluoromethyl)phenyl)pentan-1-one (3ea):[9] 462 mg, >99% yield (3 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.8 Hz, 2H), 7.72 (d, *J* = 8.8 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 1.74 (quintet, *J* = 7.2 Hz, 2H), 1.42 (sextet, *J* = 7.2 Hz, 2H), 0.96 (t, *J* =

7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 139.7, 134.2 (q, $J_{C\text{-}F}$ = 32.6 Hz), 128.4 (2C), 125.7 (q, $J_{C\text{-}F}$ = 3.8 Hz, 2C), 123.7 (q, $J_{C\text{-}F}$ = 271.2 Hz), 38.7, 26.2, 22.4, 13.9. ^{19}F (376 MHz, $CDCl_3$) δ –63.6. IR (film) 2932, 1687, 1580, 1467, 1409, 1326, 1113, 1068 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}F_3O$ 231.0991; Found 231.0991.

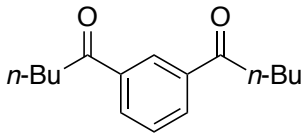


1-(4-Methoxyphenyl)pentan-1-one (3fa):[10] 379 mg, 99% yield (6 h) (Scheme 2). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 6.8 Hz, 2H), 6.92 (d, *J* = 6.8 Hz, 2H), 3.86 (s, 3H), 2.91 (t, *J* = 7.2 Hz, 2H), 1.71 (quintet, *J* = 7.2 Hz, 2H), 1.40 (sextet, *J* = 7.2 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 163.3, 130.3 (2C), 113.6 (2C), 130.1, 55.4, 38.0, 26.7, 22.5, 14.0. IR (film) 2957, 1676, 1601, 1509, 1462, 1471, 1257, 1212, 1170, 1030 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{17}O_2$ 193.1223; Found 193.1223.



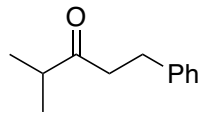
1-(Naphthalen-2-yl)pentan-1-one (3ga):[9] 384 mg, 90% yield (3 h) (Scheme 2). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.04 (dd, *J* = 8.8, 1.2 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 6.8 Hz, 1H), 7.59 (td, *J* = 6.8, 0.8 Hz, 1H), 7.54 (td, *J* = 6.8, 0.8 Hz, 1H), 3.09 (t, *J* = 8.0 Hz, 2H), 1.78 (quintet, *J* = 8.0 Hz, 2H), 1.44 (sextet, *J* = 7.6 Hz, 2H), 0.98 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 135.5, 134.4, 132.5, 129.6, 129.5, 128.4, 128.3, 127.8, 126.7, 124.0, 38.4, 26.6, 22.5, 14.0. IR (film) 2932, 1681, 1464, 1410, 1357, 1268, 1182, 1157 cm^{-1}. M.p. 54-56 °C. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{17}O$ 213.1274; Found 213.1272.

5. Products (Eqs. 1–3).

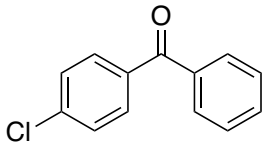


1,1'-(1,3-Phenylene)bis(pentan-1-one) (3ha'):[11] 452 mg, 92% yield (3 h) (Eq. 1). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (t, *J* = 2.0 Hz, 1H), 8.15 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.58 (t, *J* = 8.0 Hz, 1H), 3.02 (t, *J* = 7.2 Hz, 4H), 1.74 (quintet, *J* = 7.2 Hz, 4H), 1.42 (sextet, *J* = 7.2 Hz, 4H), 0.97 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.9 (2C), 137.4 (2C), 132.1 (2C), 129.0,

127.5, 38.5 (2C), 26.3 (2C), 22.4 (2C), 14.0 (2C). IR (film) 2958, 1687, 1596, 1465, 1376, 1259, 1176, 1036 cm^{-1}. M.p. 27-28 °C. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{16}H_{22}NaO_2$ 269.1512; Found 269.1506.

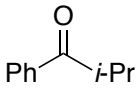


4-Methyl-1-phenylpentan-3-one (3if):[12] 70.7 mg, 20% yield (6 h) (Eq. 2). Colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.31-7.16 (m, 5H), 2.88 (t, *J* = 7.2 Hz, 2H), 2.76 (t, *J* = 7.2 Hz, 2H), 2.56 (septet, *J* = 6.8 Hz, 1H), 1.06 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.9, 141.4, 128.5 (2C), 128.3 (2C), 126.1, 42.0, 41.0, 29.8, 18.2 (2C). IR (film) 2969, 1711, 1496, 1454, 1383, 1364, 1079, 1060 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{12}H_{16}NaO$ 199.1093; Found 199.1093.

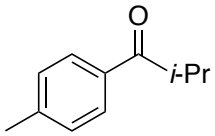


4-Chlorobenzophenone (3ji):[13] 233 mg, 54% yield (3 h) (Eq. 3). White solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.81-7.74 (m, 4H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.52-7.43 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.5, 138.9, 137.2, 135.9, 132.7, 131.5 (2C), 130.0 (2C), 128.7 (2C), 128.4 (2C). IR (film) 3062, 1660, 1585, 1484, 1447, 1399, 1316, 1273, 1173, 1090 cm^{-1}. M.p. 75-76 °C. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{10}ClO$ 217.0415; Found 217.0417.

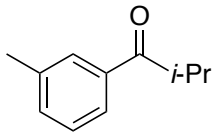
6. Products (Scheme 3).



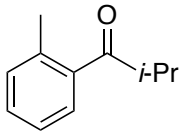
2-Methyl-1-phenylpropan-1-one (3aj):[14] 251 mg, 85% yield (6 h) (Scheme 3). Colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.2 Hz, 2H), 3.01 (septet, *J* = 6.8 Hz, 1H), 1.22 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 136.2, 132.8, 128.6 (2C), 128.3 (2C), 35.4, 19.2 (2C). IR (film) 3648, 2933, 1683, 1596, 1578, 1465, 1447, 1383, 1350, 1224, 1160 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{10}H_{13}O$ 149.0961; Found 149.0960.



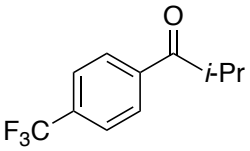
2-Methyl-1-(*p*-tolyl)propan-1-one (3bj):[15] 293 mg, 90% yield (6 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 3.53 (septet, *J* = 6.8 Hz, 1H), 2.41 (s, 3H), 1.20 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.2, 143.5, 129.3 (2C), 133.6, 128.5 (2C), 35.2, 21.6, 19.2 (2C). IR (film) 2971, 1681, 1607, 1465, 1381, 1229, 1209, 1160 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{15}O$ 163.1117; Found 163.1115.



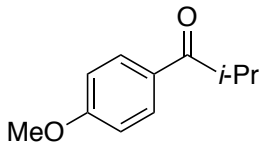
2-Methyl-1-(*m*-tolyl)propan-1-one (3cj):[15] 315 mg, 97% yield (6 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.72 (m, 2H), 7.40-7.32 (m, 2H), 3.55 (septet, *J* = 6.8 Hz, 1H), 2.41 (s, 3H), 1.21 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 138.4, 136.3, 133.6, 128.9, 128.5, 125.5, 35.4, 21.4, 19.2 (2C). IR (film) 2971, 1683, 1602, 1585, 1466, 1382, 1249, 1149, 1029 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{15}O$ 163.1117; Found 163.1116.



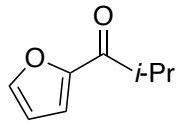
2-Methyl-1-(*o*-tolyl)propan-1-one (3dj):[15] 231 mg, 71% yield (18 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d *J*, = 7.2 Hz, 1H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.28-7.21 (m, 2H), 3.34 (septet, *J* = 6.8 Hz, 1H), 2.42 (s, 3H), 1.16 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.3, 138.6, 137.5, 131.6, 130.6, 127.4, 125.5, 38.8, 20.8, 18.5 (2C). IR (film) 3970, 1689, 1457, 1381, 1340, 1287, 1223 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{15}O$ 163.1117; Found 163.1118.



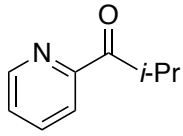
2-Methyl-1-(4-(trifluoromethyl)phenyl)propan-1-one (3ej):[15] 301 mg, 70% yield (3 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.4 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 2H), 3.55 (septet, *J* = 6.8 Hz, 1H), 1.23 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.5, 139.0, 134.2 (d, J_{C-F} = 32.6 Hz), 128.7 (2C), 125.7 (d, J_{C-F} = 3.8 Hz, 2C), 123.6 (d, J_{C-F} = 271 Hz), 35.8, 18.9 (2C). ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.6. IR (film) 2970, 1691, 1468, 1324, 1219, 1171, 1133, 1067 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{12}F_3O$ 217.0835; Found 217.0835.



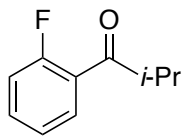
1-(4-Methoxyphenyl)-2-methylpropan-1-one (3fj):[15] 283 mg, 79% yield (9 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 9.2 Hz, 2H), 6.94 (d, J = 9.2 Hz, 2H), 3.86 (s, 3H), 3.52 (septet, J = 7.2 Hz, 1H), 1.20 (d, J = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1, 163.3, 130.6 (2C), 129.1, 113.7 (2C), 55.5, 34.9, 19.3 (2C). IR (film) 2970, 1674, 1600, 1510, 1464, 1260, 1229, 1180, 1159, 1031 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{15}O_2$ 179.1067; Found 179.1066.



1-(Furan-2-yl)-2-methylpropan-1-one (3kj):[16] 274 mg, >99% yield (3 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 1.2 Hz, 1H), 7.20 (d, J = 4.0 Hz, 1H), 6.54 (dd, J = 4.0, 1.2 Hz, 1H), 3.34 (septet, J = 6.8 Hz, 1H), 1.23 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7, 152.1, 146.2, 117.1, 112.1, 36.2, 18.8 (2C). IR (film) 2973, 1672, 1566, 1468, 1395, 1253, 1155, 1090 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_8H_{10}NaO_2$ 161.0573; Found 161.0573.

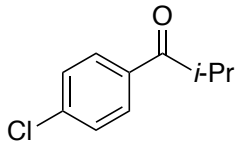


2-Methyl-1-(pyridin-2-yl)propan-1-one (3lj):[17] 299 mg, >99% yield (3 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (m, 1H), 8.05 (dd, J = 8.0, 1.2 Hz, 1H), 7.84 (td, J = 7.6, 1.6 Hz, 1H), 7.46 (m, 1H), 4.12 (septet, J = 7.2 Hz, 1H), 1.21 (d, J = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.8, 152.9, 148.9, 136.9, 126.9, 122.5, 34.2, 18.7 (2C). IR (film) 2971, 1697, 1582, 1465, 1346, 1224, 1092 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_9H_{11}NNaO$ 172.0733; Found 172.0733.

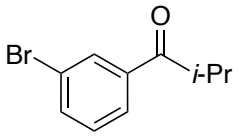


1-(2-Fluorophenyl)-2-methylpropan-1-one (3mj):[15] 333 mg, >99% yield (3 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (td, J = 7.2, 2.0 Hz, 1H), 7.50 (m, 1H), 7.22 (t, J = 7.2 Hz, 1H), 7.12 (dd, J = 10.8, 8.4 Hz, 1H), 3.41 (septet, J = 6.8 Hz, 1H), 1.21 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6 (d, $J_{C–F}$ = 3.8 Hz), 161.2 (d, $J_{C–F}$ = 252 Hz), 134.0 (d,

$J_{C–F}$ = 8.6 Hz), 130.9 (d, $J_{C–F}$ = 2.9 Hz), 125.8 (d, $J_{C–F}$ = 14.3 Hz), 124.5 (d, $J_{C–F}$ = 2.9 Hz), 116.5 (d, $J_{C–F}$ = 24.0 Hz), 40.2 (d, $J_{C–F}$ = 6.8 Hz), 18.5 (2C). ^{19}F NMR (376 MHz, $CDCl_3$) δ –111.8. IR (film) 2975, 1686, 1609, 1466, 1451, 1384, 1349, 1269, 1212, 1152, 1102 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_{11}FNaO$ 189.0686; Found 189.0686.

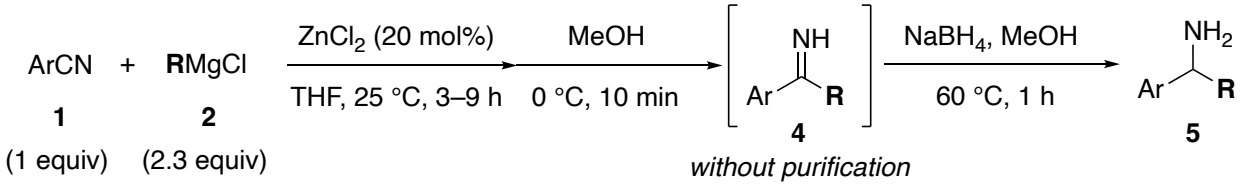


1-(4-Chlorophenyl)-2-methylpropan-1-one (3jj):[15] 353 mg, 97% yield (3 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 3.50 (septet, *J* = 7.2 Hz, 1H), 1.22 (d, *J* = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.3, 139.2, 134.4, 129.8 (2C), 128.9 (2C), 35.4, 19.1 (2C). IR (film) 2972, 1685, 1590, 1468, 1401, 1280, 1221, 1160, 1092 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{10}H_{12}ClO$ 183.0571; Found 183.0571.

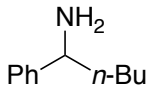


1-(3-Bromophenyl)-2-methylpropan-1-one (3nj):[18] 19.6 mg, 4% yield (3 h) (Scheme 3). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 3.49 (septet, *J* = 6.8 Hz, 1H), 1.23 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1, 138.0, 135.6, 131.4, 130.2, 126.8, 123.0, 35.6, 19.0 (2C). IR (film) 2971, 1683, 1565, 1465, 1418, 1382, 1212, 1159, 1068 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_{11}{}^{79}BrNaO$ 248.9886; Found 248.9887. Calcd for $C_{10}H_{11}{}^{81}BrNaO$ 250.9865; Found 250.9866

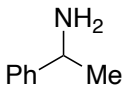
7. General procedure for the amine synthesis *via* $ZnCl_2$-catalyzed Grignard addition reaction of aromatic nitriles 1 (Scheme 4).



To a two-necked round flask, zinc chloride (54.5 mg, 0.40 mmol) was added and melt-dried (>300 °C) by a heat gun under reduced pressure (<5 Torr) for 5 min. Grignard reagent RMgCl **2** (1.0–3.0 *M* in THF or Et_2O, 4.6 mmol) and THF were added, and the solution was stirred at 25 °C for 30 min (If a Grignard reagent is >1.0 *M*, the solution of the Grignard reagent is diluted with THF to 1.0 *M*.). Nitrile **1** (2.0 mmol) was added, and the mixture was stirred at 25 °C for 3–9 h. The reaction was monitored by TLC. The mixture was then cooled to 0 °C, and methanol (3 mL) was added. The mixture was vigorously stirred at 0 °C for 10 min, and then water (20 mL) and diethyl ether (20 mL) were added. The mixture was extracted with diethyl ether (20 mL × 2). The combined organic phase was washed with brine (20 mL) and dried over $MgSO_4$. The solution was concentrated under reduced pressure, and the resultant residue was used without purification for the next step. To a solution of the residue in methanol (10 mL) was added sodium borohydride (341 mg, 9.0 mmol) at 25 °C. After stirring at 25 °C for 5 min, the mixture was stirred at 60 °C for 1 h. Then the mixtire was cooled to 25 °C, water (20 mL) and diethyl ether (20 mL) were added. The mixture was extracted with diethyl ether (20 mL × 3). The combined organic phase was washed with brine (50 mL), dried over $MgSO_4$, and concentrated under reduced pressure. The resultant residue was purified by silica gel column chromatography (eluent: *n*-hexane:EtOAc = 5:1 to 1:1) to give the desired product **5**.

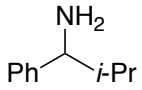


1-Phenylpentan-1-amine (5aa):[19] 290 mg, 89% yield (6 h) (Scheme 4). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.20 (m, 5H), 3.85 (t, *J* = 7.2 Hz, 1H), 1.72-1.60 (m, 2H), 1.52 (br, 2H), 1.39-1.24 (m, 3H), 1.18 (m, 1H), 0.86 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 128.4 (2C), 126.8, 126.3 (2C), 56.3, 39.4, 28.7, 22.6, 14.0. IR (film) 3290, 2929, 1601, 1492, 1451, 1378, 1070, 1027 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{18}N$ 164.1434; Found 164.1435.

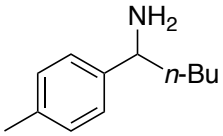


1-Phenylethylamine (5ab):[20] 182 mg, 75% yield (3 h) (Scheme 4). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.28 (m, 4H), 7.22 (m, 1H), 4.10 (q, *J* = 6.4 Hz, 1H), 1.46 (br, 2H), 1.37 (d, *J*

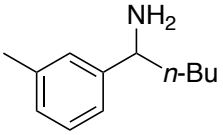
= 6.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 128.4 (2C), 126.7, 125.6 (2C), 51.3, 25.7. IR (film) 3290, 2963, 1603, 1492, 1451, 1369, 1105, 1024 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_8H_{12}N$ 122.0964; Found 122.0968.



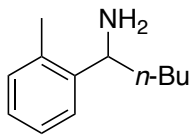
2-Methyl-1-phenylpropan-1-amine (5aj):[21] 247 mg, 83% yield (6 h) (Scheme 4). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.20 (m, 5H), 3.59 (d, *J* = 7.2 Hz, 1H), 1.85 (septet, *J* = 7.2 Hz, 1H), 1.50 (br, 2H), 0.97 (t, *J* = 7.2 Hz, 3H), 0.77 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 128.1 (2C), 127.0 (2C), 126.7, 62.5, 35.4, 19.8, 18.9. IR (film) 3305, 2957, 1602, 1491, 1453, 1383, 1364, 1161, 1027 cm^{-1}. HRMS (ESI+) *m/z*: $[M+H]^+$ Calcd for $C_{10}H_{16}N$ 150.1277; Found 150.1279.



1-(*p*-Tolyl)pentan-1-amine (5ba): 328 mg, 93% yield (9 h) (Scheme 4). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 7.6 Hz, 2H), 7.13 (d, *J* = 7.6 Hz, 2H), 3.50 (t, *J* = 6.8 Hz, 1H), 2.33 (s, 3H), 1.72-1.58 (m, 2H), 1.50 (br, 2H), 1.36-1.25 (m, 3H), 1.18 (m, 1H), 0.86 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 136.3, 129.1 (2C), 126.2 (2C), 56.0, 39.4, 28.8, 22.7, 21.0, 14.0. IR (film) 3367, 2927, 1576, 1513, 1457, 1376, 1111, 1043 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{12}H_{19}NNa$ 200.1410; Found 200.1411.



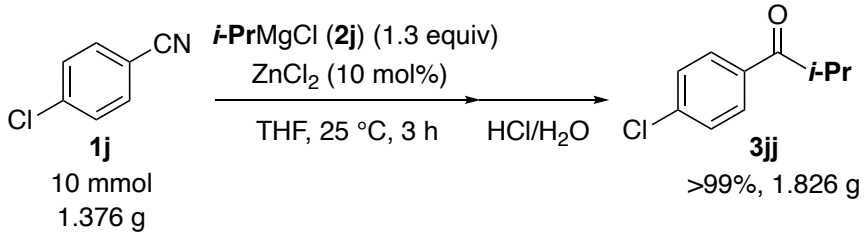
1-(*m*-Tolyl)pentan-1-amine (5ca): 332 mg, 94% yield (6 h) (Scheme 4). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.0 Hz, 1H), 7.12 (s, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 3.82 (t, *J* = 7.2 Hz, 1H), 2.34 (s, 3H), 1.70-1.60 (m, 2H), 1.53 (br, 2H), 1.39-1.25 (m, 3H), 1.18 (m, 1H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 138.0, 128.3, 127.5, 127.0, 123.3, 56.2, 39.3, 28.8, 22.7, 21.5, 14.0. IR (film) 3291, 2928, 1607, 1464, 1377, 1152, 1085, 1042 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{12}H_{19}NNa$ 200.1410; Found 200.1410.



1-(*o*-Tolyl)pentan-1-amine (5da):[22] 296 mg, 83% yield (6 h) (Scheme 4). Colorless oil. ^{1}H NMR

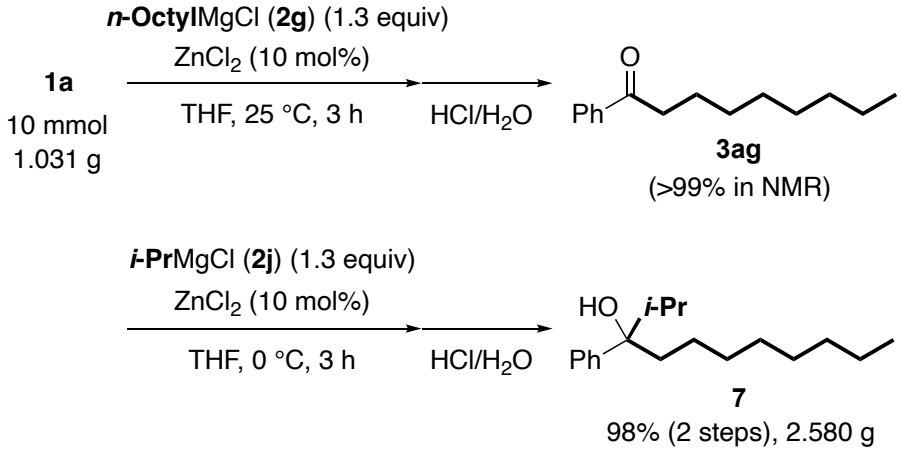
(400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.2 Hz, 1H), 7.21 (m, 1H), 7.14-7.11 (m, 2H), 4.15 (t, *J* = 6.8 Hz, 1H), 2.34 (s, 3H), 1.72-1.55 (m, 2H), 1.49 (br, 2H), 1.46-1.19 (m, 4H), 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 134.8, 130.3, 126.4 (2C), 124.9, 51.2, 38.7, 28.9, 22.8, 19.3, 14.1. IR (film) 3293, 2929, 1587, 1461, 1377, 1295, 1177, 1048 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{12}H_{19}NNa$ 200.1410; Found 200.1410.

8. Gram-scale ketone 3jj synthesis by the $ZnCl_2$-catalyzed Grignard addition reaction of aromatic nitrile 1j (Scheme 5a).

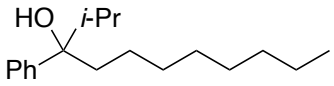


To a two-necked round flask, zinc chloride (136 mg, 1.0 mmol) was added and melt-dried (>300 °C) by a heat gun under reduced pressure (<5 Torr) for 5 min. Grignard reagent *i*-PrMgCl **2j** (2.0 *M* in THF, 6.5 mL, 13 mmol) was added, and the solution was stirred at 25 °C for 30 min. Nitrile **1j** (1.376 g, 10.0 mmol) in THF (6.5 mL) was added, and the mixture was stirred at 25 °C for 3 h. The reaction was monitored by TLC. The mixture was then cooled to 0 °C, and diethyl ether (50 mL) and 1 *M* HCl aqueous solution (100 mL) were added. The mixture was stirred at 25 °C for 1 h, and then extracted with diethyl ether (30 mL × 3). The combined organic phase was washed with brine (100 mL) and dried over $MgSO_4$. The solution was concentrated under reduced pressure, and the resultant residue was purified by silica gel column chromatography (eluent: *n*-hexane:EtOAc = 20:1 to 2:1) to give the desired product **3jj** (1.826 g, >99% yield).

9. Scalable $ZnCl_2$-catalyzed Grignard addition reaction of aromatic nitrile 1a and sequential alkyl addition to the resulting ketone (Scheme 5b).



To a two-necked round flask, zinc chloride (136 mg, 1.0 mmol) was added and melt-dried (>300 °C) by a heat gun under reduced pressure (<5 Torr) for 5 min. *n*-Octylmagnesium chloride **2g** (2.0 *M* in THF, 6.5 mL, 13 mmol) and THF (6.5 mL) were added, and the solution was stirred at 25 °C for 30 min. Nitrile **1a** (1.02 mL, 10.0 mmol) was added, and the mixture was stirred at 25 °C for 3 h. The reaction was monitored by TLC. The mixture was then cooled to 0 °C, and diethyl ether (50 mL) and 1 *M* HCl aqueous solution (100 mL) were added. The mixture was stirred at 25 °C for 1 h, and then extracted with diethyl ether (50 mL × 3). The combined organic phase was washed with brine (100 mL) and dried over $MgSO_4$. The solution was concentrated under reduced pressure to give the desired product **3ag** (ca. 2.18 g, >99% yield by ^1H NMR analysis). Without purification of **3ag** obtained, the following alkyl addition was conducted. To a two-necked round flask, zinc chloride (136 mg, 1 mmol) was added and melt-dried (>300 °C) by a heat gun under reduced pressure (<5 Torr) for 5 min. Isopropylmagnesium chloride **2j** (2.0 *M* in THF, 13 mmol, 6.5 mL) was added, and the solution was stirred at 25 °C for 30 min. The solution was cooled to 0 °C, and ketone **3ag** in THF (6.5 mL), which was obtained in the previous reaction, was added. The mixture was stirred at 0 °C for 3 h, and the reaction was monitored by TLC. To the mixture at 0 °C, diethyl ether (50 mL) and 1 *M* HCl aqueous solution (100 mL) were added. The mixture was stirred at 25 °C for 30 min, and then extracted with diethyl ether (50 mL × 3). The combined organic phase was washed with brine (100 mL), dried over $MgSO_4$, and concentrated under reduced pressure. The resultant residue was purified by silica gel column chromatography (eluent: *n*-hexane:EtOAc = 10:1 to 2:1) to give the desired product **7** (2.580 g, 98% yield in two steps).



2-Methyl-3-phenylundecan-3-ol (7):[19] 2.580 g, 98% yield (Scheme 5b). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.27 (m, 4H), 7.21 (t, *J* = 6.8 Hz, 1H), 2.02 (septet, *J* = 6.8 Hz, 1H), 1.90-1.76 (m, 2H), 1.32-1.13 (m, 12H), 0.94 (d, *J* = 6.8 Hz, 3H), 0.91 (br, 1H), 0.85 (d, *J* = 7.2 Hz, 3H), 0.71 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 127.8 (2C), 126.1, 125.8 (2C), 79.1, 39.6, 37.9, 31.9, 30.2, 29.5, 29.3, 23.6, 22.7, 17.5, 16.7, 14.1. IR (film) 1032, 1172, 1383, 1446, 1466, 2854, 2926, 3495 cm^{-1}. HRMS (ESI+) *m/z*: $[M+Na]^+$ Calcd for $C_{18}H_{30}NaO$ 285.2189; Found 285.2185.

10. Computational details.

DFT calculations were performed using the *Gaussian16*[23] program package. Geometry optimizations and vibrational-frequency analyses were performed via restricted Kohn–Sham DFT calculations using the M06 functional.[24,25] In the numerical integration, a larger grid (*ultrafinegrid*) was used.[23] Pople's 6-31G(d,p) basis set was used for the Gaussian basis functions for all atoms[26]. The polarizable continuum model (PCM)[27] was used to determine the solvent effect of tetrahydrofuran (THF). The total electronic energy values, thermal free terms, and Gibbs free energy values in THF at 298.15 K are listed in Table S1 together with the corresponding structure names as shown in the manuscript. Also, all cartesian coordinates of the stationary points are listed in Table S2.

The Grignard reaction discovered by Victor Grignard in 1900 is a prominent process to form carbon–carbon bonds benefiting from the polarity of the C(δ−)–Mg(δ+) bond. However, the mechanism of this reaction is difficult to elucidate because solutions of Grignard reagents contain a variety of chemical molecules according to the Schlenk equilibrium.

$$2\,RMgX \rightleftharpoons R_2Mg + MgX_2$$

Furthermore, the nominal reactant 'RMgX' is a condensed representation of numerous mono-, di-, and polymetallic species that coexist in the Schlenk equilibrium. The relative abundance of the molecules depends on the nature of the organic residue R and the halogen X as well as on the experimental conditions. Pioneering work based on computational approaches by Yamazaki and Yamabe[28] and Mori and Kato[29] suggest that dinuclear Grignard moieties are more reactive in nucleophilic additions than mononuclear species for the Grignard reactions with acetaldehyde and CH_3MgCl. Cascella et al.[30,31] have performed molecular-dynamics simulations using explicit solvent models, finding that the Mg(II) centers of the mono- and dinuclear species can accommodate a variable number of solvent molecules in their first coordination spheres. Moreover, the same authors examined possible pathways based on the Schlenk equilibrium for the mono- and dinuclear species in Grignard reactions in THF and concluded that the conformational space including the explicit treatment of the solvent should be considered.[31]

Fig. S1 shows the organometallic mono- and dinuclear species and the possible pathways for the Zn(II)-catalyzed Grignard reaction between benzonitrile (**1a**) and CH_3MgCl (**2b**). In the Schlenk equilibrium, there are three conceivable mononuclear species with the Zn(II) catalyst, i.e., **MeMgClZn**, **Me_2MgZn**, and **$MgCl_2$Zn**, and two mononuclear species without the Zn(II) catalyst, i.e., **MeMgCl** and **Me_2Mg**. In these calculations, the reactants, transition states, and product species are defined as **RC**, **TS**, and **PR**. respectively. Figs. S2–S4 show the Gibbs free energy diagrams for the mononuclear species with and without Zn(II) catalyst. Fig. S2 shows the Gibbs free energy difference at 298.15 K in kcal/mol from each reactant species, i.e., **RC_MeMgCl**, **RC_Me_2Mg**, and **PhCN…$MgCl_2$**, without coordinated THF. Without the Zn(II) catalyst, the free activation energy of the transition state with two methyl groups coordinated to the Mg(II) atom (**TS_Me_2Mg**) is lower than that of the transition state with the standard Grignard reactant (**TS_MeMgCl**). The binding between Mg(II) and the carbon atoms of **Me_2Mg** is weaker than that of **MeMgCl**, i.e., the bond length and bond order between Mg(II) and the carbon atoms of **Me_2Mg** (2.11 Å; 0.360) are longer and smaller than those of **MeMgCl** (2.09 Å; 0.393), respectively. The energy diagrams of the Zn(II) catalysts are also shown in Fig. S2. All chloride ions in $ZnCl_2$ were assumed to be replaced with methyl groups via reaction with CH_3MgCl. The free energy difference of **MeMgClZn**, **Me_2MgZn**, and **$MgCl_2$Zn** indicates the difference from the total free energy values of each reactant, i.e., **RC_MeMgCl**, **RC_Me_2Mg**, and **PhCN…$MgCl_2$**, and **$ZnMe_2$**, respectively. In the case of Zn(II) catalysis, the methyl group of **$ZnMe_2$** nucleophilically attacks the nitrile carbon. Especially, in the **MeMgClZn** species, there are two possible reaction mechanisms via transition states **TSa_MeMgClZn** or **TSb_MeMgClZn**, in which the Zn(II) atom of **$ZnMe_2$** coordinates to the methyl group or the Cl atom, respectively. The Gibbs free energy of **TSa_MeMgClZn** with the zinc(II)ate complex is smaller than that of **TSb_MeMgClZn**. In the absence of a catalyst, the transition state with two methyl groups coordinated to the Mg(II) atom (**TS_Me_2MgZn**) exhibits the lowest energy among the transition states. Fig. S3 shows the Gibbs free energy difference in kcal/mol for each reactant species, i.e., **RCb_MeMgCl$_{THF1}$**, **RCb_Me_2Mg$_{THF1}$**, and **PhCN…$MgCl_2$…THF1**, with one coordinated THF molecule. Compared to the energy diagrams without THF coordination, the activation barriers for the nucleophilic addition tend to decrease. The free activation energies of **TSa_Me_2Mg$_{THF1}$** and **TSb_Me_2Mg$_{THF1}$** are lower than those of the structures with the standard Grignard reactants, i.e., **TSa_MeMgCl$_{THF1}$** and **TSb_MeMgCl$_{THF1}$**. The Gibbs free energies of the transition state in the Zn(II) catalysis system, i.e., **TSa_Me_2MgZn$_{THF1}$** and **TSb_MeMgClZn$_{THF1}$**, are lower than those without Zn(II) catalyst, **TSa_Me_2Mg$_{THF1}$** and **TSb_MeMgCl$_{THF1}$**, respectively. Fig. S4 shows the Gibbs free energy difference in kcal/mol for each reactant species, **RCa_MeMgCl$_{THF2}$**, **RCa_Me_2Mg$_{THF2}$**, and **PhCN…$MgCl_2$…THF2a**, with two coordinated THF molecules. The activation barriers for the nucleophilic addition tend to decrease with increasing number of THF molecules coordinated to the Mg atoms. In the mononuclear species, the transition states with two coordinated THF molecules, i.e., **TSc_Me_2MgZn$_{THF2}$** and **TSa_Me_2Mg$_{THF2}$**, exhibit lower activation energies than

other species with and without Zn(II) catalysts, respectively.

Figs. S5–S6 show the Gibbs free energy diagrams for the dinuclear species with and without Zn(II) catalyst. To yield dimeric structures, the halide groups in **MeMgCl** or **$MgCl_2$** are required to form bridges between the Mg(II) atoms. The possible dinuclear species are **$MeMg(\mu\text{-}Cl)_2MeMg$** and **MeMg(μ-Cl)(μ-Me)MgCl** in the Schlenk equilibrium. The Mg(II) atom in the dinuclear species is coordinated to the nitrogen atom in benzonitrile. This pathway is called germinal (**gm**) when the two methyl groups are on the same Mg(II) atom and vicinal (**vi**) when they are on two different Mg(II) atoms. As mentioned in a previous study,[31] the bridging methyl groups in **MeMg(μ-Cl)(μ-Me)MgCl** are unlikely to act as a nucleophile owing to the high activation energy. Fig. S5 shows the Gibbs free energy difference in kcal/mol from the reactant species, i.e., **RC_{vi}_MeMg(μ-Cl)$_2$MeMg**, in the absence of coordinated THF molecules. Fig. S6 shows the Gibbs free energy difference in kcal/mol from the reactant species **RC_{vi}_MeMg(μ-Cl)$_2$MeMg$_{THF3}$** with three coordinated THF molecules corresponding to the mononuclear species with two coordinated THF molecules. The dinuclear species tend to be more reactive in nucleophilic additions than mononuclear species.

Table S1. Total Electronic Energy and Gibbs Free Energy (Hartree) in THF at 298.15 K

	Description in the main text	*E*	Thermal free term (298.15 K)	*G*
$ZnMe_2$		-1858.804559	0.039779	-1858.76478
MeMgCl		-700.206734	0.007852	-700.198882
Me_2Mg		-279.814964	0.038034	-279.776930
$MgCl_2$		-1120.591413	-0.023043	-1120.614456
MeMgCl...THF		-932.533321	0.115402	-932.417919
Me_2Mg...THF		-512.136958	0.146748	-511.990210
$MgCl_2$...THF		-1352.922664	0.080243	-1352.842420
PhCN…$MgCl_2$		-1444.874468	0.060614	-1444.813854
PnCN...$MgCl_2$...THF1		-1677.206329	0.169000	-1677.037328
PnCN...$MgCl_2$...THF2a		-1909.530737	0.281136	-1909.249601
PnCN...$MgCl_2$...THF2b		-1909.531099	0.283351	-1909.247748
RC_MeMgCl		-1024.485217	0.092336	-1024.392881
TS_MeMgCl	**$TS(I\text{-}V)_0$**	-1024.444519	0.098265	-1024.346254
PR_MeMgCl		-1024.504171	0.099553	-1024.404618
RCa_MeMgCl$_{THF1}$		-1256.813023	0.203990	-1256.609033
TSa_MeMgCl$_{THF1}$		-1256.777301	0.208716	-1256.568584
PRa_MeMgCl$_{THF1}$		-1256.834120	0.208362	-1256.625758
RCb_MeMgCl$_{THF1}$		-1256.812378	0.201570	-1256.610808
TSb_MeMgCl$_{THF1}$		-1256.776468	0.208128	-1256.568340
PRb_MeMgCl$_{THF1}$		-1256.831617	0.210046	-1256.621571
RCa_MeMgCl$_{THF2}$	**I**	-1489.131563	0.313206	-1488.818358
TSa_MeMgCl$_{THF2}$	**TS(I-V)**	-1489.099917	0.316260	-1488.783658
PRa_MeMgCl$_{THF2}$	**V**	-1489.165507	0.320315	-1488.845191
RCb_MeMgCl$_{THF2}$		-1489.131512	0.314797	-1488.816716
TSb_MeMgCl$_{THF2}$		-1489.092019	0.316786	-1488.775233
PRb_MeMgCl$_{THF2}$		-1489.166855	0.319494	-1488.847361
RC_Me_2Mg		-604.088749	0.124951	-603.963798
TS_Me_2Mg		-604.055526	0.129773	-603.925752
PR_Me_2Mg		-604.115591	0.132978	-603.982613
RCa_Me_2Mg_{THF1}		-836.412588	0.235415	-836.177173
TSa_Me_2Mg_{THF1}		-836.384225	0.239001	-836.145223

PRa_Me_2Mg_{THF1}	-836.440981	0.236564	-836.204417
RCb_Me_2Mg_{THF1}	-836.410894	0.233317	-836.177577
TSb_Me_2Mg_{THF1}	-836.382486	0.237542	-836.144944
PRb_Me_2Mg_{THF1}	-836.440871	0.240097	-836.200774
RCa_Me_2Mg_{THF2}	-1068.725429	0.343686	-1068.381743
TSa_Me_2Mg_{THF2}	-1068.699214	0.346571	-1068.352643
PRa_Me_2Mg_{THF2}	-1068.767112	0.350594	-1068.416517
RCb_Me_2Mg_{THF2}	-1068.726968	0.345702	-1068.381266
TSb_Me_2Mg_{THF2}	-1068.689882	0.348400	-1068.341482
PRb_Me_2Mg_{THF2}	-1068.768634	0.350799	-1068.417834
RCa_MeMgClZn	-2883.302038	0.158197	-2883.143840
TSa_MeMgClZn	-2883.275050	0.162375	-2883.112674
PRa_MeMgClZn	-2883.349705	0.165711	-2883.183994
RCb_MeMgClZn	-2883.302351	0.156949	-2883.145403
TSb_MeMgClZn	-2883.266490	0.157272	-2883.109217
PRb_MeMgClZn	-2883.346518	0.163572	-2883.182946
RCa_MeMgClZn$_{THF1}$	-3115.637468	0.267972	-3115.369497
TSa_MeMgClZn$_{THF1}$	-3115.608238	0.272292	-3115.335946
PRa_MeMgClZn$_{THF1}$	-3115.683431	0.277212	-3115.406219
RCb_MeMgClZn$_{THF1}$	-3115.636841	0.267562	-3115.369279
TSb_MeMgClZn$_{THF1}$	-3115.607420	0.272216	-3115.335204
PRb_MeMgClZn$_{THF1}$	-3115.686104	0.275363	-3115.410741
RCa_MeMgClZn$_{THF2}$	-3347.958213	0.376379	-3347.581834
TSa_MeMgClZn$_{THF2}$	-3347.933148	0.382955	-3347.550194
PRa_MeMgClZn$_{THF2}$	-3348.013925	0.387673	-3347.626252
RCb_MeMgClZn$_{THF2}$	-3347.956818	0.378046	-3347.578772
TSb_MeMgClZn$_{THF2}$	-3347.929266	0.380905	-3347.548361
PRb_MeMgClZn$_{THF2}$	-3348.007941	0.384777	-3347.623164
RCc_MeMgClZn$_{THF2}$	-3347.958289	0.377749	-3347.580540
TSc_MeMgClZn$_{THF2}$	-3347.933818	0.383193	-3347.550625
PRc_MeMgClZn$_{THF2}$	-3348.004612	0.386811	-3347.617801
RC_Me_2MgZn	-2462.920981	0.189712	-2462.731269
TS_Me_2MgZn	-2462.885265	0.193445	-2462.691820
PR_Me_2MgZn	-2462.958975	0.198407	-2462.760568
RCa_Me_2MgZn_{THF1}	-2695.240001	0.298440	-2694.941560
TSa_Me_2MgZn_{THF1}	-2695.216482	0.303460	-2694.913022
PRa_Me_2MgZn_{THF1}	-2695.288327	0.308353	-2694.979974
RCb_Me_2MgZn_{THF1}	-2695.240297	0.298281	-2694.942016
TSb_Me_2MgZn_{THF1}	-2695.213407	0.303127	-2694.910279
PRb_Me_2MgZn_{THF1}	-2695.291393	0.304469	-2694.986924
RCa_Me_2MgZn_{THF2}	-2927.557273	0.410859	-2927.146414
TSa_Me_2MgZn_{THF2}	-2927.534592	0.415275	-2927.119317
PRa_Me_2MgZn_{THF2}	-2927.615642	0.416423	-2927.199219
RCb_Me_2MgZn_{THF2}	-2927.557291	0.407791	-2927.149500
TSb_Me_2MgZn_{THF2}	-2927.530667	0.412219	-2927.118448
PRb_Me_2MgZn_{THF2}	-2927.618116	0.416686	-2927.201431
RCc_Me_2MgZn_{THF2}	-2927.557675	0.408227	-2927.149449
TSc_Me_2MgZn_{THF2}	-2927.533875	0.414697	-2927.119178
PRc_Me_2MgZn_{THF2}	-2927.604792	0.418755	-2927.186038
RC_$MgCl_2$Zn	-3303.689607	0.125812	-3303.563796
TS_$MgCl_2$Zn	-3303.655140	0.127571	-3303.527569
PR_$MgCl_2$Zn	-3303.736677	0.129871	-3303.606806
RCa_$MgCl_2Zn_{THF1}$	-3536.024658	0.236939	-3535.787719
TSa_$MgCl_2Zn_{THF1}$	-3535.990430	0.238498	-3535.751931
PRa_$MgCl_2Zn_{THF1}$	-3536.067482	0.243454	-3535.824028
RCb_$MgCl_2Zn_{THF1}$	-3536.028744	0.235720	-3535.793024
TSb_$MgCl_2Zn_{THF1}$	-3535.988839	0.236061	-3535.752778
PRb_$MgCl_2Zn_{THF1}$	-3536.072221	0.241460	-3535.830761
RCa_$MgCl_2Zn_{THF2}$	-3768.354887	0.348323	-3768.006565
TSa_$MgCl_2Zn_{THF2}$	-3768.314593	0.349725	-3767.964868

PRa_MgCl$_2$Zn$_{THF2}$		-3768.401176	0.353896	-3768.047280
RCb_MgCl$_2$Zn$_{THF2}$		-3768.350949	0.344655	-3768.006293
TSb_MgCl$_2$Zn$_{THF2}$		-3768.311744	0.345949	-3767.965794
PRb_MgCl$_2$Zn$_{THF2}$		-3768.396262	0.353433	-3768.042830
RCc_MgCl$_2$Zn$_{THF2}$		-3768.352285	0.344054	-3768.008230
TSc_MgCl$_2$Zn$_{THF2}$		-3768.316514	0.349752	-3767.966762
PRc_MgCl$_2$Zn$_{THF2}$		-3768.388382	0.355576	-3768.032806
RC$_{gm}$_MeMg(μ-Cl)$_2$MeMg		-1724.722133	0.121853	-1724.600280
TS$_{gm}$_MeMg(μ-Cl)$_2$MeMg		-1724.682595	0.125506	-1724.557089
PR$_{gm}$_MeMg(μ-Cl)$_2$MeMg		-1724.740428	0.127041	-1724.613388
RC$_{vi}$_MeMg(μ-Cl)$_2$MeMg		-1724.722310	0.121951	-1724.600359
TS$_{vi}$_MeMg(μ-Cl)$_2$MeMg		-1724.685266	0.124169	-1724.561098
PR$_{vi}$_MeMg(μ-Cl)$_2$MeMg		-1724.766572	0.127625	-1724.638947
RC$_{gm}$_MeMg(μ-Cl)(μ-Me)MgCl		-1724.718908	0.124733	-1724.594175
TS$_{gm}$_MeMg(μ-Cl)(μ-Me)MgCl		-1724.680226	0.126596	-1724.553630
PR$_{gm}$_MeMg(μ-Cl)(μ-Me)MgCl		-1724.735803	0.130775	-1724.605028
RC$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMg		-1724.719472	0.124203	-1724.595269
TS$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMg		-1724.682773	0.128076	-1724.554696
PR$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMg		-1724.763370	0.131190	-1724.632180
RC$_{gm}$_MeMg(μ-Cl)$_2$MeMg$_{THF3}$		-2421.692771	0.453794	-2421.238977
TS$_{gm}$_MeMg(μ-Cl)$_2$MeMg$_{THF3}$		-2421.668330	0.456664	-2421.211666
PR$_{gm}$_MeMg(μ-Cl)$_2$MeMg$_{THF3}$		-2421.731539	0.460124	-2421.271414
RC$_{vi}$_MeMg(μ-Cl)$_2$MeMg$_{THF3}$		-2421.692922	0.451936	-2421.240986
TS$_{vi}$_MeMg(μ-Cl)$_2$MeMg$_{THF3}$		-2421.664983	0.455969	-2421.209014
PR$_{vi}$_MeMg(μ-Cl)$_2$MeMg$_{THF3}$		-2421.745179	0.463832	-2421.281347
RC$_{gm}$_MeMg(μ-Cl)(μ-Me)MgCl$_{THF3}$	**II$_g$**	-2421.693754	0.455481	-2421.238272
TS$_{gm}$_MeMg(μ-Cl)(μ-Me)MgCl$_{THF3}$	**TS(II$_g$-VI$_g$)**	-2421.668514	0.458937	-2421.209577
PR$_{gm}$_MeMg(μ-Cl)(μ-Me)MgCl$_{THF3}$	**VI$_g$**	-2421.733978	0.469853	-2421.264125
RC$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMg$_{THF3}$	**II$_v$**	-2421.693886	0.45612	-2421.237767
TS$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMg$_{THF3}$	**TS(II$_v$-VI$_v$)**	-2421.663582	0.456501	-2421.207081
PR$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMg$_{THF3}$	**VI$_v$**	-2421.754009	0.462434	-2421.291574
TS_MgCl(μ-Cl)(μ-Me)MeMg$_{THF3}$	**TS(II$_v$- II$_v$′)**	-2421.688774	0.455153	-2421.233621
RC$_{vi}$_MgCl(μ-Cl)Me$_2$Mg$_{THF3}$	**II$_v$′**	-2421.689668	0.456017	-2421.233651
RC$_{gm}$_MeMg(μ-Cl)$_2$MeMgZn		-3583.541308	0.185919	-3583.355389
TS$_{gm}$_MeMg(μ-Cl)$_2$MeMgZn		-3583.513754	0.189886	-3583.323868
PR$_{gm}$_MeMg(μ-Cl)$_2$MeMgZn		-3583.589418	0.191758	-3583.397660
RC$_{vi}$_MeMg(μ-Cl)$_2$MeMgZn		-3583.547731	0.184082	-3583.363649
TS$_{vi}$_MeMg(μ-Cl)$_2$MeMgZn		-3583.502271	0.191667	-3583.310604
PR$_{vi}$_MeMg(μ-Cl)$_2$MeMgZn		-3583.554454	0.194280	-3583.360174
RC$_{gm}$_MeMg(μ-Cl)(μ-Me)MgClZn		-3583.537650	0.187875	-3583.349774
TS$_{gm}$_MeMg(μ-Cl)(μ-Me)MgClZn		-3583.510990	0.192709	-3583.318281
PR$_{gm}$_MeMg(μ-Cl)(μ-Me)MgClZn		-3583.586955	0.193335	-3583.393619
RC$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMgZn		-3583.549416	0.193758	-3583.355658
TS$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMgZn		-3583.501879	0.192302	-3583.309577
PR$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMgZn		-3583.585288	0.196147	-3583.389141
RC$_{gm}$_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$		-4280.518958	0.519834	-4279.999125
TS$_{gm}$_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$		-4280.501087	0.522843	-4279.978244
PR$_{gm}$_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$		-4280.571553	0.523490	-4280.048063
RC$_{vi}$_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$		-4280.517944	0.520713	-4279.997231
TS$_{vi}$_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$		-4280.478574	0.524483	-4279.972387
PR$_{vi}$_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$		-4280.565304	0.525611	-4280.039692
RC$_{gm}$_MeMg(μ-Cl)(μ-Me)MgClZn$_{THF3}$	**III$_g$**	-4280.520080	0.520386	-4279.999693
TS$_{gm}$_MeMg(μ-Cl)(μ-Me)MgClZn$_{THF3}$	**TS(III$_g$-IV$_g$)**	-4280.502392	0.523681	-4279.978580
PR$_{gm}$_MeMg(μ-Cl)(μ-Me)MgClZn$_{THF3}$	**IV$_g$**	-4280.570356	0.527469	-4280.042887
RC$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMgZn$_{THF3}$		-4280.521623	0.524528	-4279.997095
TS$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMgZn$_{THF3}$		-4280.497356	0.521461	-4279.975895
PR$_{vi}$_MgCl(μ-Cl)(μ-Me)MeMgZn$_{THF3}$		-4280.572839	0.528871	-4280.043968
RC$_{vi}$_MgCl(μ-Cl)Me$_2$MgZn$_{THF3}$	**III$_v$**	-4280.523916	0.519265	-4280.00465
TS$_{vi}$_MgCl(μ-Cl)Me$_2$MgZn$_{THF3}$	**TS(III$_v$-IV$_v$)**	-4280.498870	0.521913	-4279.976957

PR_{vi}_MgCl(μ-Cl)Me_2MgZn_{THF3}	**IV_v**	-4280.571306	0.528750	-4280.042556

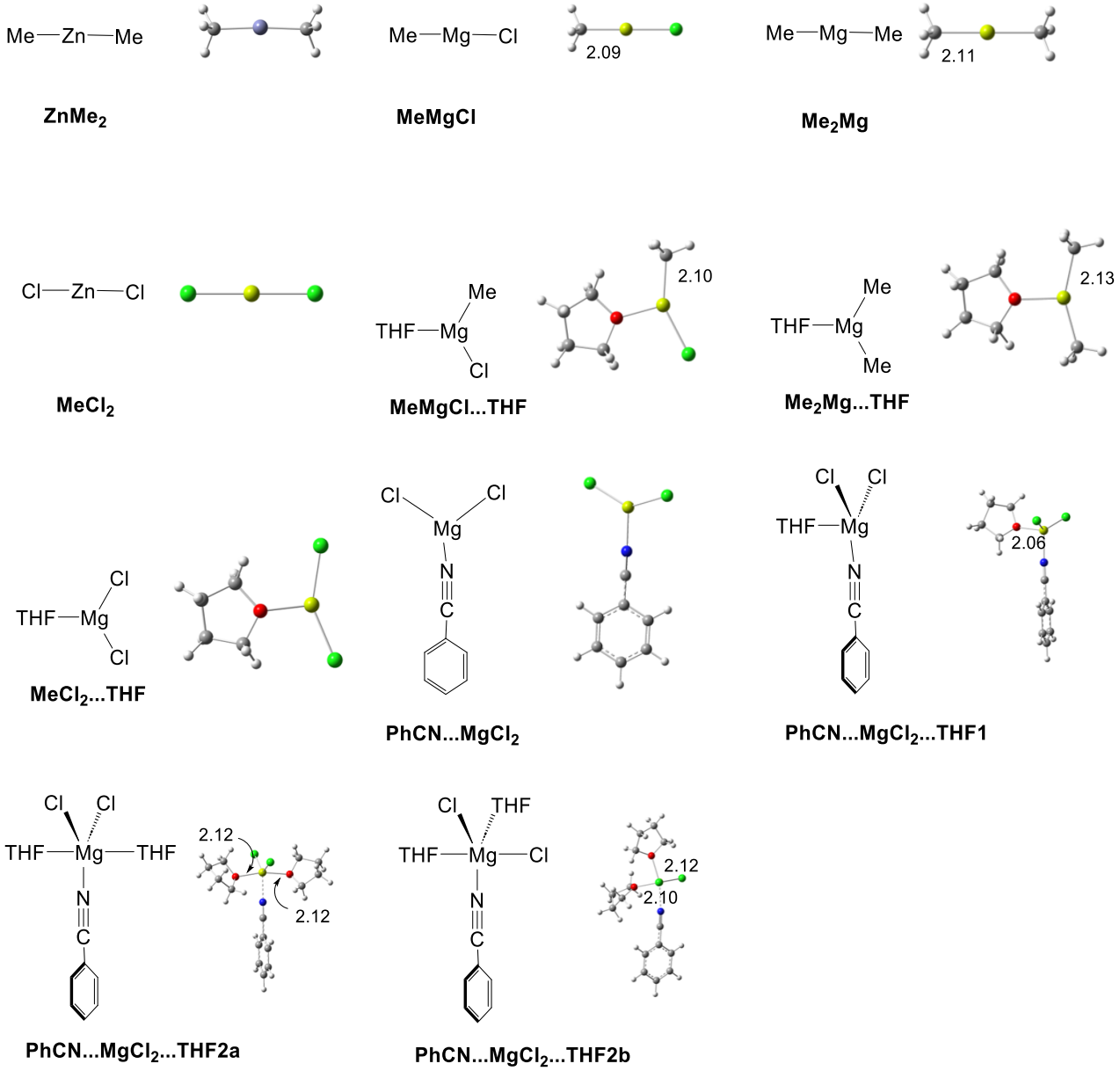


Fig. S1. Structures optimized at M06/6-31G(d,p) level. The bond lengths are shown in Angstrom.

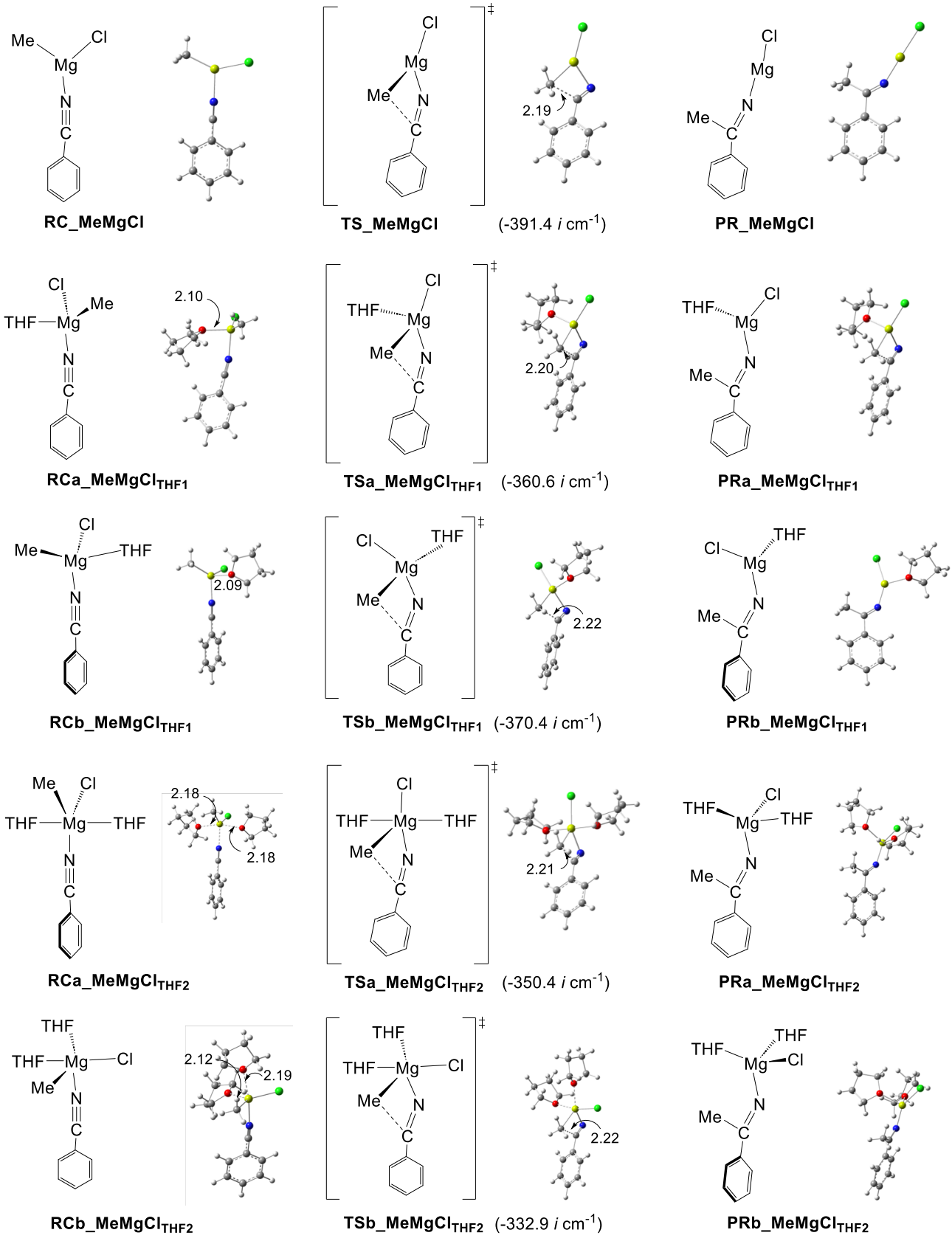


Fig. S1. *Continued.*

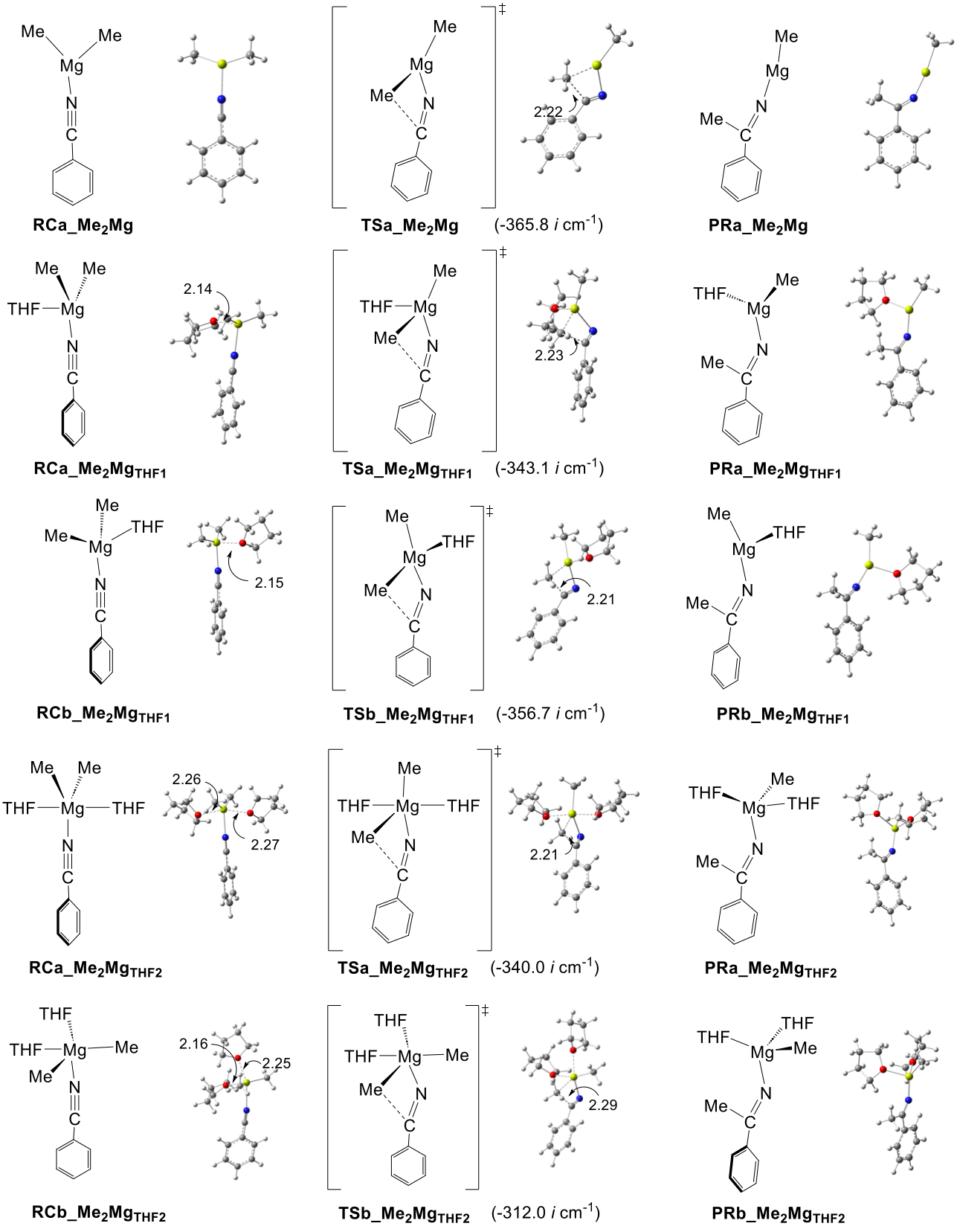


Fig. S1. *Continued.*

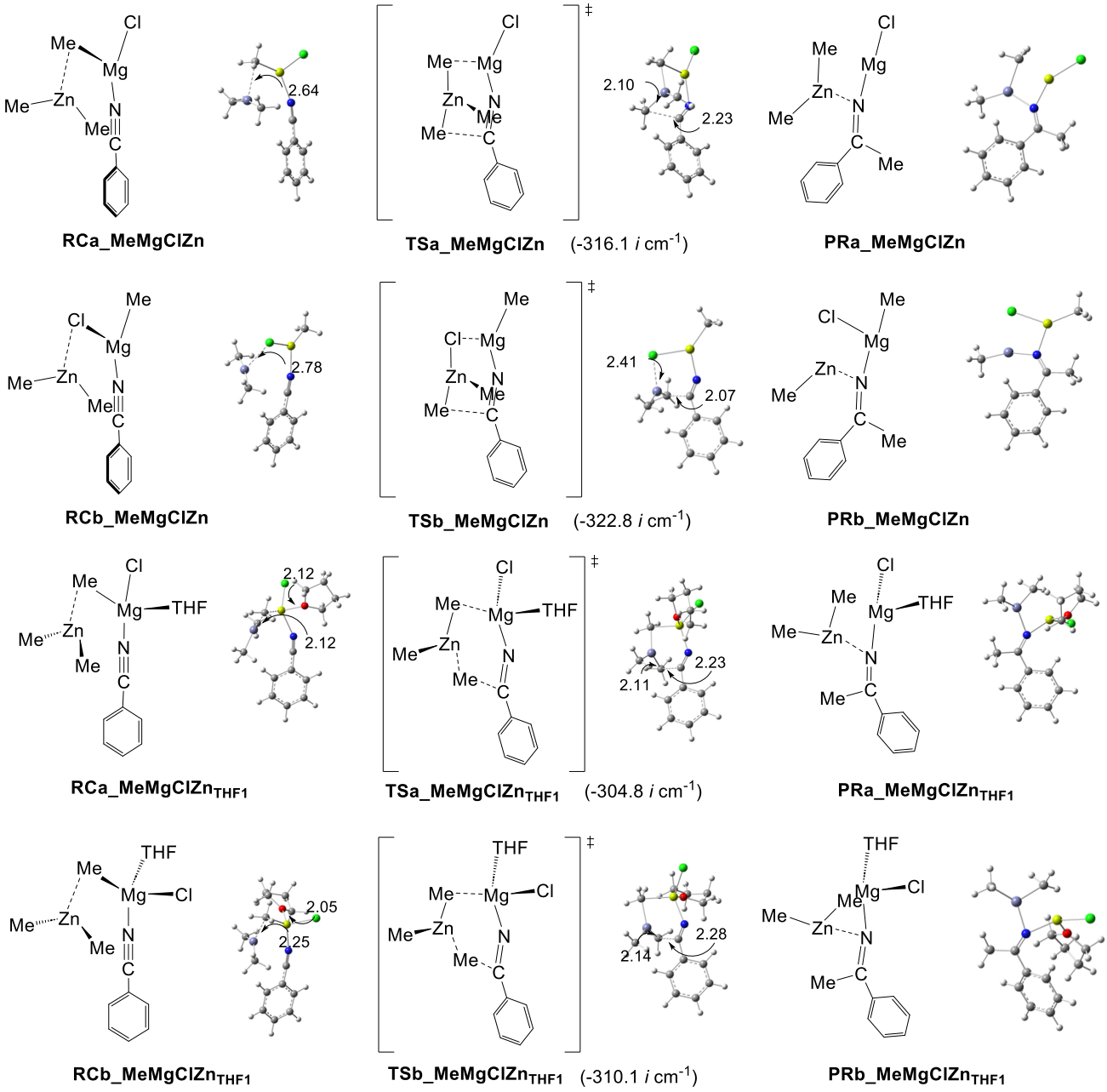


Fig. S1. *Continued.*

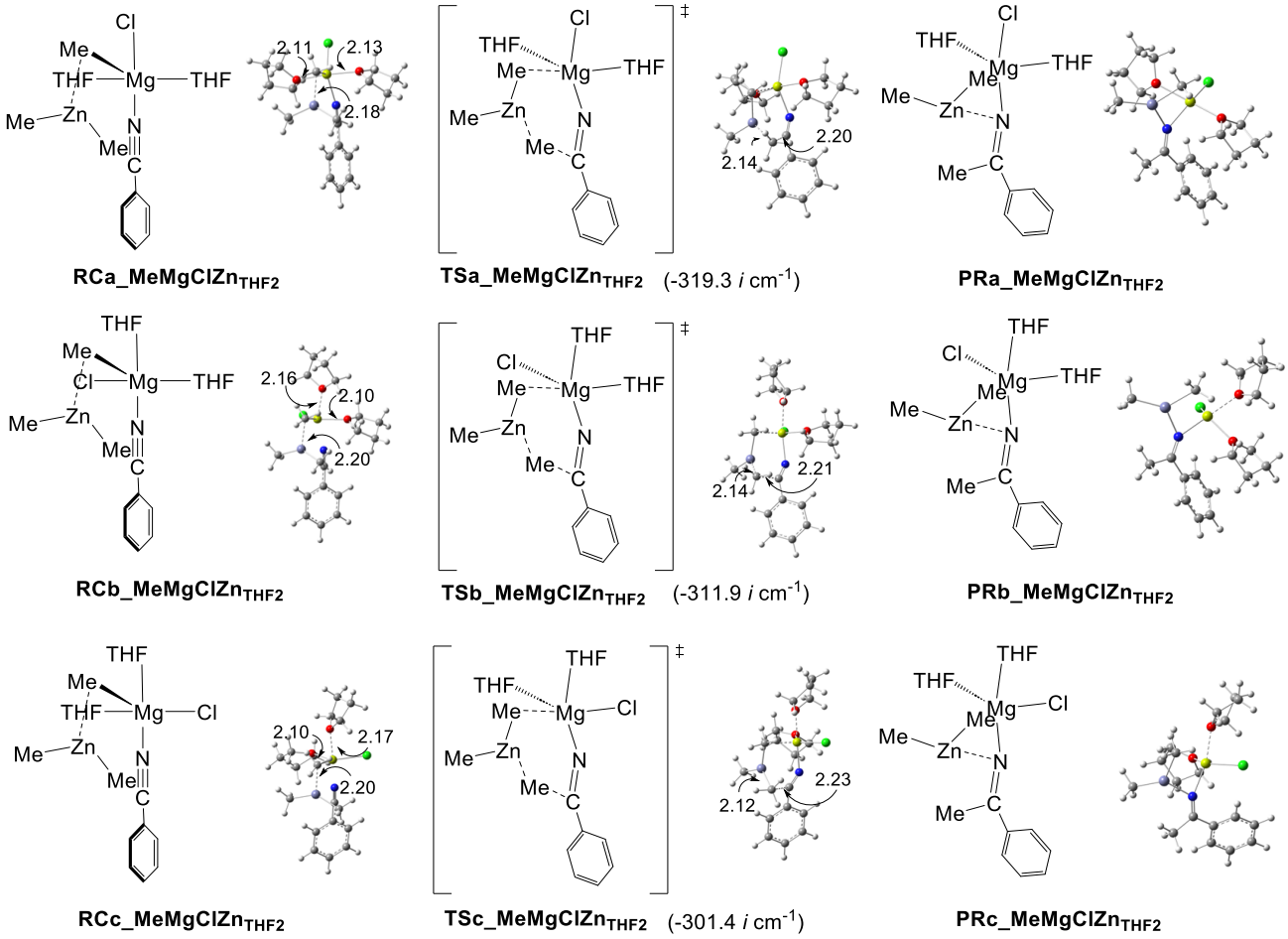
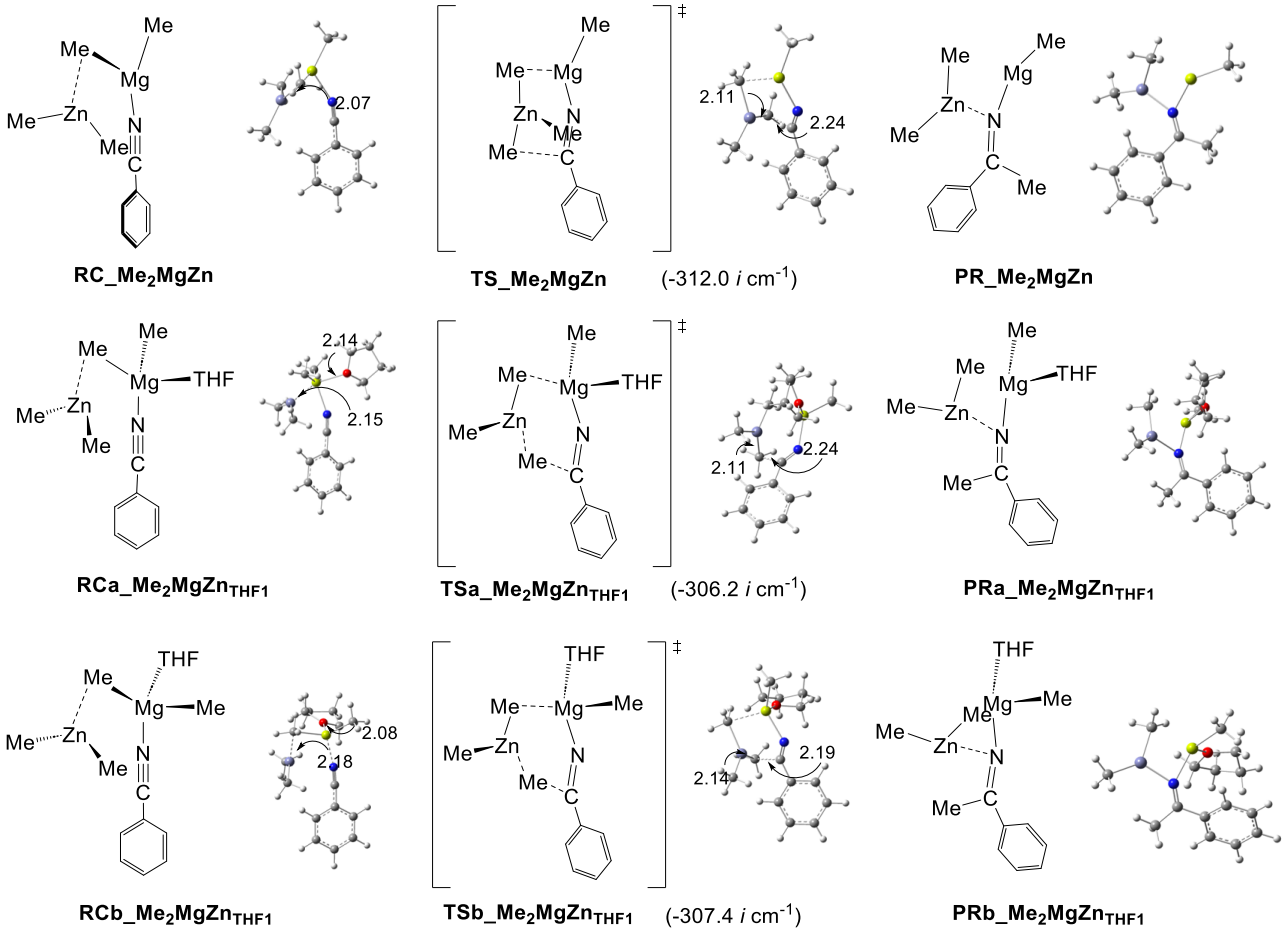


Fig. S1. *Continued.*



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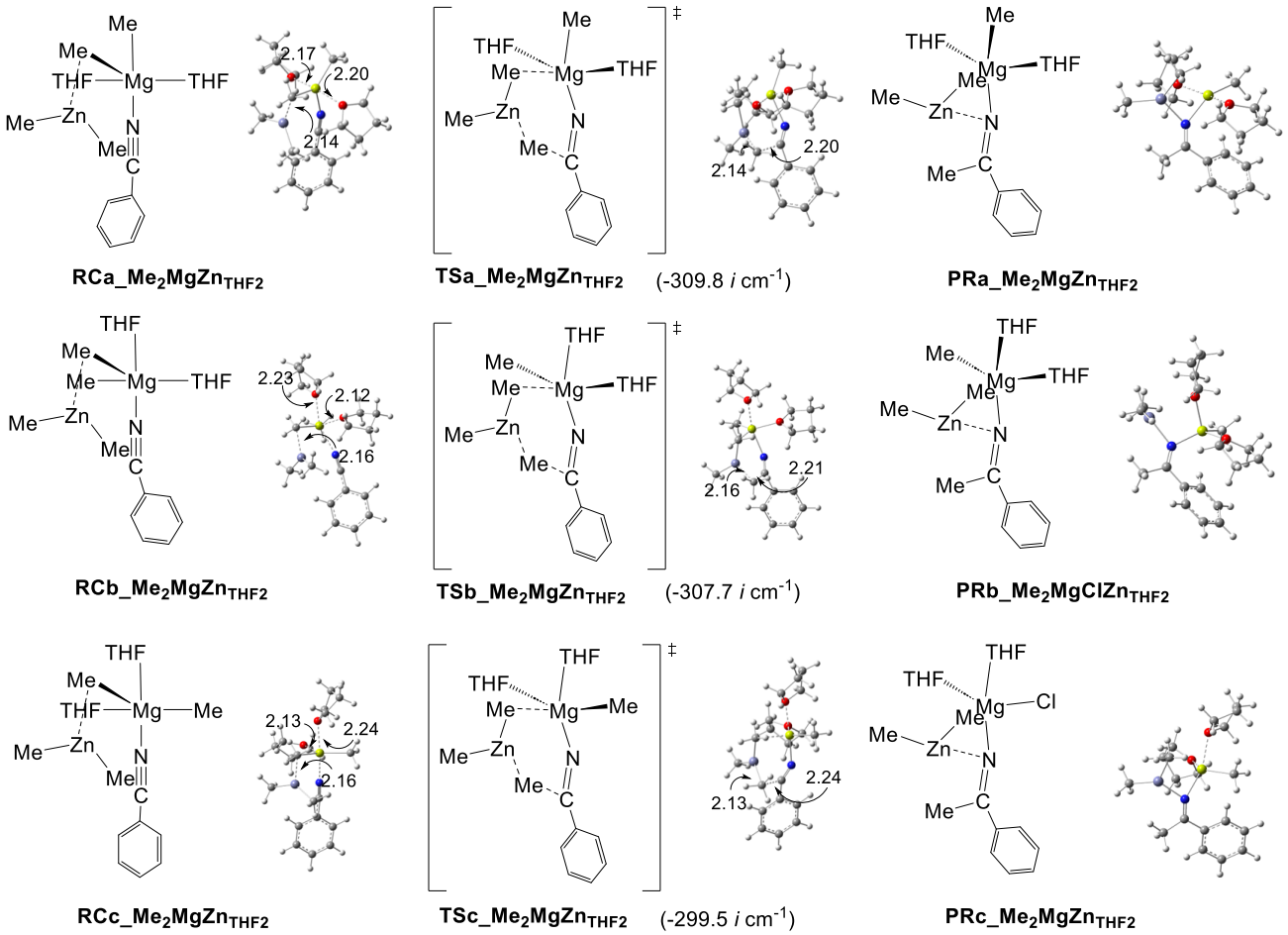

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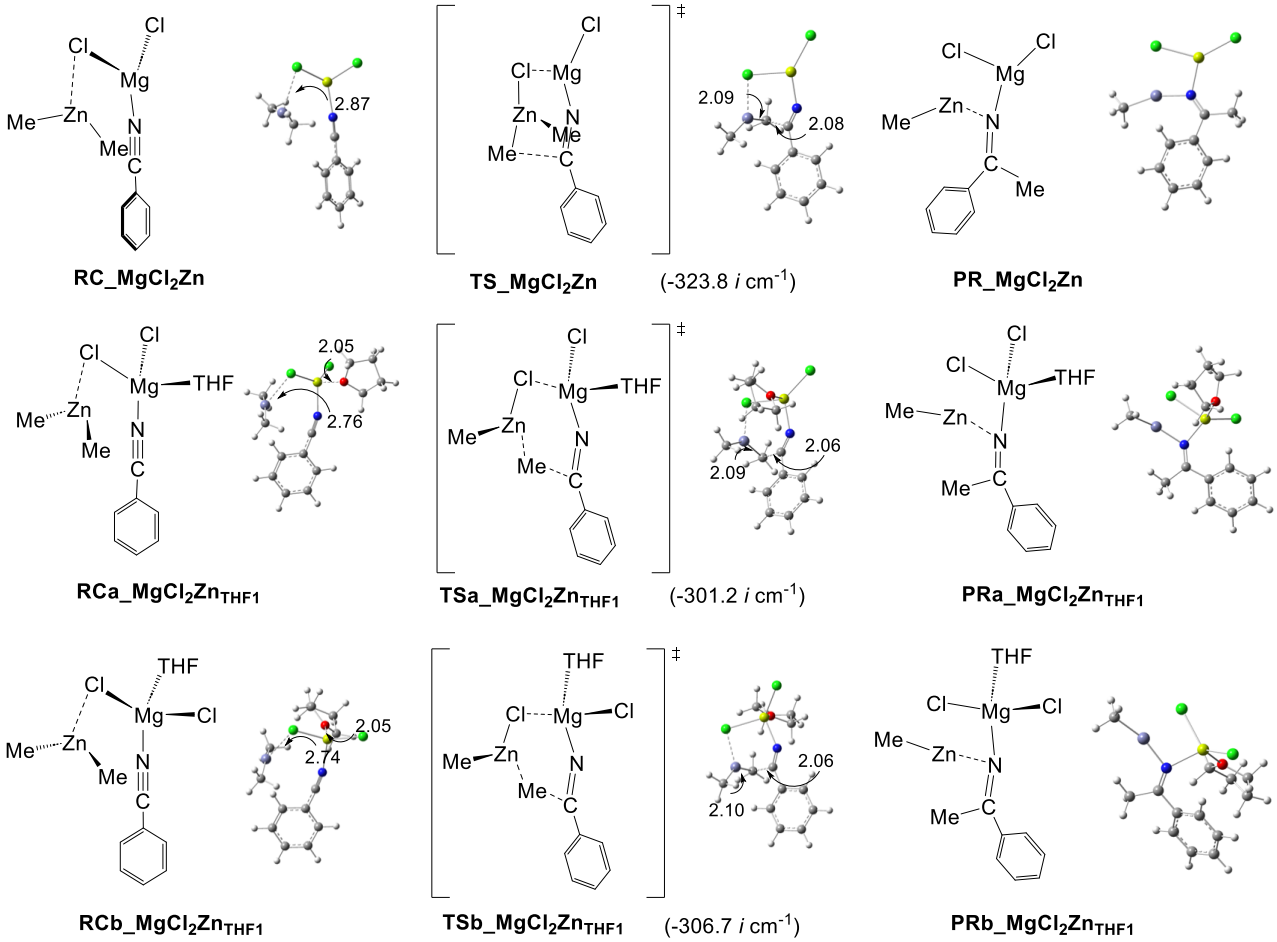

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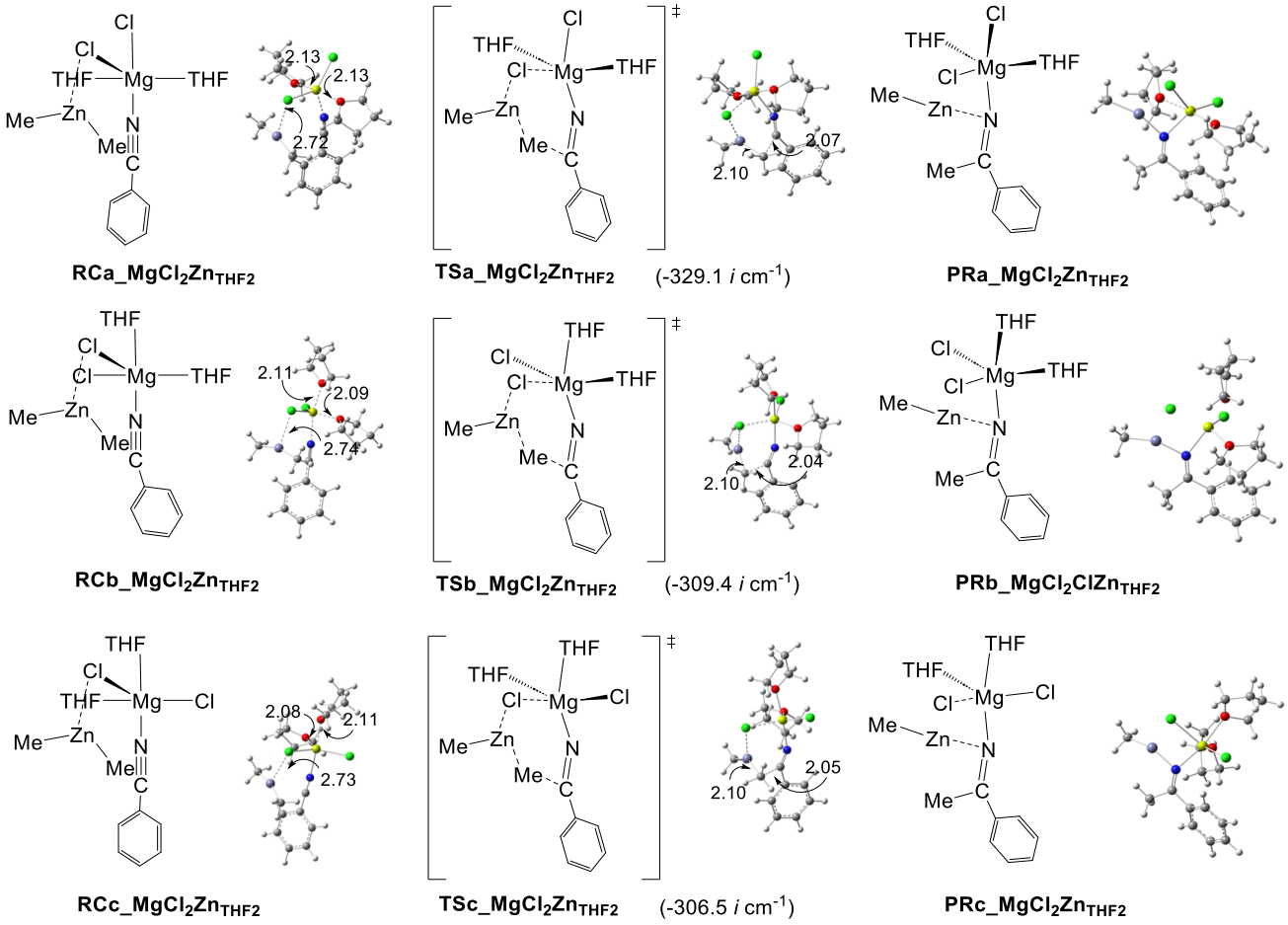

Fig. S1. *Continued.*

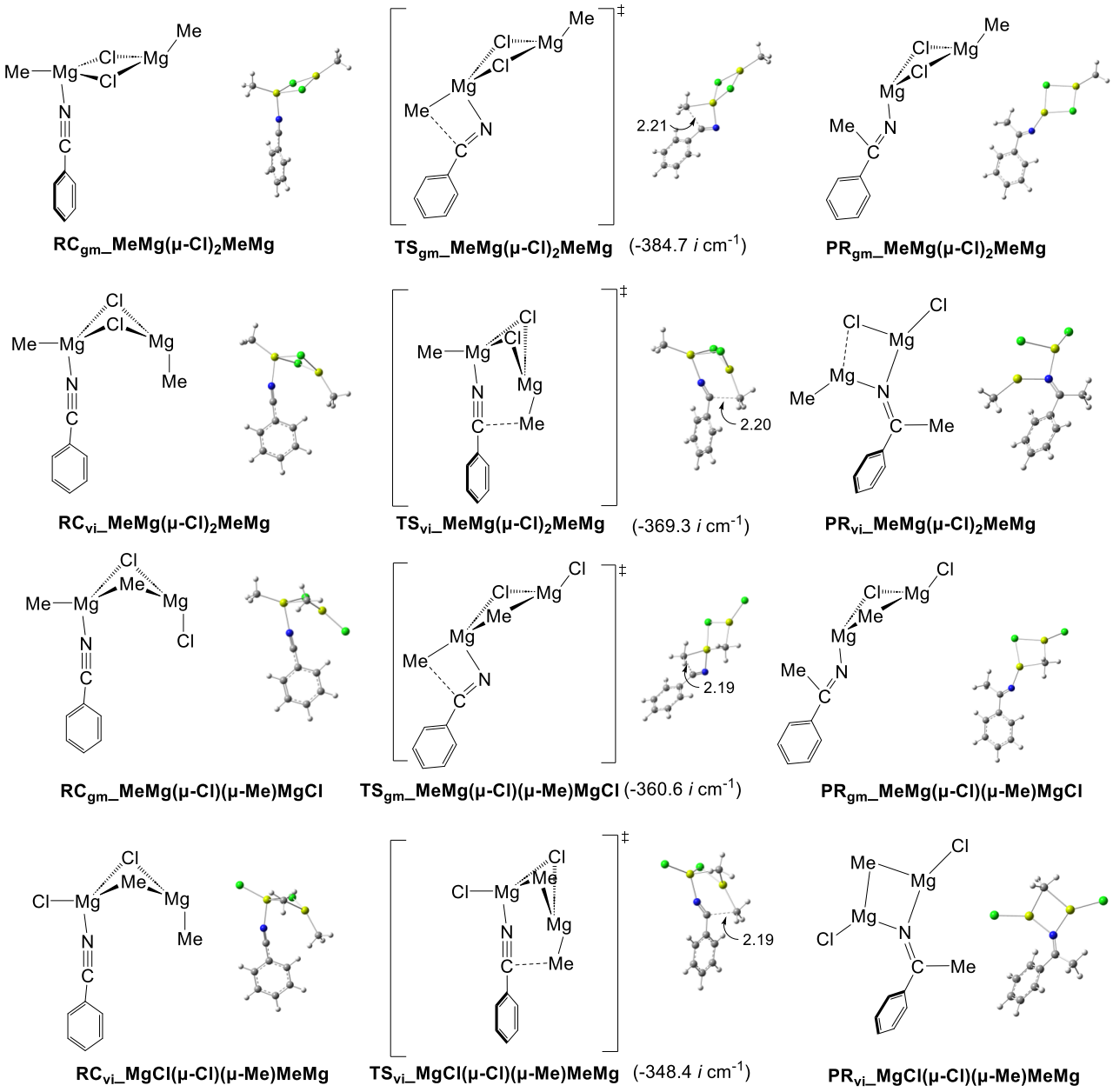

Fig. S1. *Continued.*

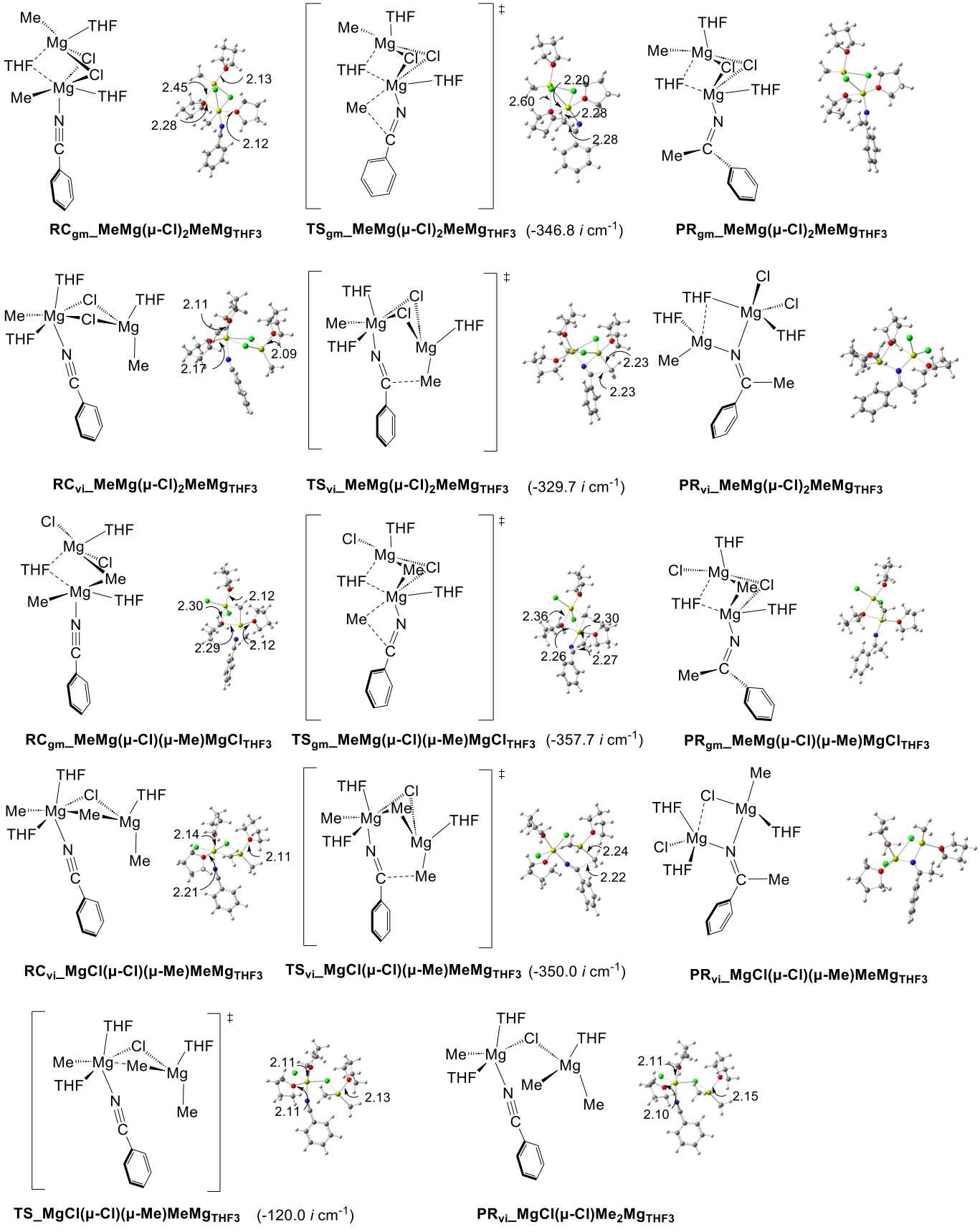

Fig. S1. *Continued.*

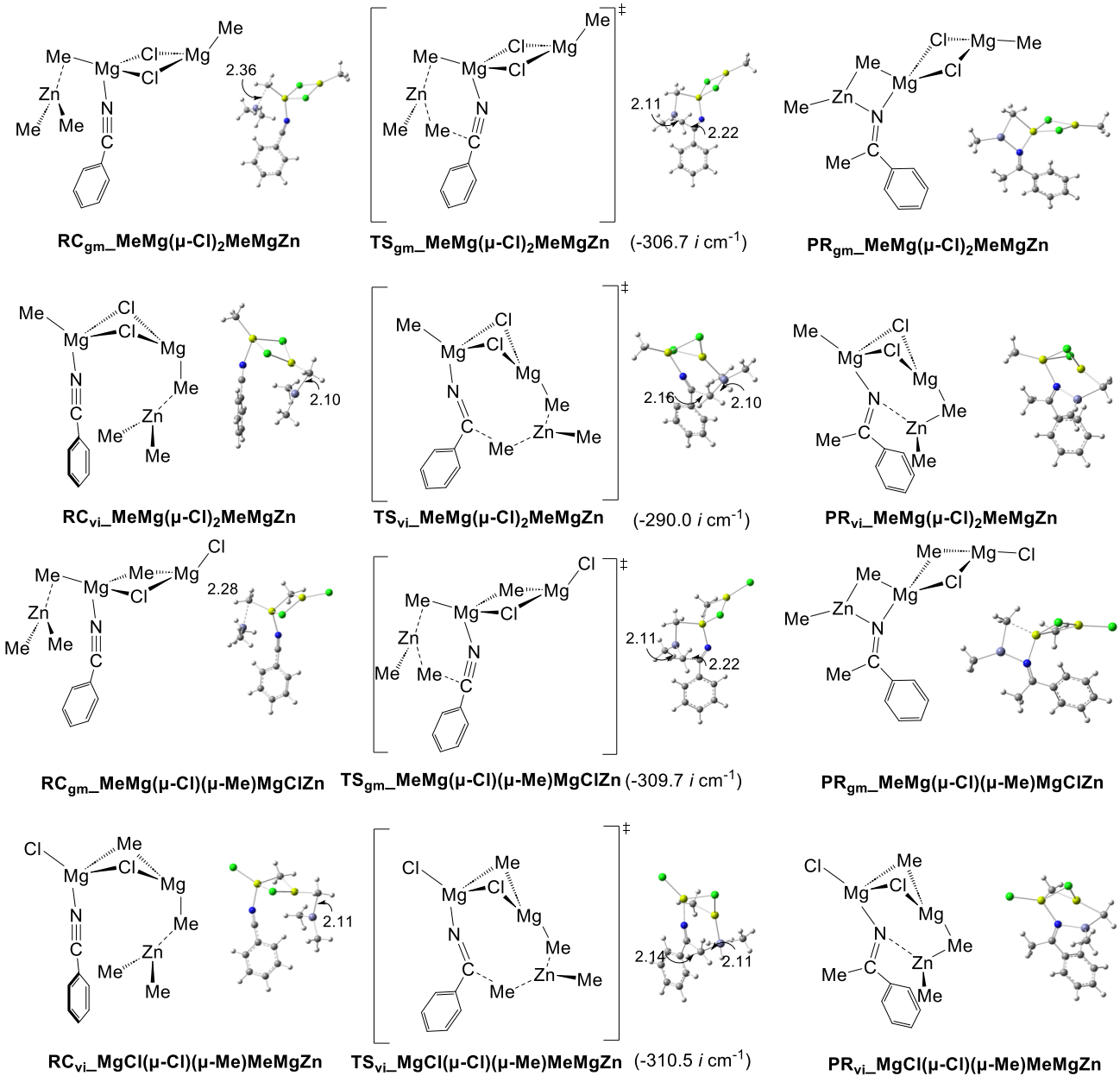

Fig. S1. *Continued.*

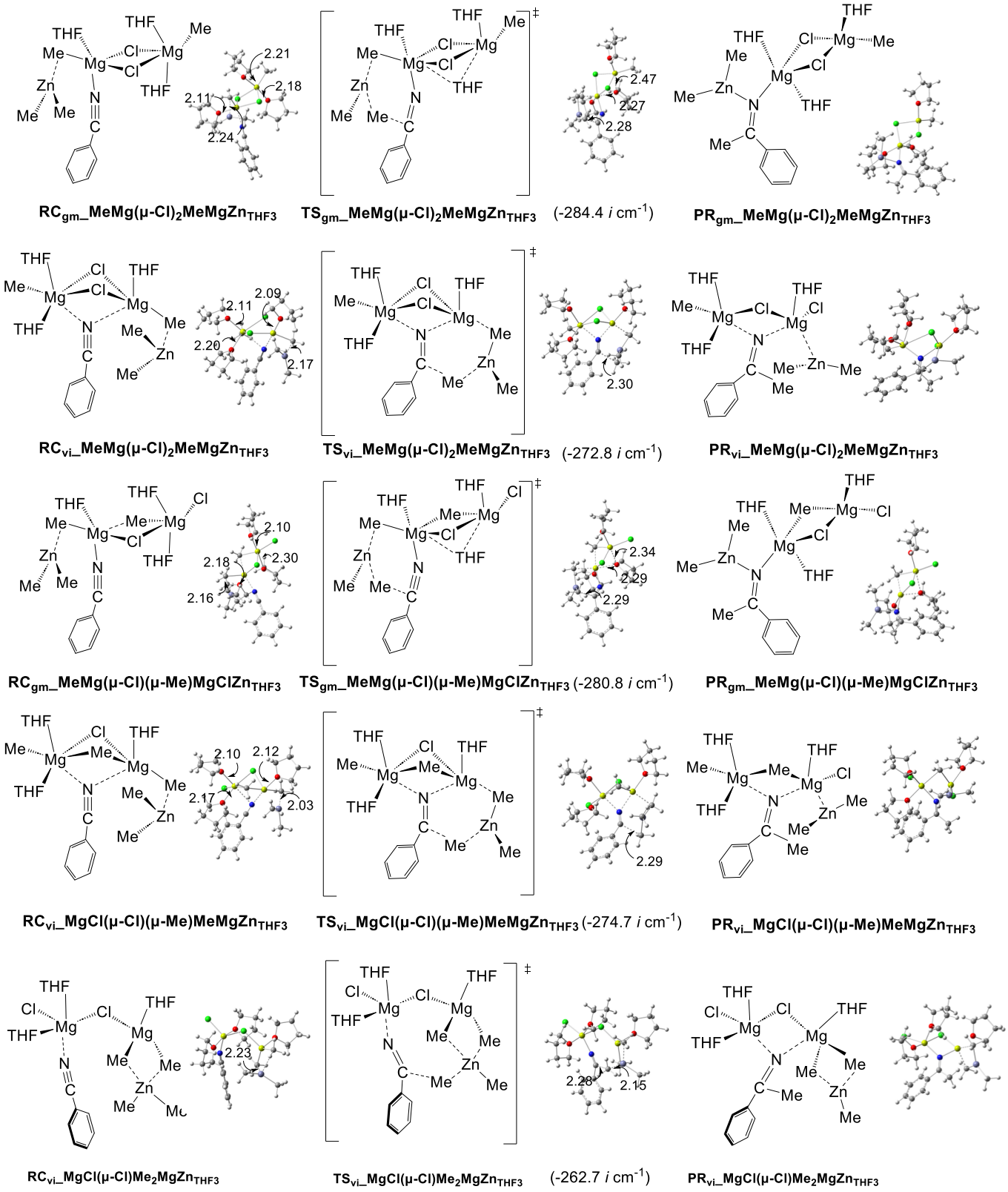

Fig. S1. *Continued.*

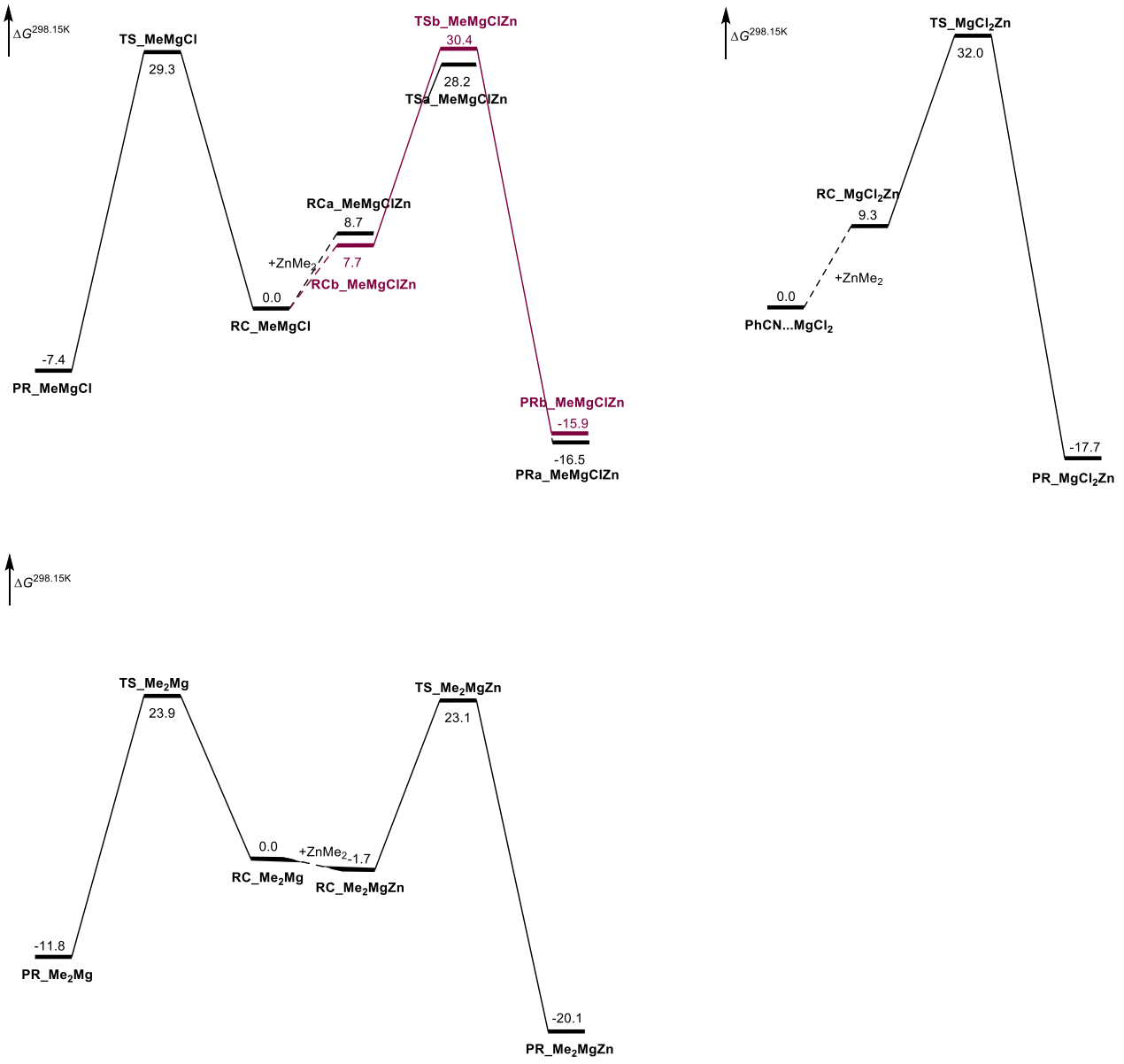

Fig. S2. Gibbs free energy (298.15 K) diagram of the mononuclear species for the Grignard reaction pathways when not coordinated with THF (kcal/mol).

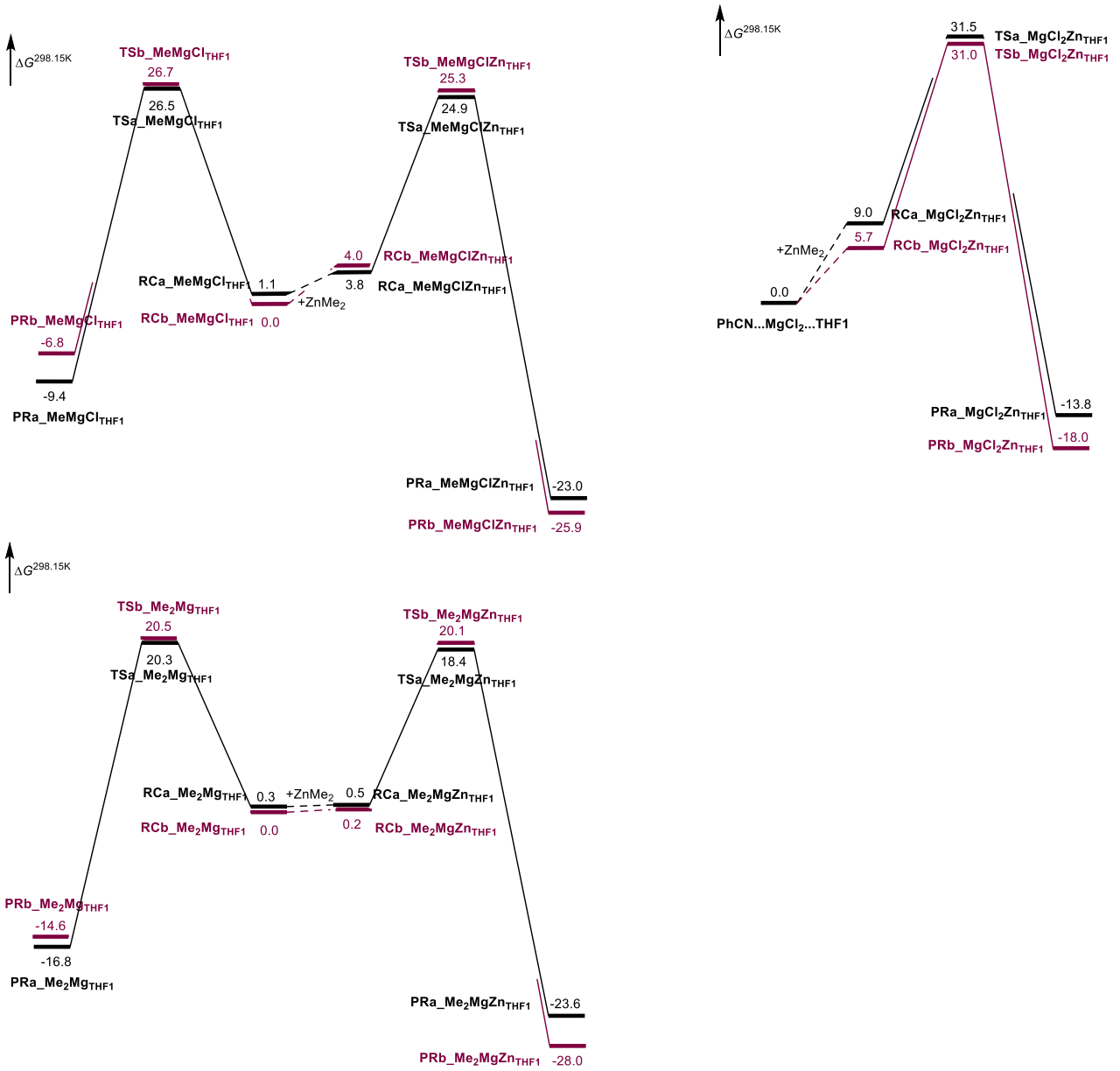

Fig. S3. Gibbs free energy (298.15 K) diagram of the mononuclear species for the Grignard reaction pathways when coordinated with one THF (kcal/mol)

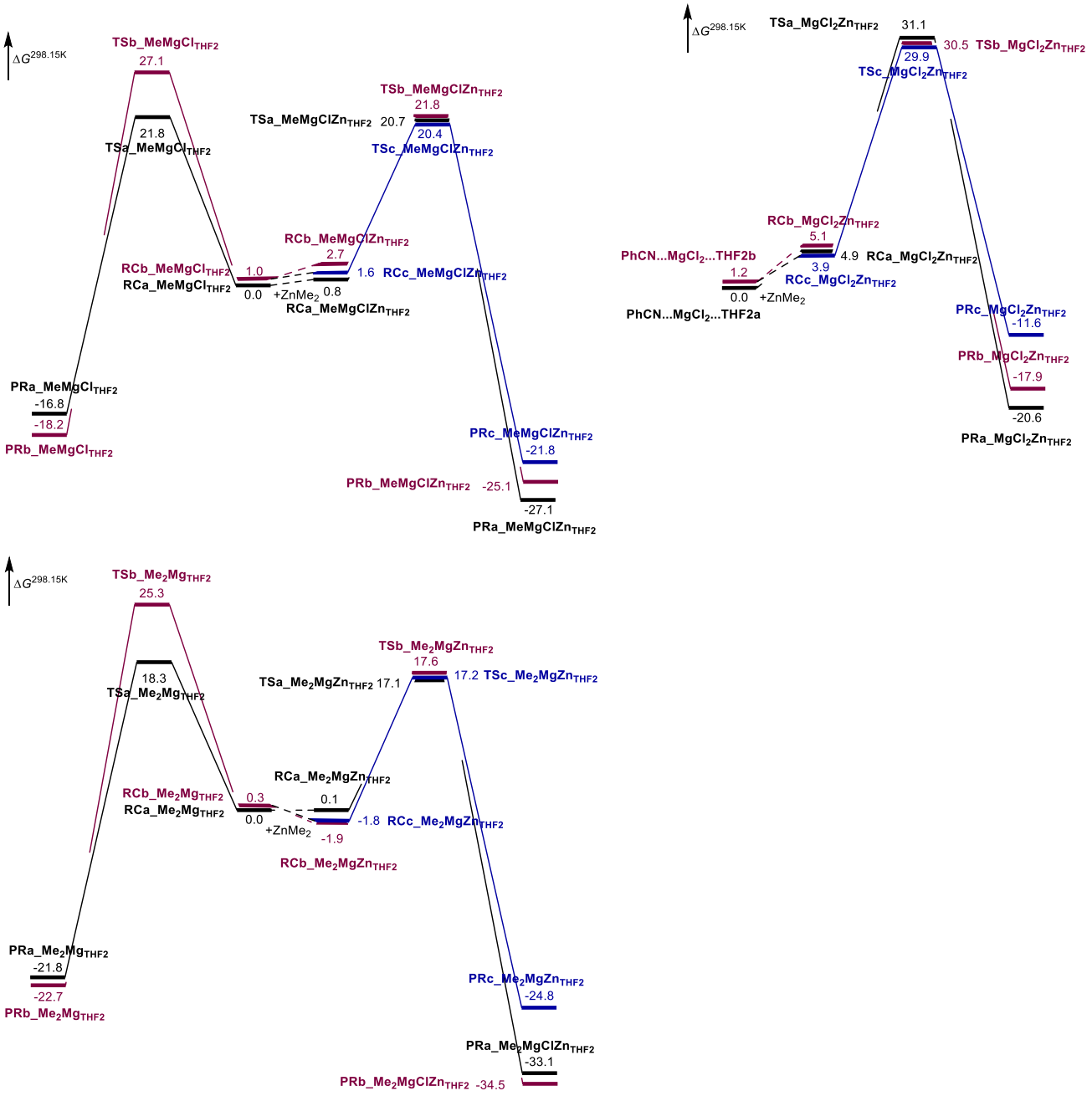

Fig. S4. Gibbs free energy (298.15 K) diagram of the mononuclear species for the Grignard reaction pathways when coordinated with two THFs (kcal/mol)

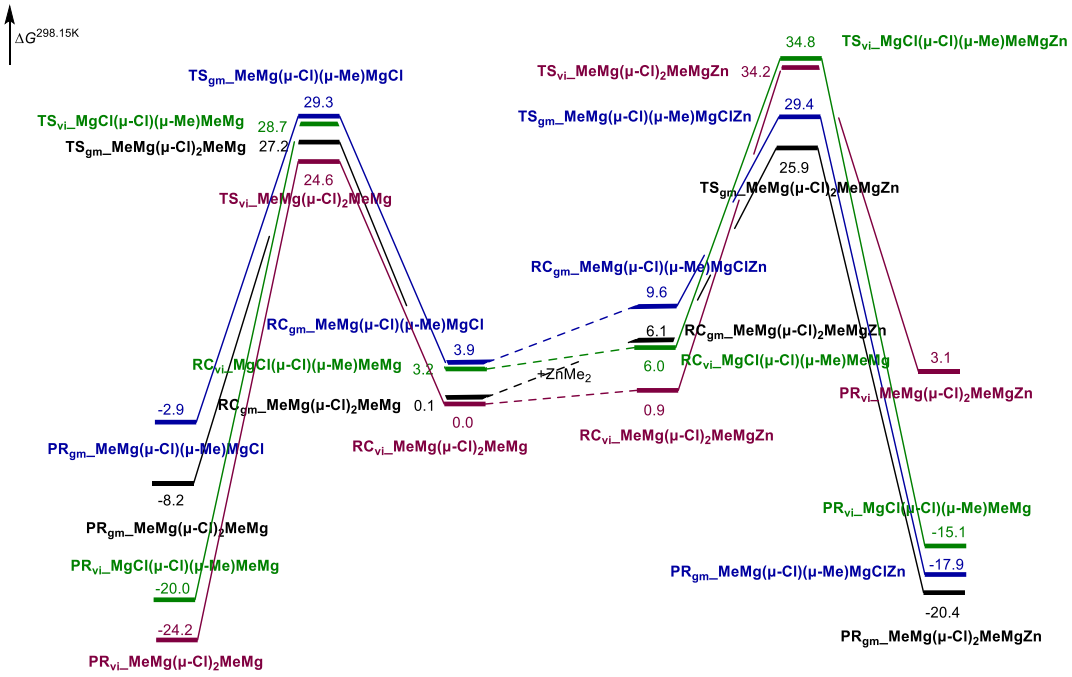

Fig. S5. Gibbs free energy (298.15 K) diagram of the binonuclear species for the Grignard reaction pathways when not coordinated with THF (kcal/mol)

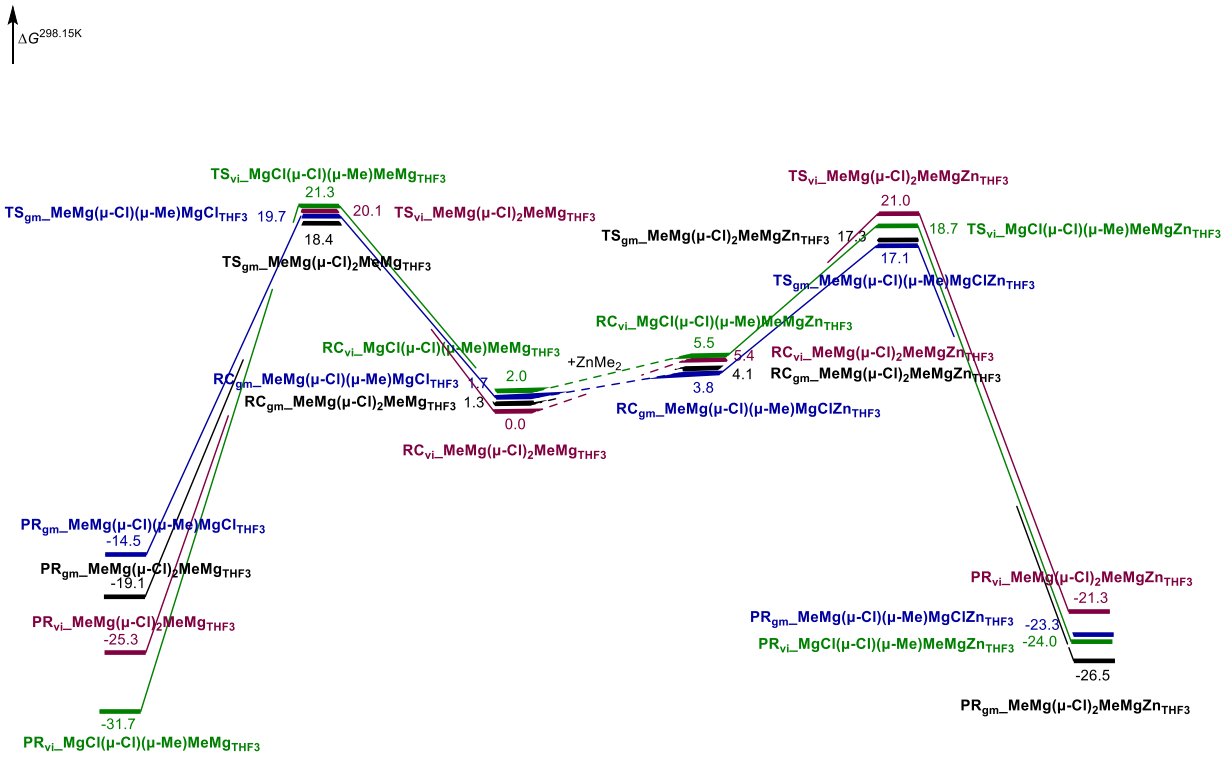

Fig. S6. Gibbs free energy (298.15 K) diagram of the binonuclear species for the Grignard reaction pathways coordinated with 3 THFs (kcal/mol)

Table S2. Cartesian coordinates of stationary points at M06(6-31G(d,p) level are given below:

$ZnMe_2$

Atom	Coordinate (Å)		
	x	y	z
Zn	0.000000	0.026133	-0.000158
C	-1.919681	-0.037210	0.000307
H	-2.339301	0.078469	1.007239
H	-2.369725	0.747554	-0.620063
H	-2.290191	-0.994765	-0.386656
C	1.919682	-0.037209	0.000300
H	2.290268	-0.993458	-0.389802
H	2.369852	0.749648	-0.617316
H	2.339094	0.075061	1.007707

MeMgCl

Atom	Coordinate (Å)		
	x	y	z
Mg	-0.508816	0.000105	0.000306
C	-2.598631	-0.000106	0.000071
H	-3.018705	-0.104766	1.009591
H	-3.015031	0.927846	-0.415527
H	-3.015119	-0.823007	-0.596976
Cl	1.808614	-0.000041	-0.000070

Me_2Mg

Atom	Coordinate (Å)		
	x	y	z
Mg	-0.508816	0.000105	0.000306
C	-2.598631	-0.000106	0.000071
H	-3.018705	-0.104766	1.009591
H	-3.015031	0.927846	-0.415527
H	-3.015119	-0.823007	-0.596976
C	1.621184	-0.000029	-0.000040
H	1.977998	0.816933	0.591701
H	1.977859	-0.921057	0.411532
H	1.977695	0.103969	-1.003526

$MgCl_2$

Atom	Coordinate (Å)		
	x	y	z
Mg	-0.508816	0.000105	0.000306
Cl	-2.858816	-0.000132	0.000042
Cl	1.841184	-0.000043	-0.000075

MeMgCl...THF

Atom	Coordinate (Å)		
	x	y	z
Mg	1.388245	0.592410	0.022931
C	1.512155	2.691890	0.017725
H	0.951200	3.113284	-0.830509
H	1.074457	3.139086	0.922650
H	2.532323	3.091915	-0.059481
Cl	2.476703	-1.464665	0.037275
O	-0.601303	0.052606	-0.175321
C	-1.658411	1.041381	-0.201602
C	-1.161438	-1.273178	0.001085
C	-2.860363	0.329390	0.379028
H	-1.322097	1.912949	0.368354
H	-1.825548	1.342838	-1.244394
C	-2.659319	-1.088936	-0.142354
H	-0.713011	-1.936411	-0.744002
H	-0.884686	-1.630208	1.001235
H	-3.803598	0.781895	0.062234
H	-2.821008	0.346261	1.475246
H	-2.955495	-1.152445	-1.196420
H	-3.220751	-1.842893	0.415524

Me_2Mg...THF

Atom	Coordinate (Å)		
	x	y	z
Mg	-1.766417	-0.002189	0.017945
C	-2.272801	-2.069903	0.003313
H	-1.793948	-2.599387	-0.836297
H	-1.935882	-2.595020	0.911402
H	-3.348667	-2.282650	-0.082571
O	0.334268	0.008886	-0.094259
C	1.160267	-1.173752	-0.159004
C	1.155640	1.185043	0.071266
C	2.527272	-0.719918	0.310783
H	0.698213	-1.947787	0.461556
H	1.182642	-1.525714	-1.199564
C	2.570522	0.715503	-0.201134
H	0.793375	1.956638	-0.615090
H	1.038376	1.549650	1.101099
H	3.331294	-1.348943	-0.080410
H	2.580199	-0.736857	1.406500
H	2.778447	0.730354	-1.278157
H	3.317385	1.337037	0.299906
C	-2.298561	2.059213	0.033305
H	-3.376669	2.258639	0.122341
H	-1.822280	2.607740	0.861685
H	-1.973655	2.574362	-0.884855

$MgCl_2$...THF

Atom	Coordinate (Å)		
	x	y	z
Mg	-1.268708	-0.000031	0.019818
Cl	-1.905109	2.205064	0.016627
O	0.758941	0.005353	-0.099051
C	1.594111	-1.179944	-0.185636
C	1.585747	1.190687	0.062877
C	2.944875	-0.726794	0.321320
H	1.120553	-1.969852	0.403859
H	1.632823	-1.493979	-1.236484
C	3.001055	0.710940	-0.182028
H	1.232807	1.949967	-0.640450
H	1.446600	1.562541	1.085798
H	3.757602	-1.352738	-0.055743
H	2.969892	-0.752619	1.417601
H	3.233808	0.731687	-1.253469
H	3.737331	1.327479	0.339792
Cl	-1.902725	-2.205903	0.006578

PhCN…$MgCl_2$

Atom	Coordinate (Å)		
	x	y	z
C	-3.057270	-0.517845	-0.657811
C	-2.596832	0.653400	-0.039202
C	-3.480846	1.562159	0.557035
C	-4.839072	1.289559	0.528005
C	-5.304591	0.129282	-0.087414
C	-4.419720	-0.771145	-0.677118
H	-2.345418	-1.203506	-1.113047
H	-3.098552	2.461969	1.029810
H	-5.537812	1.983721	0.984957
H	-6.371536	-0.075380	-0.108127
H	-4.793920	-1.671559	-1.154639

C	-1.201860	0.909785	-0.032188
N	-0.056945	1.089006	-0.045188
Mg	2.063538	1.208762	-0.155214
Cl	2.661448	3.420487	-0.117419
Cl	3.449390	-0.626765	-0.462643

PnCN...$MgCl_2$...THF1

Atom	Coordinate (Å)		
	x	y	z
C	3.833659	-0.391083	1.147475
C	5.187283	-0.674656	1.055510
C	5.848403	-0.535473	-0.162958
C	5.163926	-0.112442	-1.300114
C	3.809692	0.174578	-1.227801
C	3.149485	0.032539	0.000252
H	3.302395	-0.492696	2.089337
H	5.729361	-1.004998	1.936484
H	6.909843	-0.759106	-0.226839
H	5.687697	-0.005747	-2.245316
H	3.260129	0.507286	-2.103414
C	1.760731	0.325935	0.080952
N	0.628016	0.562502	0.143258
Mg	-1.449432	1.053636	0.290067
O	-2.121704	-0.656441	-0.632578
C	-1.707493	-1.963242	-0.153850
C	-3.501725	-0.709328	-1.078077
C	-2.829346	-2.902226	-0.549370
H	-0.740540	-2.198342	-0.609077
H	-1.590941	-1.903776	0.937519
C	-4.046256	-1.987331	-0.481130
H	-4.010721	0.199559	-0.739862
H	-3.504849	-0.726146	-2.175278
H	-2.895488	-3.765015	0.118392
H	-2.682828	-3.269194	-1.572322
H	-4.344139	-1.821121	0.561873
H	-4.910175	-2.367284	-1.032593
Cl	-2.157648	0.714918	2.473058
Cl	-1.974657	2.739984	-1.199364

PnCN...$MgCl_2$...THF2a

Atom	Coordinate (Å)		
	x	y	z
C	4.111154	-0.000047	1.354595
C	5.496564	0.000016	1.299258
C	6.146274	0.000183	0.067140
C	5.417903	0.000289	-1.120263
C	4.032176	0.000229	-1.084134
C	3.383413	0.000061	0.157535
H	3.588663	-0.000174	2.306832
H	6.071970	-0.000065	2.220181
H	7.232365	0.000232	0.032035
H	5.932035	0.000420	-2.076748
H	3.448882	0.000310	-2.000486
C	1.960338	0.000008	0.196823
N	0.801584	-0.000030	0.218445
Mg	-1.388653	-0.000006	0.305684
Cl	-2.441625	-0.000031	-1.826085
O	-1.163061	2.111714	0.252903
C	-2.301867	2.932528	0.605990
C	-0.426986	2.737681	-0.823232
C	-2.007567	4.286419	-0.001243
H	-3.205099	2.483061	0.166455
H	-2.396730	2.920356	1.694684
C	-1.293342	3.891282	-1.287555
H	0.536554	3.078733	-0.421071
H	-0.247480	1.989446	-1.603191
H	-1.338892	4.863011	0.650253
H	-2.915733	4.872250	-0.166864
H	-0.706114	4.698665	-1.733512
H	-2.019296	3.539253	-2.031293
O	-1.162974	-2.111740	0.252845
C	-0.426682	-2.737684	-0.823154
C	-2.301731	-2.932661	0.605823
C	-1.292889	-3.891351	-1.287587
H	-0.247083	-1.989460	-1.603101
H	0.536812	-3.078672	-0.420829
C	-2.007244	-4.286535	-0.001362
H	-2.396717	-2.920492	1.694506
H	-3.204964	-2.483297	0.166188
H	-0.705540	-4.698691	-1.733466
H	-2.018777	-3.539386	-2.031420
H	-1.338606	-4.863070	0.650222
H	-2.915343	-4.872439	-0.167092
Cl	-2.438785	-0.000087	2.415063

PnCN...$MgCl_2$...THF2b

Atom	Coordinate (Å)		
	x	y	z
C	-4.282995	0.459506	0.955952
C	-5.661876	0.604607	0.948602
C	-6.447022	-0.242325	0.169701
C	-5.861180	-1.239455	-0.606685
C	-4.483565	-1.398136	-0.610973
C	-3.698454	-0.544669	0.173459
H	-3.653072	1.108608	1.559187
H	-6.126199	1.378836	1.552216
H	-7.527296	-0.124228	0.168108
H	-6.480652	-1.895767	-1.210774
H	-4.010254	-2.170176	-1.210690
C	-2.280757	-0.684618	0.177037
N	-1.125194	-0.775477	0.186599
Mg	1.114035	-0.734981	0.080466
O	0.718775	1.290958	-0.307862
C	0.530897	1.739230	-1.669244
C	0.030849	2.172305	0.606908
C	-0.024969	3.141822	-1.542265
H	1.496355	1.670086	-2.181781
H	-0.184438	1.062977	-2.161177
C	-0.859788	3.025784	-0.271899
H	-0.508812	1.560456	1.338058
H	0.785685	2.770822	1.135535
H	-0.602620	3.440137	-2.420823
H	0.787706	3.865131	-1.401345
H	-1.801945	2.501661	-0.483350
H	-1.098450	3.988691	0.187077
O	3.114741	-0.149227	-0.308198
C	3.663687	0.995458	0.384267
C	4.136383	-1.159807	-0.470912
C	5.029505	0.552219	0.868035
H	3.723441	1.828947	-0.329607
H	2.983883	1.268541	1.198200
C	5.441421	-0.438292	-0.213501
H	3.964293	-1.954567	0.270491
H	4.029444	-1.585710	-1.471936
H	4.933723	0.039060	1.833735
H	5.721687	1.389918	0.989129
H	6.238076	-1.120112	0.096082
H	5.772228	0.091567	-1.115720
Cl	1.125503	-2.346454	-1.642935
Cl	1.462981	-0.941922	2.403241

RC_MeMgCl

Atom	Coordinate (Å)		
	x	y	z
C	2.568195	1.184515	-0.305667
C	3.948786	1.079239	-0.370213
C	4.570015	-0.133272	-0.079532
C	3.818007	-1.250242	0.277471
C	2.436186	-1.163831	0.346081
C	1.816250	0.058055	0.053320
H	2.067067	2.121887	-0.529288
H	4.542772	1.944716	-0.648238
H	5.652767	-0.208629	-0.132164
H	4.310712	-2.191475	0.502160
H	1.833852	-2.024725	0.621278
C	0.398570	0.156924	0.118046
N	-0.756766	0.238314	0.168812
Mg	-2.931697	0.447400	0.150119
Cl	-3.653975	-1.724889	-0.278333
C	-3.636950	2.428806	0.187639
H	-3.170075	3.031184	0.980217
H	-3.434197	2.954817	-0.756399
H	-4.721958	2.497170	0.348102

TS_MeMgCl

Atom	Coordinate (Å)		
	x	y	z
C	-2.141510	1.027358	-0.504050
C	-3.510645	1.058482	-0.275112
C	-4.158233	-0.052301	0.259959
C	-3.437617	-1.205762	0.553449
C	-2.069948	-1.249863	0.314690
C	-1.417350	-0.128767	-0.207618
H	-1.636465	1.892010	-0.925630
H	-4.075677	1.955445	-0.514181
H	-5.228678	-0.018939	0.445765
H	-3.941005	-2.075844	0.966575
H	-1.495635	-2.147940	0.528971
C	0.013219	-0.269720	-0.476777
N	0.813288	-0.994637	-1.008799
Mg	2.313182	0.167414	-0.200798
Cl	4.533044	-0.213410	0.225649
C	0.706947	1.433497	0.710112
H	0.253532	2.263440	0.161022
H	0.070472	1.183195	1.562515
H	1.631337	1.852552	1.162186

PR_MeMgCl

Atom	Coordinate (Å)		
	x	y	z
C	-1.785113	-1.192965	0.045043
C	-3.049637	-1.761450	0.014305
C	-4.179794	-0.947403	-0.047648
C	-4.027237	0.433969	-0.076930
C	-2.754722	0.999381	-0.044556
C	-1.612077	0.194748	0.016327
H	-0.888300	-1.807051	0.091857
H	-3.159659	-2.843773	0.038011
H	-5.173330	-1.389291	-0.073121
H	-4.902394	1.078309	-0.125837
H	-2.661346	2.082730	-0.068827
C	-0.210403	0.757228	0.046356
N	0.797501	-0.000924	0.084251
Mg	2.723559	-0.196893	0.087792
Cl	5.019949	-0.429610	-0.083485
C	-0.129978	2.274986	0.023908
H	-0.591306	2.692638	-0.880905
H	-0.652405	2.723320	0.879424
H	0.918164	2.584701	0.054547

RCa_MeMgCl$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-2.858058	0.504520	-0.755104
C	-4.215333	0.776301	-0.831355
C	-5.129764	-0.058723	-0.193248
C	-4.696194	-1.170569	0.525150
C	-3.342384	-1.456848	0.612588
C	-2.426841	-0.614614	-0.030195
H	-2.130405	1.143062	-1.250875
H	-4.561863	1.640265	-1.390504
H	-6.192381	0.159426	-0.256878
H	-5.416160	-1.816224	1.019112
H	-2.987177	-2.319211	1.169146
C	-1.031790	-0.885625	0.055059
N	0.109351	-1.082722	0.118578
Mg	2.318875	-1.080482	0.327782
Cl	3.083252	-1.582193	-1.827489
C	2.870543	-1.596339	2.300878
H	2.000594	-1.631640	2.976172
H	3.374475	-2.567752	2.407698
H	3.555745	-0.851643	2.736076
O	2.131292	1.006226	0.236076
C	1.630341	1.688326	1.408151
C	1.710066	1.703083	-0.960073
C	0.536479	2.595956	0.888809
H	1.292242	0.932092	2.125458
H	2.455133	2.255936	1.858841
C	1.094549	3.000192	-0.470900
H	2.582360	1.830797	-1.607336
H	0.975201	1.074706	-1.483524
H	0.344479	3.441915	1.553934
H	-0.400188	2.034047	0.770237
H	1.864994	3.771429	-0.350811
H	0.335689	3.381148	-1.160032

TSa_MeMgCl$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-2.675626	1.057638	-0.488088
C	-4.004219	1.409583	-0.283908
C	-4.934556	0.437753	0.071031
C	-4.536972	-0.888742	0.221489
C	-3.208977	-1.246506	0.032242
C	-2.275633	-0.271867	-0.324483
H	-1.938601	1.804169	-0.778563
H	-4.313431	2.444287	-0.406340
H	-5.974119	0.713396	0.228672
H	-5.265954	-1.648723	0.489958
H	-2.894276	-2.280350	0.147761
C	-0.871915	-0.580647	-0.590241
N	-0.004160	-0.479527	-1.415870
Mg	1.330334	-1.172853	0.022092
Cl	3.097463	-2.622696	-0.258315
C	-0.398125	-1.327617	1.425894
H	-0.918520	-0.519009	1.947843
H	-1.030871	-2.219971	1.448628
H	0.476508	-1.571370	2.066972
O	2.146731	0.648606	0.543392
C	1.291563	1.730655	0.987091
C	3.231331	1.187126	-0.264836
C	1.573777	2.852155	0.015742
H	0.257279	1.370074	0.981781
H	1.571386	1.993778	2.015453

C	3.075346	2.694285	-0.193422
H	4.174974	0.806557	0.135801
H	3.107073	0.818995	-1.292764
H	1.286428	3.830854	0.408402
H	1.031765	2.677278	-0.923567
H	3.622904	3.099682	0.665836
H	3.445882	3.185375	-1.096730

PRa_MeMgCl$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.109425	-0.436880	-1.128372
C	-4.405626	-0.226698	-1.574521
C	-5.366201	0.295751	-0.709313
C	-5.013065	0.601948	0.599717
C	-3.709355	0.389824	1.041881
C	-2.734929	-0.132251	0.184606
H	-2.341710	-0.845474	-1.782147
H	-4.673598	-0.470697	-2.600614
H	-6.384032	0.461649	-1.055193
H	-5.754934	1.008591	1.283749
H	-3.458210	0.636898	2.070884
C	-1.306525	-0.378748	0.611993
N	-0.452570	-0.849316	-0.192080
Mg	1.462436	-1.262709	-0.214088
Cl	3.170070	-2.800489	0.050250
C	-1.003102	-0.006011	2.056723
H	-1.201713	1.057127	2.251705
H	-1.617268	-0.575946	2.766681
H	0.051451	-0.205818	2.276914
O	2.401072	0.550412	-0.244347
C	1.678924	1.797416	-0.082422
C	3.823937	0.803782	-0.359390
C	2.683890	2.869859	-0.443920
H	0.792164	1.761380	-0.721744
H	1.356616	1.874063	0.964921
C	3.989952	2.253557	0.044912
H	4.348563	0.086884	0.278759
H	4.118227	0.632049	-1.402801
H	2.450383	3.828277	0.026800
H	2.712695	3.018151	-1.530391
H	4.069551	2.340603	1.135410
H	4.879957	2.705715	-0.400144

RCb_MeMgCl$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.613708	0.037174	1.131230
C	-4.960028	0.353968	1.225754
C	-5.707840	0.572267	0.071030
C	-5.117391	0.476207	-1.187001
C	-3.772347	0.160112	-1.300550
C	-3.024626	-0.058654	-0.136421
H	-3.015404	-0.137570	2.020796
H	-5.428041	0.430206	2.202681
H	-6.762905	0.819422	0.152401
H	-5.708070	0.647383	-2.082001
H	-3.296506	0.079721	-2.273591
C	-1.643588	-0.387523	-0.237432
N	-0.517975	-0.655511	-0.309129
Mg	1.563339	-1.318567	-0.277723
C	2.288710	-2.577765	-1.809825
H	1.658761	-3.449021	-2.041279
H	2.405794	-2.026792	-2.756890
H	3.285542	-2.982500	-1.575651
O	2.266996	0.613307	-0.668714
C	1.873740	1.733875	0.164070
C	3.672631	0.720117	-0.994447
C	3.090465	2.639182	0.226693
H	0.991515	2.200928	-0.285203
H	1.609630	1.336047	1.153518
C	4.235705	1.647335	0.058584
H	4.100915	-0.288855	-0.993599
H	3.766015	1.140211	-2.005103
H	3.134127	3.202803	1.162339
H	3.083739	3.355599	-0.604005
H	4.406038	1.095466	0.991841
H	5.176339	2.111302	-0.249672
Cl	1.964233	-1.407481	2.044682

TSb_MeMgCl$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.632532	0.862407	-0.655930
C	-4.974165	0.571802	-0.441651
C	-5.339733	-0.632921	0.150764
C	-4.362428	-1.550212	0.529357
C	-3.018924	-1.261820	0.330995
C	-2.651922	-0.052992	-0.263417
H	-3.333159	1.795671	-1.126935
H	-5.735276	1.287294	-0.741651
H	-6.389835	-0.859820	0.316248
H	-4.648804	-2.495025	0.983703
H	-2.252970	-1.975457	0.623159
C	-1.261811	0.287289	-0.556986
N	-0.508780	0.599504	-1.440063
Mg	0.929302	0.931690	0.012473
C	-0.551502	0.269504	1.541562
H	-1.401367	0.837515	1.929559
H	-0.706668	-0.792037	1.759620
H	0.316125	0.576776	2.165288
O	2.110480	-0.736501	-0.138729
C	2.855711	-1.218149	1.011032
C	2.876961	-0.956624	-1.350498
C	4.020659	-1.990622	0.428032
H	3.195245	-0.344623	1.585851
H	2.175606	-1.814193	1.627064
C	4.283478	-1.231748	-0.867776
H	2.441612	-1.813890	-1.878817
H	2.784404	-0.065764	-1.980856
H	3.727972	-3.025619	0.213690
H	4.879107	-2.009872	1.104093
H	4.870210	-1.797820	-1.595643
H	4.801710	-0.287023	-0.660099
Cl	2.431726	2.630799	0.446084

PRb_MeMgCl$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.029058	-1.218837	-0.404288
C	-4.195371	-1.964671	-0.488233
C	-5.415533	-1.397695	-0.122265
C	-5.451482	-0.081939	0.324551
C	-4.277727	0.663333	0.403094
C	-3.046132	0.107283	0.040598
H	-2.064549	-1.639686	-0.680438
H	-4.158182	-2.993845	-0.839847
H	-6.332093	-1.979949	-0.185684
H	-6.397704	0.370316	0.613972
H	-4.332220	1.690845	0.755185
C	-1.745505	0.872529	0.116839
N	-0.642934	0.321818	-0.166134

Mg	1.258283	0.781641	-0.192163
C	-1.890797	2.321599	0.559325
H	-2.571189	2.882306	-0.095159
H	-2.299794	2.395715	1.576098
H	-0.914739	2.816482	0.543775
O	2.518063	-0.764722	0.360281
C	2.872398	-1.772208	-0.623031
C	3.643628	-0.526650	1.246981
C	4.194939	-2.338900	-0.150628
H	2.056386	-2.498858	-0.671990
H	2.974524	-1.279547	-1.600919
C	4.828741	-1.130988	0.528766
H	3.724617	0.553094	1.409870
H	3.436053	-1.028411	2.200270
H	4.788265	-2.737161	-0.977584
H	4.030680	-3.144794	0.574706
H	5.214088	-0.426489	-0.219636
H	5.641517	-1.389896	1.212039
Cl	2.796022	2.452829	-0.683427

RCa_MeMgCl$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.065909	-0.001707	1.292978
C	-5.448275	-0.001826	1.185207
C	-6.050403	-0.004921	-0.070855
C	-5.276268	-0.007922	-1.228827
C	-3.892565	-0.007837	-1.139165
C	-3.291612	-0.004713	0.125897
H	-3.580359	0.000658	2.264684
H	-6.058572	0.000501	2.083481
H	-7.134349	-0.005004	-0.148094
H	-5.752885	-0.010343	-2.204658
H	-3.274376	-0.010134	-2.032381
C	-1.870219	-0.004613	0.228243
N	-0.713970	-0.004389	0.312790
Mg	1.506834	-0.002227	0.610191
Cl	2.615868	-0.005063	-1.539339
C	2.331563	0.042744	2.574146
H	2.208665	-0.888673	3.150266
H	3.416100	0.245820	2.574280
H	1.891185	0.837871	3.199139
O	1.228890	-2.158156	0.429245
C	2.368322	-2.954305	0.813726
C	0.589530	-2.747623	-0.721839
C	2.167915	-4.286722	0.123267
H	3.283928	-2.455325	0.460123
H	2.394569	-3.004228	1.906218
C	1.520704	-3.851230	-1.185535
H	-0.388507	-3.137609	-0.406745
H	0.439096	-1.964879	-1.473598
H	1.481679	-4.919027	0.700969
H	3.106406	-4.831712	-0.011031
H	0.990938	-4.654414	-1.705399
H	2.279018	-3.439932	-1.863710
O	1.221235	2.152988	0.413211
C	0.583032	2.740346	-0.739352
C	2.359447	2.950067	0.797884
C	1.504212	3.857403	-1.192011
H	0.446360	1.959775	-1.496173
H	-0.401461	3.117279	-0.428659
C	2.147150	4.287327	0.120957
H	2.393240	2.987121	1.890814
H	3.275179	2.459996	0.432165
H	0.967086	4.660141	-1.704973
H	2.266921	3.460268	-1.873791
H	1.454937	4.907601	0.704556
H	3.080477	4.842295	-0.008507

TSa_MeMgCl$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	3.516553	0.210752	-0.017424
C	4.858766	-0.047643	0.226657
C	5.339283	-1.354150	0.172164
C	4.476389	-2.403369	-0.129351
C	3.132112	-2.151818	-0.380682
C	2.654144	-0.842450	-0.328838
H	3.122154	1.224969	0.029597
H	5.532788	0.772086	0.461860
H	6.389933	-1.554058	0.366864
H	4.851105	-3.422880	-0.171133
H	2.449224	-2.963613	-0.621057
C	1.254813	-0.561724	-0.639603
N	0.459867	-0.390030	-1.521118
Mg	-0.911955	0.176423	-0.023589
Cl	-3.102762	1.104908	-0.005895
C	0.643168	-0.447500	1.483684
H	1.441952	0.208567	1.844784
H	-0.241853	-0.233640	2.126153
H	0.917419	-1.486428	1.700877
O	-1.743150	-1.773553	0.028346
C	-2.465034	-2.253484	-1.129438
C	-2.366758	-2.262568	1.234557
C	-3.734535	-2.872684	-0.580146
H	-2.649299	-1.409519	-1.803809
H	-1.830775	-2.987608	-1.643233
C	-3.273963	-3.386109	0.778761
H	-1.574318	-2.572517	1.923270
H	-2.940485	-1.440700	1.689051
H	-4.132838	-3.653793	-1.233286
H	-4.503813	-2.100945	-0.452672
H	-2.704218	-4.317003	0.666302
H	-4.093902	-3.567442	1.478801
O	-0.097021	2.160832	-0.027229
C	-0.123458	2.956957	1.173955
C	-0.286578	3.004918	-1.183736
C	0.017541	4.389782	0.702088
H	-1.086777	2.792401	1.680444
H	0.687044	2.613887	1.825855
C	-0.721027	4.346769	-0.630319
H	0.669648	3.065341	-1.721472
H	-1.033143	2.540010	-1.837674
H	1.074623	4.640227	0.547442
H	-0.403858	5.104894	1.413640
H	-0.470891	5.175050	-1.298747
H	-1.805515	4.350115	-0.463661

PRa_MeMgCl$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.354924	-0.396847	-1.169946
C	-5.721992	-0.264218	-0.937768
C	-6.190536	0.009825	0.341961
C	-5.280760	0.152612	1.389087
C	-3.920512	0.023886	1.151059
C	-3.430515	-0.253281	-0.129733
H	-4.013092	-0.612990	-2.179775
H	-6.422706	-0.376772	-1.762560
H	-7.258075	0.111116	0.524712
H	-5.638548	0.364942	2.394714
H	-3.190109	0.133362	1.950293

C	-1.937156	-0.380180	-0.328768
N	-1.124795	-0.165949	0.615402
Mg	0.826966	-0.125670	0.888553
Cl	2.141044	-0.355372	2.800857
C	-1.516474	-0.772449	-1.740708
H	-1.821679	-0.017936	-2.479675
H	-0.426787	-0.872414	-1.782934
H	-1.968090	-1.722529	-2.057269
O	1.532947	1.617572	0.049734
C	2.568582	2.503525	0.534475
C	0.939814	2.146729	-1.159285
C	2.843930	3.434299	-0.626922
H	2.184022	3.038909	1.412209
H	3.423049	1.893054	0.843026
C	1.461683	3.565560	-1.257019
H	1.274665	1.527495	-2.004552
H	-0.148049	2.061045	-1.066889
H	3.542735	2.966318	-1.332625
H	3.270220	4.387131	-0.302811
H	1.483042	3.928831	-2.287650
H	0.835514	4.244649	-0.665747
O	1.889229	-1.264231	-0.488307
C	1.699509	-2.700303	-0.527932
C	3.277366	-0.943722	-0.752031
C	3.098554	-3.277549	-0.503502
H	1.080721	-2.993225	0.328386
H	1.162819	-2.948283	-1.453267
C	3.879699	-2.226747	-1.284056
H	3.303840	-0.099839	-1.450122
H	3.746462	-0.643564	0.196312
H	3.144487	-4.277074	-0.943297
H	3.464595	-3.334143	0.529536
H	3.688850	-2.326383	-2.359667
H	4.959324	-2.274261	-1.120239

RCb_MeMgCl$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.259856	0.571483	0.947021
C	-5.630652	0.769976	0.879289
C	-6.426949	-0.111081	0.151502
C	-5.859241	-1.195385	-0.513275
C	-4.489754	-1.407456	-0.455628
C	-3.692757	-0.520160	0.277235
H	-3.623543	1.247026	1.513321
H	-6.079912	1.612917	1.396224
H	-7.500756	0.048692	0.102320
H	-6.486530	-1.878383	-1.078604
H	-4.031274	-2.247997	-0.968647
C	-2.281844	-0.718868	0.344508
N	-1.131983	-0.861302	0.405455
Mg	1.201880	-0.852544	0.431781
C	1.544504	-0.900169	2.532873
H	0.999550	-1.678953	3.088693
H	2.609389	-1.042537	2.785330
H	1.259191	0.053528	3.011168
O	0.774185	1.108582	-0.250098
C	0.632606	1.395739	-1.655017
C	0.096408	2.105116	0.536535
C	0.135287	2.825477	-1.707732
H	1.605099	1.228338	-2.130384
H	-0.098741	0.694146	-2.083703
C	-0.735550	2.890203	-0.457914
H	-0.489672	1.597292	1.311204
H	0.855793	2.734125	1.023823
H	-0.404863	3.046541	-2.631944
H	0.976377	3.525527	-1.622909
H	-1.693638	2.383101	-0.636461
H	-0.944414	3.907943	-0.117749
O	3.212783	-0.187917	-0.140390
C	3.698722	0.994240	0.525097
C	4.268594	-1.160248	-0.238847
C	5.121960	0.673974	0.950062
H	3.651671	1.830027	-0.188175
H	3.037850	1.218780	1.371335
C	5.543922	-0.359772	-0.087356
H	4.157832	-1.894114	0.576032
H	4.154627	-1.680972	-1.193568
H	5.124144	0.223212	1.950951
H	5.759893	1.561832	0.975640
H	6.391926	-0.974689	0.226533
H	5.802879	0.127587	-1.035864
Cl	1.210605	-2.462767	-1.335903

TSb_MeMgCl$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.050909	-1.153371	0.113576
C	-5.410550	-1.050540	0.375921
C	-6.054328	0.179518	0.260920
C	-5.338150	1.308692	-0.124335
C	-3.978383	1.212062	-0.397552
C	-3.334978	-0.020794	-0.278895
H	-3.533795	-2.106947	0.202774
H	-5.970841	-1.933450	0.672642
H	-7.117974	0.256997	0.471873
H	-5.839878	2.268707	-0.215871
H	-3.409335	2.085863	-0.707102
C	-1.917761	-0.119315	-0.618260
N	-1.124032	-0.113959	-1.517736
Mg	0.336073	-0.584974	-0.077091
C	-1.247599	-0.287467	1.487917
H	-1.882700	-1.118435	1.810776
H	-0.322056	-0.360940	2.104352
H	-1.717579	0.657981	1.782050
O	0.755268	1.540993	0.018466
C	1.353786	2.123219	-1.157573
C	1.337470	2.131447	1.198345
C	2.641565	2.749447	-0.670013
H	1.483635	1.334055	-1.907399
H	0.663024	2.871647	-1.569462
C	2.217559	3.263633	0.700891
H	0.526805	2.447513	1.862608
H	1.937511	1.366359	1.712647
H	3.011739	3.530760	-1.338828
H	3.417381	1.978390	-0.563734
H	1.636565	4.188135	0.597326
H	3.055555	3.461150	1.374834
O	2.500371	-0.592126	0.031911
C	3.292546	-1.002714	-1.100600
C	3.172352	-1.140385	1.178678
C	4.743744	-1.010771	-0.604289
H	2.954977	-2.000411	-1.413421
H	3.098132	-0.290798	-1.909983
C	4.621977	-0.797661	0.913364
H	2.741484	-0.681546	2.075012
H	2.994566	-2.226097	1.211123
H	5.340251	-0.224022	-1.074958
H	5.219526	-1.968103	-0.836531
H	4.802774	0.252205	1.175804
H	5.313327	-1.416730	1.490846
Cl	0.417476	-2.967990	-0.207631

PRb_MeMgCl$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.492703	-0.852743	-0.108858
C	-5.682004	-0.261317	0.310595
C	-5.730200	1.102809	0.572819
C	-4.578195	1.872206	0.413102
C	-3.395936	1.277001	-0.001401
C	-3.328135	-0.094452	-0.270136
H	-4.481531	-1.921727	-0.309234
H	-6.574545	-0.871727	0.431416
H	-6.658915	1.566110	0.898481
H	-4.607153	2.941606	0.613191
H	-2.483816	1.856397	-0.133115
C	-2.011066	-0.691772	-0.712019
N	-0.959852	0.006523	-0.777847
Mg	0.960266	-0.260780	-1.168040
C	-2.067961	-2.177667	-1.043246
H	-2.799460	-2.399160	-1.831882
H	-1.081947	-2.513677	-1.381941
H	-2.355382	-2.778237	-0.168391
O	1.609381	-1.454020	0.403183
C	0.735749	-2.012662	1.411650
C	2.975154	-1.442910	0.871489
C	1.571920	-2.037117	2.674174
H	-0.161807	-1.386235	1.460282
H	0.446119	-3.023616	1.094938
C	2.967353	-2.302875	2.119001
H	3.615715	-1.812755	0.064703
H	3.253436	-0.400968	1.094735
H	1.231319	-2.796863	3.382452
H	1.538430	-1.061815	3.177018
H	3.077422	-3.361394	1.853929
H	3.771713	-2.037793	2.810087
O	1.843877	1.384152	-0.278729
C	1.282462	1.910771	0.943356
C	3.054111	2.092683	-0.628725
C	1.996502	3.228808	1.154666
H	0.197983	1.975989	0.807472
H	1.495569	1.198714	1.756869
C	3.382517	2.922037	0.596728
H	3.816785	1.353835	-0.897126
H	2.845471	2.716789	-1.507079
H	2.005529	3.533936	2.204255
H	1.514420	4.021353	0.569418
H	3.959965	2.328483	1.317601
H	3.962930	3.814469	0.348868
Cl	2.468473	-0.735052	-2.882962

RC_Me$_2$Mg

Atom	Coordinate (Å)		
	x	y	z
C	2.179835	-1.116994	0.499651
C	3.565918	-1.098970	0.471327
C	4.239219	0.012591	-0.029958
C	3.533288	1.115060	-0.505798
C	2.147033	1.114449	-0.483317
C	1.473974	-0.005911	0.020785
H	1.639431	-1.976490	0.885805
H	4.123445	-1.954715	0.840403
H	5.325703	0.019766	-0.050133
H	4.065350	1.977974	-0.895226
H	1.581401	1.966260	-0.849941
C	0.049675	-0.015143	0.043315
N	-1.110146	-0.020670	0.058833
Mg	-3.355464	0.001633	-0.010626
C	-3.953760	-1.977541	-0.520441
H	-3.506178	-2.329991	-1.462585
H	-3.660505	-2.716458	0.241539
H	-5.041020	-2.092370	-0.643974
C	-3.950584	1.984413	0.485994
H	-3.653743	2.723125	-0.274644
H	-5.038283	2.100098	0.604961
H	-3.506602	2.336173	1.430135

TS_Me$_2$Mg

Atom	Coordinate (Å)		
	x	y	z
C	-1.668226	1.010883	-0.556126
C	-3.039687	1.092217	-0.354723
C	-3.730496	0.023463	0.210987
C	-3.050030	-1.137694	0.564003
C	-1.679879	-1.231450	0.354335
C	-0.984162	-0.152956	-0.200220
H	-1.128068	1.841843	-1.001691
H	-3.572562	1.995529	-0.639814
H	-4.802841	0.095545	0.373745
H	-3.587185	-1.975760	1.000333
H	-1.137671	-2.137371	0.614630
C	0.444718	-0.340776	-0.444151
N	1.241931	-1.075646	-0.960282
Mg	2.767373	0.097997	-0.130330
C	1.141865	1.372010	0.783609
H	0.657075	2.195051	0.250287
H	0.514069	1.094539	1.635720
H	2.060370	1.807663	1.227002
C	4.808141	-0.238938	0.270607
H	4.956720	-1.158214	0.854545
H	5.405581	-0.356436	-0.644460
H	5.279055	0.570626	0.845716

PR_Me$_2$Mg

Atom	Coordinate (Å)		
	x	y	z
C	1.415504	-1.197191	-0.000693
C	2.724074	-1.656662	-0.000467
C	3.782958	-0.749433	0.000282
C	3.514586	0.614535	0.000808
C	2.198279	1.069733	0.000518
C	1.126102	0.171324	-0.000236
H	0.571131	-1.883414	-0.001140
H	2.924672	-2.726276	-0.000817
H	4.810661	-1.105774	0.000439
H	4.333132	1.331253	0.001483
H	2.014190	2.141653	0.001117
C	-0.319299	0.614183	-0.000259
N	-1.264150	-0.222108	0.000653
Mg	-3.210522	-0.465268	-0.000141
C	-0.521792	2.122848	-0.000925
H	-0.068305	2.596819	0.880067
H	-0.067236	2.596255	-0.881680
H	-1.593115	2.343430	-0.001605
C	-5.311841	-0.457632	0.000574
H	-5.724087	0.057624	-0.878470
H	-5.753100	-1.464153	0.002072
H	-5.724050	0.060332	0.878032

RCa_Me$_2$Mg$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z

C	2.723996	0.757092	0.506766
C	4.068314	1.096034	0.525853
C	5.020343	0.197154	0.050428
C	4.636425	-1.045702	-0.447564
C	3.295916	-1.399813	-0.475031
C	2.342327	-0.493542	0.003874
H	1.967466	1.444616	0.877759
H	4.375364	2.062717	0.913984
H	6.072586	0.467903	0.068961
H	5.384772	-1.741394	-0.815528
H	2.979918	-2.365132	-0.859932
C	0.960209	-0.839950	-0.013083
N	-0.170179	-1.101733	-0.018773
Mg	-2.407381	-1.426505	0.199526
C	-3.092835	-2.164493	-1.686047
H	-2.313292	-2.131041	-2.466083
H	-3.462683	-3.201666	-1.685369
H	-3.924472	-1.557008	-2.081375
O	-2.506254	0.700744	-0.028963
C	-2.241847	1.278860	-1.324075
C	-1.993914	1.561476	1.009055
C	-1.201408	2.349445	-1.070637
H	-1.915752	0.476564	-1.994799
H	-3.176783	1.703739	-1.714563
C	-1.610690	2.851885	0.309214
H	-2.766365	1.674108	1.776334
H	-1.118504	1.075437	1.465188
H	-1.202595	3.126331	-1.839911
H	-0.198333	1.902969	-1.035699
H	-2.477547	3.519213	0.228433
H	-0.815645	3.388226	0.835172
C	-2.724575	-1.710707	2.297440
H	-2.863393	-2.754099	2.620431
H	-1.889978	-1.321783	2.904984
H	-3.618464	-1.171900	2.653657

TSa_Me_2Mg_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	2.372054	-1.212560	-0.330367
C	3.672791	-1.648101	-0.106168
C	4.691331	-0.722788	0.099369
C	4.409253	0.641153	0.081279
C	3.110104	1.083867	-0.129347
C	2.088821	0.155608	-0.338733
H	1.568598	-1.925822	-0.504119
H	3.891072	-2.712849	-0.095942
H	5.708681	-1.064216	0.272778
H	5.205988	1.364263	0.235129
H	2.882583	2.146910	-0.141406
C	0.712548	0.563228	-0.611501
N	-0.176236	0.514851	-1.415424
Mg	-1.397193	1.526783	-0.005476
C	0.369798	1.441735	1.409005
H	0.846709	0.596577	1.916055
H	1.080970	2.275334	1.397153
H	-0.456802	1.754423	2.080137
O	-2.419395	-0.210466	0.560243
C	-1.712983	-1.383510	1.023620
C	-3.491800	-0.610759	-0.332356
C	-2.045872	-2.452486	0.008483
H	-0.649362	-1.130634	1.092314
H	-2.082977	-1.640536	2.025250
C	-3.503693	-2.128074	-0.297655
H	-4.419117	-0.144366	0.013907
H	-3.260747	-0.232781	-1.338716
H	-1.894090	-3.463429	0.395806
H	-1.426573	-2.322515	-0.889138
H	-4.150638	-2.490306	0.510546
H	-3.860429	-2.556789	-1.237705
C	-2.756667	3.111639	-0.322434
H	-3.156454	3.523986	0.616172
H	-2.334010	3.964994	-0.872195
H	-3.632384	2.782415	-0.903464

PRa_Me_2Mg_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	2.936408	0.570036	-1.052865
C	4.214452	0.345184	-1.542459
C	5.134881	-0.380770	-0.787214
C	4.759421	-0.874373	0.456872
C	3.474312	-0.645373	0.942900
C	2.540013	0.080482	0.196208
H	2.199555	1.133887	-1.621385
H	4.499660	0.736538	-2.517122
H	6.138322	-0.558759	-1.167595
H	5.469393	-1.441447	1.055436
H	3.204935	-1.041472	1.919510
C	1.132755	0.355131	0.677817
N	0.307796	1.007999	-0.020386
Mg	-1.575570	1.621337	0.011941
C	0.810849	-0.227885	2.049232
H	0.921828	-1.321484	2.062718
H	1.473034	0.165030	2.832655
H	-0.222869	0.016556	2.315644
O	-2.621209	-0.171844	-0.110254
C	-2.022720	-1.487342	-0.079293
C	-4.043256	-0.272155	-0.350232
C	-3.070676	-2.398702	-0.681957
H	-1.077187	-1.441913	-0.627816
H	-1.810304	-1.747702	0.967092
C	-4.361961	-1.746517	-0.199985
H	-4.559186	0.377851	0.363701
H	-4.248516	0.089399	-1.366944
H	-2.956672	-3.435643	-0.355226
H	-3.014475	-2.374956	-1.777309
H	-4.543502	-1.993762	0.853222
H	-5.243054	-2.040072	-0.776531
C	-2.962280	3.211189	0.098733
H	-2.510480	4.213150	0.088554
H	-3.672027	3.187209	-0.742759
H	-3.579698	3.166886	1.009060

RCb_Me_2Mg_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	3.684016	0.177905	1.158443
C	5.018180	-0.195258	1.099524
C	5.564980	-0.644245	-0.100315
C	4.783432	-0.723018	-1.250611
C	3.447820	-0.353170	-1.209211
C	2.901626	0.096773	-0.000434
H	3.242198	0.530469	2.086093
H	5.634147	-0.135787	1.991971
H	6.611264	-0.935266	-0.139360
H	5.216955	-1.073205	-2.182750
H	2.824499	-0.407326	-2.097181
C	1.528996	0.476600	0.049480
N	0.411053	0.783449	0.088542
Mg	-1.717661	1.484928	0.143241
C	-2.066593	2.710907	-1.574029

H	-1.384258	3.568701	-1.683313
H	-1.972428	2.136414	-2.511288
H	-3.081308	3.141210	-1.598819
O	-2.341896	-0.466599	-0.491688
C	-2.088718	-1.579830	0.393985
C	-3.698127	-0.530635	-0.978964
C	-3.309976	-2.474499	0.284039
H	-1.154092	-2.059693	0.085155
H	-1.965553	-1.180849	1.411300
C	-4.410889	-1.466839	-0.026629
H	-4.100121	0.489300	-1.001917
H	-3.685390	-0.922857	-2.005360
H	-3.485876	-3.048193	1.198006
H	-3.197223	-3.181756	-0.547063
H	-4.705727	-0.928488	0.883414
H	-5.305038	-1.915041	-0.468310
C	-2.306869	1.492194	2.205100
H	-1.626984	0.915689	2.855285
H	-2.383614	2.486844	2.671534
H	-3.298994	1.028053	2.345143

TSb_Me$_2$Mg$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.479944	0.992897	-0.007602
C	-4.777936	0.560544	0.234555
C	-5.085235	-0.796075	0.174815
C	-4.092398	-1.723874	-0.127561
C	-2.791933	-1.299299	-0.371181
C	-2.487413	0.061670	-0.317541
H	-3.227319	2.050012	0.040663
H	-5.552269	1.285650	0.471391
H	-6.101390	-1.131274	0.366500
H	-4.331300	-2.783264	-0.173507
H	-2.007384	-2.015687	-0.605363
C	-1.131385	0.516944	-0.617773
N	-0.382394	0.876005	-1.483371
Mg	1.054672	1.205805	0.024637
C	-0.457260	0.373958	1.485002
H	-1.272317	0.958121	1.924736
H	-0.705218	-0.689673	1.577311
H	0.423744	0.538030	2.140737
O	2.233074	-0.520244	-0.146857
C	2.803909	-1.101175	1.051290
C	3.216416	-0.527189	-1.208764
C	4.125943	-1.700117	0.614190
H	2.954897	-0.299102	1.789495
H	2.088036	-1.823955	1.454270
C	4.538184	-0.757513	-0.510193
H	2.968605	-1.339505	-1.903932
H	3.153200	0.428625	-1.741136
H	3.979527	-2.715658	0.226602
H	4.847536	-1.747136	1.433863
H	5.297390	-1.174248	-1.177044
H	4.917394	0.187468	-0.099107
C	2.397214	2.810180	0.328487
H	3.042852	2.634751	1.204195
H	3.082193	2.940007	-0.524281
H	1.928954	3.791398	0.491064

PRb_Me$_2$Mg$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-2.182517	-0.577743	-0.940820
C	-3.182286	-1.463339	-1.315353
C	-4.429393	-1.412702	-0.693638
C	-4.659586	-0.468429	0.300337
C	-3.651306	0.417473	0.672456
C	-2.395034	0.377748	0.058560
H	-1.200545	-0.594770	-1.411306
H	-2.993410	-2.198636	-2.095215
H	-5.215860	-2.105829	-0.983936
H	-5.629314	-0.419267	0.791319
H	-3.854853	1.146911	1.453293
C	-1.262335	1.307240	0.438908
N	-0.142751	1.256765	-0.133531
Mg	1.746991	1.514377	-0.564374
C	-1.585926	2.281741	1.563004
H	-2.422748	2.943426	1.300974
H	-1.872559	1.762045	2.487507
H	-0.705107	2.897138	1.764014
O	2.416907	-0.431651	-0.244043
C	1.562715	-1.522741	0.170149
C	3.800272	-0.747361	0.035880
C	2.414289	-2.324343	1.129603
H	0.651819	-1.087275	0.592379
H	1.293498	-2.110128	-0.719170
C	3.794226	-2.194258	0.493765
H	4.388010	-0.566278	-0.869792
H	4.154585	-0.069102	0.823720
H	2.074223	-3.358940	1.225229
H	2.403582	-1.864490	2.125779
H	3.879726	-2.869275	-0.366549
H	4.616634	-2.412471	1.180159
C	3.417066	2.737664	-0.987191
H	4.056935	2.865749	-0.100568
H	4.066993	2.306382	-1.763995
H	3.167391	3.752445	-1.328251

RCa_Me$_2$Mg$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	3.930230	0.024893	1.318187
C	5.314090	0.031559	1.226552
C	5.931286	0.029924	-0.022031
C	5.170171	0.021488	-1.188499
C	3.785442	0.014753	-1.114030
C	3.168677	0.016544	0.143151
H	3.433574	0.026207	2.284289
H	5.913701	0.038158	2.132068
H	7.016083	0.035333	-0.086657
H	5.657765	0.020293	-2.158994
H	3.177654	0.008334	-2.014463
C	1.744543	0.010917	0.225110
N	0.586405	0.007182	0.288082
Mg	-1.697971	0.005161	0.435728
C	-2.381677	-0.095935	2.476814
H	-2.459567	0.869153	3.005268
H	-3.372898	-0.569067	2.587849
H	-1.706133	-0.713391	3.095769
O	-1.318837	2.238858	0.397857
C	-2.490757	2.999425	0.740290
C	-0.710497	2.792541	-0.781129
C	-2.404933	4.269894	-0.082734
H	-3.383253	2.412279	0.472547
H	-2.493999	3.161311	1.822825
C	-1.728359	3.761835	-1.349851
H	0.219597	3.302529	-0.489045
H	-0.464548	1.969640	-1.461469
H	-1.769655	5.011427	0.418598
H	-3.385639	4.721741	-0.256872
H	-1.269283	4.550013	-1.953482

H	-2.449968	3.219472	-1.974736
O	-1.310826	-2.213244	0.307705
C	-0.761258	-2.728101	-0.917991
C	-2.420639	-3.025761	0.718892
C	-1.683916	-3.856407	-1.347841
H	-0.710896	-1.910150	-1.647026
H	0.257886	-3.085701	-0.713062
C	-2.236730	-4.339261	-0.012028
H	-2.402040	-3.100080	1.810583
H	-3.360468	-2.533804	0.418997
H	-1.162020	-4.630974	-1.917023
H	-2.497510	-3.462888	-1.970975
H	-1.499408	-4.965497	0.506413
H	-3.167884	-4.906145	-0.100990
C	-2.623462	0.065803	-1.520249
H	-3.388165	0.856154	-1.624692
H	-1.905083	0.263368	-2.337943
H	-3.132989	-0.869509	-1.813256

TSa_Me_2Mg_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	3.368913	0.025538	0.107063
C	4.684231	-0.343498	0.353401
C	5.085169	-1.665549	0.172226
C	4.169125	-2.618178	-0.262848
C	2.852337	-2.253726	-0.521138
C	2.451706	-0.929491	-0.336722
H	3.039168	1.052880	0.251645
H	5.400123	0.401850	0.690519
H	6.114622	-1.952768	0.371131
H	4.480679	-3.649861	-0.405467
H	2.129770	-2.988328	-0.869308
C	1.081531	-0.543176	-0.658299
N	0.294426	-0.336614	-1.535923
Mg	-1.071531	0.310709	-0.021777
C	0.476364	-0.374995	1.498662
H	1.305704	0.244507	1.857201
H	-0.394613	-0.125551	2.144446
H	0.709920	-1.425285	1.712190
O	-1.881230	-1.745359	0.054070
C	-2.674283	-2.120988	-1.088546
C	-2.549981	-2.145736	1.264087
C	-4.041761	-2.462735	-0.533133
H	-2.679635	-1.282775	-1.794490
H	-2.200292	-2.986110	-1.572975
C	-3.678650	-3.058081	0.822367
H	-1.816021	-2.623444	1.921647
H	-2.939381	-1.244769	1.763853
H	-4.599061	-3.146808	-1.179081
H	-4.632962	-1.547042	-0.402608
H	-3.316855	-4.087050	0.702411
H	-4.508186	-3.068633	1.534797
O	-0.048824	2.289310	-0.063558
C	-0.050261	3.064890	1.144380
C	-0.363935	3.133220	-1.188317
C	0.076525	4.504159	0.689103
H	-0.999783	2.896009	1.678325
H	0.774311	2.713456	1.773916
C	-0.736496	4.483069	-0.600211
H	0.525402	3.191658	-1.830152
H	-1.179431	2.669306	-1.757193
H	1.125947	4.745934	0.478515
H	-0.297341	5.214489	1.431705
H	-0.508365	5.310744	-1.277483
H	-1.809223	4.514421	-0.370792
C	-3.020921	1.195178	-0.091364
H	-3.056437	2.261143	0.188683
H	-3.431338	1.152002	-1.115793
H	-3.776585	0.696799	0.538772

PRa_Me_2Mg_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	-4.188589	-0.684248	-1.103317
C	-5.562360	-0.509295	-0.951888
C	-6.072309	0.044675	0.216506
C	-5.196322	0.421137	1.234313
C	-3.829829	0.241952	1.078044
C	-3.297416	-0.312011	-0.090965
H	-3.814810	-1.120560	-2.027001
H	-6.235805	-0.808187	-1.752737
H	-7.144757	0.182774	0.335664
H	-5.585854	0.855558	2.153160
H	-3.124750	0.524149	1.857567
C	-1.797348	-0.485056	-0.204419
N	-1.017899	-0.175654	0.740077
Mg	0.932582	-0.155714	1.161645
C	-1.329685	-1.050025	-1.543052
H	-1.662763	-0.430296	-2.387830
H	-0.236300	-1.092420	-1.556312
H	-1.721980	-2.060974	-1.722543
O	1.556810	1.611308	0.239943
C	2.530845	2.570094	0.698084
C	0.990349	2.029247	-1.021116
C	2.795009	3.455745	-0.503039
H	2.100483	3.133159	1.536937
H	3.410636	2.024350	1.056765
C	1.431603	3.468800	-1.185975
H	1.397914	1.383206	-1.813449
H	-0.092923	1.878859	-0.968257
H	3.545419	2.994952	-1.158795
H	3.153422	4.448324	-0.217956
H	1.470834	3.774294	-2.234854
H	0.745816	4.142063	-0.657196
O	2.011120	-1.198039	-0.367665
C	1.933890	-2.639551	-0.339765
C	3.380679	-0.789050	-0.580449
C	3.356072	-3.098477	-0.103810
H	1.228067	-2.933138	0.446514
H	1.544166	-2.988260	-1.306581
C	4.138895	-2.062768	-0.902677
H	3.398010	-0.037479	-1.378108
H	3.750627	-0.329825	0.348013
H	3.526709	-4.127944	-0.429453
H	3.601608	-3.023456	0.963649
H	4.081973	-2.286577	-1.975145
H	5.193630	-1.997639	-0.622568
C	2.051562	-0.620136	2.908562
H	1.739633	-0.087934	3.820270
H	1.980555	-1.692040	3.157589
H	3.131028	-0.419175	2.803920

RCb_Me_2Mg_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	-4.182466	0.434517	0.954266
C	-5.538032	0.719864	0.882827
C	-6.368088	-0.040908	0.063072
C	-5.848858	-1.091201	-0.689879
C	-4.495065	-1.387639	-0.629930
C	-3.663073	-0.621136	0.194363

H	-3.521676	1.014761	1.593956
H	-5.948966	1.536607	1.469206
H	-7.429576	0.186317	0.011376
H	-6.501754	-1.681263	-1.326517
H	-4.075007	-2.203087	-1.211846
C	-2.265913	-0.908684	0.262353
N	-1.126338	-1.124998	0.324809
Mg	1.339874	-1.146519	0.173454
C	1.737859	-1.359535	2.279457
H	1.241978	-2.208209	2.778885
H	2.814299	-1.480962	2.496725
H	1.430589	-0.468406	2.856893
O	0.797466	0.911011	-0.177483
C	0.579616	1.355376	-1.526567
C	0.125646	1.777684	0.749506
C	0.018626	2.756749	-1.391011
H	1.534645	1.294467	-2.060212
H	-0.139750	0.675714	-2.009327
C	-0.789308	2.634380	-0.103863
H	-0.397134	1.158594	1.487261
H	0.881792	2.383716	1.271082
H	-0.576046	3.056733	-2.257978
H	0.831780	3.482887	-1.262399
H	-1.732529	2.105010	-0.299637
H	-1.025012	3.594171	0.363808
O	3.332639	-0.220793	-0.309770
C	3.772868	0.863304	0.525133
C	4.419974	-1.122395	-0.550854
C	5.217512	0.552928	0.885271
H	3.674917	1.797266	-0.048451
H	3.115579	0.920827	1.401410
C	5.667833	-0.303730	-0.292539
H	4.350167	-1.973245	0.147297
H	4.323577	-1.504190	-1.572127
H	5.257741	-0.034084	1.812020
H	5.817360	1.455987	1.029923
H	6.543188	-0.922575	-0.075714
H	5.896666	0.325269	-1.162355
C	1.336806	-2.361105	-1.605029
H	1.578894	-1.765067	-2.503949
H	2.086746	-3.171070	-1.596115
H	0.376949	-2.855523	-1.829763

TSb_Me$_2$Mg$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.072548	-1.297606	0.045224
C	-5.422037	-1.139872	0.330456
C	-6.014329	0.117849	0.239922
C	-5.255284	1.219662	-0.143052
C	-3.905588	1.068232	-0.439064
C	-3.313092	-0.192897	-0.346203
H	-3.595806	-2.273017	0.119050
H	-6.014872	-2.001429	0.626926
H	-7.070211	0.238638	0.468813
H	-5.716153	2.201614	-0.215270
H	-3.303823	1.920878	-0.745970
C	-1.909043	-0.349764	-0.700187
N	-1.093509	-0.388604	-1.573002
Mg	0.357569	-0.906300	-0.063256
C	-1.262866	-0.537025	1.488844
H	-1.872797	-1.392336	1.805161
H	-0.346129	-0.561369	2.119557
H	-1.785351	0.386901	1.765589
O	0.692782	1.291353	0.063198
C	1.242538	1.959988	-1.085483
C	1.225377	1.875917	1.264326
C	2.451405	2.710994	-0.568592
H	1.469149	1.209301	-1.851374
H	0.482204	2.641178	-1.493797
C	1.973553	3.119268	0.819838
H	0.396281	2.072111	1.952167
H	1.909359	1.152866	1.734601
H	2.730103	3.554543	-1.205848
H	3.310393	2.030660	-0.488292
H	1.291181	3.975583	0.750837
H	2.783922	3.383435	1.504783
O	2.639698	-0.640843	-0.034199
C	3.428096	-0.948533	-1.190106
C	3.326804	-1.257547	1.059876
C	4.886965	-0.952492	-0.710267
H	3.123260	-1.932611	-1.576661
H	3.211528	-0.192055	-1.951780
C	4.771620	-0.869361	0.820701
H	2.890901	-0.879151	1.991210
H	3.177413	-2.348204	1.016448
H	5.451710	-0.108943	-1.118066
H	5.392758	-1.869940	-1.026366
H	4.936246	0.157983	1.167909
H	5.477445	-1.521521	1.342164
C	0.600050	-3.034043	-0.058142
H	1.374868	-3.455456	-0.720152
H	0.833529	-3.426069	0.947299
H	-0.342947	-3.528475	-0.349379

PRb_Me$_2$Mg$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	4.361131	-0.859214	0.048274
C	5.520501	-0.266681	-0.447435
C	5.536967	1.088744	-0.754848
C	4.382965	1.848030	-0.562925
C	3.231322	1.251548	-0.071267
C	3.195265	-0.111083	0.244110
H	4.374378	-1.921450	0.282322
H	6.414766	-0.869498	-0.592490
H	6.442064	1.552935	-1.140453
H	4.386693	2.910663	-0.798734
H	2.317113	1.821030	0.087822
C	1.907311	-0.707988	0.770805
N	0.858900	-0.015669	0.896587
Mg	-1.046259	-0.256164	1.465148
C	1.993675	-2.192675	1.110715
H	2.765116	-2.401429	1.864527
H	1.028289	-2.531771	1.501677
H	2.243089	-2.800544	0.228903
O	-1.753926	-1.591220	-0.022267
C	-0.948943	-2.091115	-1.112316
C	-3.147069	-1.589190	-0.391702
C	-1.873648	-2.095860	-2.312640
H	-0.071183	-1.441674	-1.204554
H	-0.612566	-3.105524	-0.857383
C	-3.219669	-2.405843	-1.666892
H	-3.725539	-2.000050	0.441971
H	-3.458421	-0.545367	-0.556735
H	-1.571453	-2.826724	-3.067489
H	-1.895532	-1.105964	-2.788090
H	-3.291856	-3.474950	-1.432329
H	-4.077576	-2.133296	-2.287292
O	-1.925098	1.305256	0.364917
C	-1.429304	1.700550	-0.927714
C	-3.045697	2.124457	0.750938

C	-2.048847	3.059758	-1.177014
H	-0.334746	1.679059	-0.881794
H	-1.768981	0.963065	-1.673939
C	-3.406589	2.904353	-0.499008
H	-3.842418	1.467614	1.118846
H	-2.729528	2.783472	1.570683
H	-2.116576	3.300355	-2.241311
H	-1.461078	3.843323	-0.683072
H	-4.082251	2.316690	-1.134586
H	-3.895620	3.854847	-0.269953
C	-2.259061	-0.416143	3.208144
H	-1.942399	-1.173274	3.941353
H	-2.319678	0.531730	3.766972
H	-3.300949	-0.671801	2.950689

RCa_MeMgClZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.843046	-0.437461	-0.652554
C	-2.378392	0.756268	-0.082151
C	-3.252841	1.656430	0.539396
C	-4.604435	1.352790	0.585239
C	-5.073540	0.169253	0.019098
C	-4.198434	-0.722693	-0.597111
H	-2.138791	-1.117935	-1.127336
H	-2.868377	2.573378	0.976263
H	-5.295145	2.040101	1.064403
H	-6.134763	-0.060976	0.059331
H	-4.574298	-1.642380	-1.035232
C	-0.985615	1.029413	-0.135699
N	0.158464	1.210817	-0.193211
Mg	2.322117	0.964079	-0.170239
C	3.485610	-0.814825	-0.312984
H	3.651330	-1.375179	0.616925
H	3.287003	-1.537207	-1.115700
Cl	3.032590	3.175629	-0.136981
H	4.468726	-0.383118	-0.562640
Zn	1.109943	-1.851081	0.199879
C	1.184068	-1.731672	2.131641
H	0.353448	-2.253763	2.622249
H	2.113787	-2.157289	2.530544
H	1.145365	-0.687993	2.474940
C	0.504039	-2.140453	-1.618473
H	-0.415533	-2.738308	-1.673322
H	0.301794	-1.192786	-2.137799
H	1.254010	-2.666755	-2.223394

TSa_MeMgClZn

Atom	Coordinate (Å)		
	x	y	z
C	2.780570	0.419042	0.390554
C	1.964802	-0.690570	0.171535
C	2.529824	-1.909307	-0.224662
C	3.904495	-2.013230	-0.381597
C	4.716682	-0.903822	-0.161389
C	4.153477	0.311272	0.219408
H	2.327895	1.363155	0.682282
H	1.879983	-2.762201	-0.403445
H	4.342863	-2.961473	-0.680760
H	5.793022	-0.985847	-0.289177
H	4.786591	1.178677	0.384533
C	0.509783	-0.647070	0.259393
N	-0.460476	-1.274092	-0.066456
Mg	-2.440645	-0.691351	-0.136428
C	-2.585951	1.497097	0.223500
H	-3.139251	1.199687	1.130509
H	-2.348150	2.549286	0.439725
Cl	-4.448406	-1.809221	-0.129625
H	-3.316028	1.580504	-0.595381
Zn	-0.512074	1.399003	-0.069574
C	0.106029	0.853982	1.863698
H	0.957840	0.368755	2.345852
H	0.199329	1.922896	2.129377
H	-0.810056	0.461751	2.320742
C	0.415072	2.228508	-1.588191
H	0.954428	1.491069	-2.197232
H	-0.266329	2.765260	-2.259834
H	1.165363	2.954597	-1.247511

PRa_MeMgClZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.970503	-1.685117	-0.493316
C	-1.951284	-0.924645	0.091552
C	-2.300805	0.247753	0.767922
C	-3.622045	0.664509	0.842435
C	-4.623843	-0.089205	0.236335
C	-4.294167	-1.264412	-0.431529
H	-2.732040	-2.605843	-1.020533
H	-1.514680	0.833921	1.236229
H	-3.871363	1.578854	1.375900
H	-5.659815	0.236703	0.288408
H	-5.071252	-1.857863	-0.906957
C	-0.517099	-1.335020	0.006299
N	0.440391	-0.496709	0.076536
Mg	2.450795	-0.399075	0.086245
C	2.630183	1.852322	0.166984
H	3.198261	2.042741	-0.754716
H	2.347863	2.849200	0.529290
Cl	4.459602	-1.526905	0.097014
H	3.378109	1.543640	0.920489
Zn	0.562954	1.487499	-0.122223
C	-0.268193	-2.812426	-0.174670
H	-0.577883	-3.134642	-1.177107
H	0.796691	-3.036401	-0.065669
H	-0.841471	-3.412510	0.541606
C	-0.702708	2.864264	-0.694445
H	-0.209356	3.710502	-1.188786
H	-1.450623	2.468975	-1.393702
H	-1.263785	3.272857	0.156903

RCb_MeMgClZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.727795	-0.632848	-0.418420
C	-2.390820	0.710845	-0.205723
C	-3.359778	1.655521	0.157906
C	-4.674966	1.244416	0.307186
C	-5.016669	-0.089827	0.096936
C	-4.048822	-1.024323	-0.263862
H	-1.955361	-1.345099	-0.700337
H	-3.074958	2.691192	0.319067
H	-5.436343	1.965607	0.588843
H	-6.049865	-0.404779	0.216035
H	-4.324942	-2.061976	-0.425656
C	-1.036583	1.116441	-0.355762
N	0.069401	1.444169	-0.476639
Mg	2.203022	1.824741	-0.385847
Zn	1.211649	-1.653404	0.468991
C	1.663782	-0.921190	2.197535
H	1.134660	-1.397514	3.031990
H	2.738139	-1.011350	2.404644

H	1.427607	0.151989	2.252654
C	0.363647	-2.478874	-1.058661
H	-0.501886	-3.108712	-0.814810
H	0.026919	-1.716042	-1.775720
H	1.066307	-3.115805	-1.612037
Cl	3.115258	-0.256652	-0.994781
C	2.855396	3.638058	0.451985
H	2.373016	4.513763	-0.005642
H	2.642846	3.699386	1.529003
H	3.938595	3.789151	0.345446

TSb_MeMgClZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.626299	-0.466118	0.424576
C	-1.822151	0.642126	0.161217
C	-2.406298	1.833946	-0.281803
C	-3.782624	1.915842	-0.437332
C	-4.581866	0.806479	-0.172325
C	-4.001706	-0.385340	0.252116
H	-2.170314	-1.394478	0.760874
H	-1.766500	2.687646	-0.490619
H	-4.233839	2.848077	-0.766757
H	-5.659848	0.871454	-0.296129
H	-4.622357	-1.254137	0.453941
C	-0.358801	0.622043	0.283805
N	0.560486	1.303672	-0.099262
Mg	2.632898	1.428412	-0.136271
Zn	0.534603	-1.416122	-0.038578
C	0.056026	-0.658994	1.852171
H	-0.754159	-0.155893	2.383513
H	-0.047206	-1.720749	2.148177
H	1.011280	-0.275982	2.222794
C	-0.185402	-2.421616	-1.532893
H	-0.660522	-1.746377	-2.255369
H	0.587360	-2.986854	-2.064926
H	-0.952534	-3.133772	-1.206570
C	3.972014	3.043669	-0.229596
H	3.893033	3.699122	0.649268
H	5.025229	2.737291	-0.292908
H	3.780511	3.679346	-1.105901
Cl	2.908014	-1.013524	0.084026

PRb_MeMgClZn

Atom	Coordinate (Å)		
	x	y	z
C	2.911142	1.520443	-0.475373
C	1.849284	0.814939	0.101182
C	2.123993	-0.405607	0.727379
C	3.413563	-0.917840	0.763473
C	4.455630	-0.218304	0.161792
C	4.200344	1.000988	-0.457839
H	2.729981	2.475826	-0.962049
H	1.322473	-0.945322	1.226437
H	3.606372	-1.860117	1.270111
H	5.466255	-0.617919	0.185157
H	5.009954	1.553740	-0.927585
C	0.452868	1.343190	0.063500
N	-0.574599	0.582725	0.020195
Mg	-2.603953	1.064502	0.099537
Zn	-0.549638	-1.309052	-0.210441
C	0.323521	2.844336	0.078741
H	0.656838	3.265231	-0.878298
H	-0.717566	3.146474	0.228757
H	0.949628	3.293897	0.857589
C	0.036481	-3.101300	-0.576591
H	-0.673591	-3.647093	-1.207332
H	1.009205	-3.111257	-1.082771
H	0.152559	-3.672041	0.352686
Cl	-3.137528	-1.294385	0.273796
C	-3.605766	2.903473	-0.103031
H	-4.699104	2.816085	-0.171137
H	-3.401067	3.580495	0.739774
H	-3.281552	3.439095	-1.007837

RCa_MeMgClZn$_{THF1}$

Atom	Coordinate (Å)		
	X	y	z
C	-3.676148	0.108389	-0.079333
C	-2.875228	1.233377	0.164060
C	-3.437608	2.502907	0.342819
C	-4.815503	2.640588	0.276470
C	-5.617793	1.527214	0.035144
C	-5.051947	0.266826	-0.142633
H	-3.209117	-0.865338	-0.219796
H	-2.797221	3.359504	0.532035
H	-5.266668	3.618739	0.413968
H	-6.697082	1.643720	-0.014955
H	-5.684912	-0.595232	-0.331117
C	-1.468016	1.041737	0.237113
N	-0.331031	0.816509	0.299462
Mg	1.412594	-0.509246	0.421773
C	1.486163	-1.879450	-1.372667
H	2.559296	-1.824025	-1.119597
H	1.384329	-2.913151	-1.733258
H	1.344368	-1.242226	-2.255933
Zn	-0.305583	-2.256553	-0.297475
C	-0.295405	-1.901909	1.701735
H	-1.358449	-1.739103	1.931406
H	-0.003708	-2.842762	2.189904
H	0.225220	-1.127841	2.286275
C	-1.811012	-2.731375	-1.477505
H	-2.727060	-3.031828	-0.950249
H	-2.082556	-1.880472	-2.120036
H	-1.562772	-3.556286	-2.159303
O	2.439547	0.991887	-0.658850
C	2.327681	2.371681	-0.237896
C	3.787189	0.732365	-1.124130
C	3.537689	3.061236	-0.829579
H	1.367265	2.755633	-0.593119
H	2.342960	2.404323	0.862092
C	4.587582	1.961065	-0.744338
H	4.150401	-0.183017	-0.643509
H	3.744444	0.578378	-2.210203
H	3.807195	3.967144	-0.280161
H	3.349335	3.334774	-1.875203
H	4.956093	1.865880	0.284865
H	5.444498	2.117917	-1.404782
Cl	3.039146	-0.546810	2.114862

TSa_MeMgClZn$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	3.628744	0.005588	-0.400478
C	2.704076	-0.505835	0.509694
C	3.026632	-1.624958	1.284999
C	4.277609	-2.213498	1.159468
C	5.197942	-1.704462	0.247500
C	4.869337	-0.601366	-0.536834
H	3.360524	0.871785	-1.001233
H	2.291776	-2.015540	1.984580
H	4.533405	-3.072783	1.773665

H	6.175942	-2.168409	0.148010
H	5.585951	-0.208606	-1.252987
C	1.354914	0.029142	0.658577
N	0.253127	-0.327055	0.973609
Mg	-1.596701	0.580511	0.803559
C	-1.273410	2.533082	-0.221204
H	-1.403943	2.959204	0.787978
H	-0.879312	3.387297	-0.790126
Cl	-3.099657	0.614750	2.549467
O	-2.418209	-0.704058	-0.573831
C	-2.047459	-2.108189	-0.507585
C	-3.785677	-0.576998	-1.039717
H	-1.073081	-2.221539	-0.992504
H	-1.953786	-2.383901	0.552183
C	-3.184608	-2.847722	-1.181240
C	-4.377922	-1.956139	-0.858052
H	-4.279106	0.201516	-0.447882
H	-3.759856	-0.270097	-2.093090
H	-3.288128	-3.868531	-0.804622
H	-3.025082	-2.895495	-2.265156
H	-5.241598	-2.127764	-1.505481
H	-4.690662	-2.095014	0.184905
H	-2.276732	2.398206	-0.659192
Zn	0.450130	1.538818	-0.854286
C	1.720831	2.229821	0.686020
H	2.744946	2.027337	1.003249
H	1.776908	3.166761	0.100810
H	1.105271	2.431485	1.570179
C	0.812341	0.753916	-2.619868
H	1.632718	1.264510	-3.141324
H	1.108294	-0.301078	-2.534628
H	-0.060091	0.786793	-3.284696

PRa_MeMgClZn$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	4.048821	0.905669	-0.053280
C	2.748318	0.433045	-0.257990
C	2.580861	-0.871280	-0.734388
C	3.676165	-1.686658	-0.984183
C	4.964904	-1.212013	-0.752006
C	5.147718	0.085338	-0.285093
H	4.208914	1.918729	0.309245
H	1.575150	-1.234988	-0.936819
H	3.525520	-2.693326	-1.366456
H	5.824286	-1.850456	-0.941743
H	6.150928	0.463164	-0.103076
C	1.552751	1.290723	0.011126
N	0.427816	0.790490	0.332284
Mg	-0.605244	-0.815232	1.003320
C	-2.407147	0.432170	1.839972
H	-2.261097	-0.465421	2.468791
H	-2.616124	1.199400	2.599620
Cl	-0.174546	-2.720061	2.241536
O	-1.492401	-1.474982	-0.757535
C	-1.417403	-0.722656	-1.989285
C	-2.751462	-2.199529	-0.741997
H	-0.727113	0.111683	-1.825424
H	-1.015629	-1.374389	-2.777958
C	-2.852935	-0.336146	-2.250821
C	-3.580056	-1.630622	-1.893039
H	-2.538609	-3.268393	-0.846272
H	-3.219517	-2.030678	0.234558
H	-3.026310	-0.015307	-3.281354
H	-3.142930	0.482726	-1.577092
H	-4.622647	-1.472393	-1.605424
H	-3.568690	-2.316461	-2.747617
H	-3.361922	0.260357	1.322913
Zn	-1.319781	1.719295	0.626467
C	1.763218	2.779066	-0.120387
H	2.339189	3.037046	-1.016433
H	0.792012	3.282803	-0.150423
H	2.320256	3.168444	0.741672
C	-2.031284	3.219212	-0.415847
H	-1.708223	4.199399	-0.040975
H	-1.685836	3.156471	-1.457737
H	-3.128296	3.235082	-0.444357

RCb_MeMgClZn$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.603721	0.202652	-0.332394
C	-2.952867	-0.872472	0.289836
C	-3.633519	-2.054601	0.605846
C	-4.979422	-2.156004	0.290590
C	-5.633072	-1.092859	-0.329180
C	-4.950204	0.081271	-0.638999
H	-3.047628	1.111803	-0.555774
H	-3.107539	-2.871953	1.090337
H	-5.521875	-3.065888	0.529348
H	-6.688660	-1.180333	-0.572046
H	-5.469627	0.904937	-1.119518
C	-1.572842	-0.729479	0.593811
N	-0.446618	-0.558408	0.811313
Mg	1.497387	0.325550	1.062035
C	1.975460	2.350104	0.465199
H	3.042984	2.068475	0.531858
H	1.972105	3.061214	-0.375763
H	1.766081	2.956623	1.358054
Zn	0.095790	1.952017	-0.705622
C	0.348853	0.694342	-2.202318
H	-0.605365	0.475908	-2.702509
H	1.022039	1.077886	-2.982610
H	0.758427	-0.275649	-1.887223
C	-1.252045	3.055007	0.213328
H	-2.100187	3.360500	-0.414893
H	-1.682572	2.525302	1.077201
H	-0.815575	3.979449	0.617023
O	2.557899	-0.914357	-0.179500
C	3.472389	-0.462536	-1.208227
C	2.371336	-2.347119	-0.261480
C	3.601960	-1.642160	-2.148062
H	3.043545	0.433722	-1.668509
H	4.426528	-0.207052	-0.729119
C	3.463948	-2.824759	-1.194925
H	2.427611	-2.754435	0.753307
H	1.369619	-2.538494	-0.672191
H	4.547406	-1.632260	-2.696418
H	2.780213	-1.636459	-2.875925
H	4.397684	-2.982059	-0.641693
H	3.199320	-3.759837	-1.695222
Cl	2.127572	-0.206065	3.232659

TSb_MeMgClZn$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	3.481755	0.001944	-0.337758
C	2.454687	0.605107	0.388576
C	2.718603	1.729032	1.177340
C	4.004010	2.252995	1.224476
C	5.029062	1.646852	0.504225
C	4.768218	0.517869	-0.269026

H	3.265531	-0.879206	-0.937838
H	1.908203	2.181508	1.744639
H	4.206190	3.133586	1.828513
H	6.035875	2.054593	0.545819
H	5.570848	0.040213	-0.824466
C	1.092302	0.076718	0.427921
N	0.197309	-0.052120	1.223875
Mg	-1.720479	-0.689690	0.775191
C	-1.619526	-2.248015	-0.835598
H	-2.454448	-1.623531	-1.200667
H	-1.349407	-2.803146	-1.745141
H	-2.053864	-3.015235	-0.178782
Zn	0.415837	-1.833370	-0.676530
C	0.642548	0.030789	-1.700322
H	1.610070	0.328965	-2.106216
H	0.106365	-0.513694	-2.500297
H	0.035206	0.922357	-1.505809
C	1.786867	-3.176864	-0.256841
H	2.512109	-3.308484	-1.070973
H	2.364215	-2.894434	0.633874
H	1.350402	-4.163366	-0.056788
O	-2.190613	1.027422	-0.267582
C	-2.982783	1.141172	-1.472589
C	-1.917524	2.338766	0.282913
C	-2.951601	2.616204	-1.816601
H	-2.532367	0.499161	-2.238037
H	-3.997978	0.784200	-1.251651
C	-2.873003	3.263976	-0.438813
H	-2.065158	2.287953	1.366870
H	-0.865643	2.586260	0.077146
H	-3.825608	2.924308	-2.395788
H	-2.052044	2.849837	-2.400371
H	-3.855663	3.253070	0.047709
H	-2.511422	4.295096	-0.462243
Cl	-3.464043	-1.076261	2.231188

PRb_MeMgClZn$_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-2.327096	2.303294	-0.180766
C	-1.353844	1.631339	0.566950
C	-1.770582	0.780976	1.596633
C	-3.120514	0.590463	1.860865
C	-4.081240	1.244297	1.091012
C	-3.680794	2.101201	0.070399
H	-2.029411	2.977476	-0.981378
H	-1.016572	0.288531	2.209079
H	-3.425497	-0.063806	2.674221
H	-5.138636	1.092811	1.293435
H	-4.424549	2.617631	-0.531572
C	0.103228	1.773049	0.257301
N	0.917542	0.819770	0.474156
Mg	0.891397	-1.208870	0.404428
C	2.712062	-1.350594	-0.991347
H	1.952512	-2.034776	-1.412689
H	3.210488	-0.985540	-1.900890
H	3.447500	-1.998676	-0.496347
Zn	2.770797	0.588245	-0.188595
C	0.530712	3.078559	-0.365890
H	0.085611	3.946211	0.134269
H	1.621800	3.154862	-0.334639
H	0.220577	3.120613	-1.419103
C	4.383659	1.677870	-0.004225
H	4.228769	2.717419	-0.320946
H	4.714833	1.714698	1.041384
H	5.225355	1.289497	-0.591205
O	-0.694664	-1.581095	-0.858988
C	-0.903052	-0.827938	-2.076790
C	-1.929910	-2.223591	-0.449490
C	-2.243485	-1.298477	-2.600033
H	-0.920958	0.242569	-1.823305
H	-0.059397	-1.024459	-2.746840
C	-3.000056	-1.583561	-1.307614
H	-1.829098	-3.300237	-0.635037
H	-2.062858	-2.057230	0.625083
H	-2.125223	-2.216777	-3.188048
H	-2.725365	-0.546108	-3.230027
H	-3.864743	-2.238229	-1.444105
H	-3.342646	-0.646393	-0.847396
Cl	0.803341	-2.921290	1.969503

RCa_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	3.673003	-0.353460	-2.123360
C	4.994591	-0.768911	-2.074025
C	5.515948	-1.299565	-0.895670
C	4.723634	-1.419489	0.243870
C	3.399299	-1.010238	0.215376
C	2.882308	-0.477846	-0.974449
H	3.249664	0.060670	-3.033972
H	5.620951	-0.680064	-2.956703
H	6.552789	-1.623806	-0.865995
H	5.139378	-1.834316	1.157331
H	2.751782	-1.088730	1.088174
C	1.518039	-0.076107	-0.984780
N	0.398578	0.227750	-0.940493
Mg	-1.612769	0.520213	-0.053254
Cl	-3.538559	0.967065	-1.391083
C	-1.839806	0.445470	2.158973
H	-2.890032	0.340490	1.824551
H	-1.765659	1.466917	2.556647
C	0.269230	-2.383322	1.629569
H	1.066581	-2.887790	2.196075
H	-0.658029	-2.931822	1.851742
H	0.481056	-2.576408	0.567170
H	-1.839823	-0.221313	3.038461
Zn	0.142929	-0.446957	2.053542
C	1.513423	0.818150	2.743584
H	1.107303	1.602803	3.399283
H	2.272122	0.286672	3.337786
H	2.076270	1.343284	1.954988
O	-1.080550	2.582605	-0.103137
C	-0.949785	3.256231	-1.377973
C	-0.200602	3.200996	0.859489
C	0.030425	4.394240	-1.144246
H	-0.560396	2.529243	-2.104757
H	-1.943504	3.574738	-1.705485
C	0.862242	3.872630	0.021538
H	-0.777314	3.933775	1.442632
H	0.169614	2.420679	1.529106
H	-0.501291	5.306575	-0.847212
H	0.616876	4.620895	-2.038850
H	1.396842	4.656105	0.565686
H	1.593462	3.127779	-0.323193
O	-1.944817	-1.536759	-0.386205
C	-3.087104	-2.161992	0.235064
C	-1.589152	-2.236515	-1.590738
C	-3.584341	-3.174743	-0.777214
H	-2.747803	-2.630634	1.169469
H	-3.825455	-1.385973	0.467122
C	-2.294005	-3.571868	-1.482212

H	-1.943280	-1.653369	-2.454811
H	-0.497219	-2.311456	-1.630882
H	-4.269277	-2.691059	-1.485875
H	-4.107792	-4.011923	-0.307780
H	-2.450501	-4.044721	-2.455449
H	-1.707639	-4.254187	-0.852631

TSa_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	3.358931	0.704862	-1.468174
C	4.655966	0.454742	-1.899090
C	5.377736	-0.604878	-1.357520
C	4.803352	-1.415025	-0.381076
C	3.515404	-1.159367	0.069441
C	2.790493	-0.098984	-0.476443
H	2.776849	1.520215	-1.892348
H	5.102118	1.086637	-2.662602
H	6.391189	-0.801215	-1.698158
H	5.364132	-2.247483	0.035645
H	3.055706	-1.783180	0.832625
C	1.408747	0.175193	-0.091449
N	0.339546	0.402997	-0.582987
Mg	-1.674379	0.478665	0.022169
Cl	-3.785638	0.751726	-1.012357
C	-1.526911	0.054933	2.285148
H	-2.447145	-0.547718	2.239996
H	-1.833386	1.114401	2.281359
C	0.626731	-2.769017	1.590768
H	1.473630	-3.066616	2.225101
H	-0.229074	-3.385060	1.899249
H	0.881470	-3.080814	0.566374
H	-1.190924	-0.071179	3.325415
Zn	0.229866	-0.840485	1.670202
C	1.804247	0.561474	2.045944
H	1.243865	0.814055	2.963654
H	2.697493	-0.003552	2.329705
H	2.139530	1.525240	1.644093
O	-1.430731	2.597168	0.185152
C	-1.460975	3.331373	-1.064874
C	-0.459468	3.194540	1.071596
C	-0.590733	4.552488	-0.838432
H	-1.045429	2.683356	-1.851542
H	-2.504414	3.550468	-1.307091
C	0.422272	4.034941	0.175674
H	-0.994665	3.810006	1.808168
H	0.068224	2.391696	1.595042
H	-1.179029	5.369710	-0.403209
H	-0.140013	4.913924	-1.766532
H	0.943622	4.825827	0.721594
H	1.171369	3.399633	-0.317649
O	-1.700254	-1.596016	-0.454466
C	-2.736064	-2.474714	0.034225
C	-1.172301	-2.095255	-1.702091
C	-3.073430	-3.369652	-1.139167
H	-2.328550	-3.038124	0.885983
H	-3.576695	-1.857976	0.370676
C	-1.718958	-3.502760	-1.823828
H	-1.531202	-1.443976	-2.513312
H	-0.079509	-2.036525	-1.657776
H	-3.788177	-2.863887	-1.801355
H	-3.505364	-4.324247	-0.827022
H	-1.781473	-3.835630	-2.863337
H	-1.080931	-4.206320	-1.273244

PRa_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	2.128312	0.302402	1.780653
C	3.312974	-0.129508	2.361828
C	4.505265	0.541722	2.096064
C	4.495451	1.658520	1.266830
C	3.302751	2.096917	0.697993
C	2.105559	1.411287	0.928583
H	1.192180	-0.212685	1.994664
H	3.306539	-0.989274	3.028144
H	5.435594	0.201862	2.544560
H	5.419944	2.192672	1.060548
H	3.313335	2.969622	0.048365
C	0.832323	1.806664	0.243728
N	-0.079850	0.958567	0.000933
Mg	-0.487212	-1.029022	-0.287750
Cl	-0.672811	-3.021491	0.958336
C	-1.574096	-0.470897	-2.416140
H	-1.388643	-1.553733	-2.290219
H	-0.908388	-0.187547	-3.243370
C	-3.047925	2.606158	-1.051739
H	-2.843528	3.437455	-1.739237
H	-4.066837	2.258698	-1.272294
H	-3.073833	3.042492	-0.042176
H	-2.592182	-0.466314	-2.830233
Zn	-1.728164	1.152576	-1.144216
C	0.729666	3.252018	-0.187227
H	-0.309579	3.482499	-0.442697
H	1.079586	3.946894	0.585241
H	1.342733	3.430951	-1.081431
O	1.288331	-1.548857	-1.290427
C	2.273734	-2.431702	-0.694820
C	1.940378	-0.624276	-2.192486
C	3.550456	-2.185009	-1.471844
H	2.386116	-2.155410	0.362567
H	1.892724	-3.454645	-0.752738
C	3.412735	-0.716040	-1.852063
H	1.735388	-0.947329	-3.222406
H	1.505357	0.369350	-2.035765
H	3.584606	-2.812933	-2.370836
H	4.439809	-2.397168	-0.871470
H	4.050763	-0.418801	-2.688868
H	3.644005	-0.071886	-0.992276
O	-2.459797	-0.358788	0.514607
C	-3.685567	-1.073740	0.218252
C	-2.527384	0.203449	1.847548
C	-4.440982	-1.124662	1.530413
H	-4.227203	-0.503609	-0.549429
H	-3.419934	-2.058490	-0.181076
C	-3.998175	0.172309	2.197432
H	-1.930448	-0.430893	2.519367
H	-2.083875	1.203203	1.804751
H	-4.112535	-1.987731	2.123466
H	-5.521843	-1.198515	1.383713
H	-4.172163	0.193686	3.276457
H	-4.510618	1.031430	1.744453

RCb_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.250514	1.610911	0.744702
C	-5.636725	1.589873	0.764739
C	-6.319450	0.390650	0.572384
C	-5.624176	-0.797311	0.359167
C	-4.237644	-0.796425	0.337768
C	-3.557357	0.413876	0.531683

H	-3.701731	2.536684	0.892911
H	-6.187809	2.510799	0.931010
H	-7.406047	0.382224	0.589483
H	-6.164495	-1.727612	0.210683
H	-3.669004	-1.710957	0.178557
C	-2.135219	0.390249	0.499242
N	-0.980426	0.291672	0.446964
Mg	1.229811	-0.277355	0.447920
C	1.544229	-1.724163	-1.181411
H	2.361063	-2.184386	-0.600199
H	2.011558	-1.038170	-1.907408
C	-1.290476	-3.070956	0.353177
H	-2.166155	-3.671994	0.067096
H	-0.523066	-3.789398	0.675764
H	-1.578408	-2.516344	1.258608
H	1.191306	-2.557891	-1.808982
Zn	-0.649699	-1.875744	-1.085486
C	-1.291864	-0.997560	-2.739808
H	-0.467071	-0.588842	-3.343865
H	-1.839554	-1.682172	-3.403064
H	-1.979380	-0.159560	-2.547913
O	1.336005	1.651609	-0.375185
C	1.373579	2.793863	0.507708
C	0.719443	2.012761	-1.632661
C	1.109089	3.983012	-0.390790
H	0.584656	2.677420	1.266044
H	2.348290	2.800142	1.007115
C	0.131712	3.389505	-1.399027
H	1.505403	2.025793	-2.401299
H	-0.020198	1.246963	-1.893386
H	2.033470	4.296900	-0.891687
H	0.707614	4.838143	0.159013
H	0.046784	3.967887	-2.322633
H	-0.868502	3.303876	-0.953609
Cl	1.127324	-0.550446	2.793452
O	3.372766	0.010352	0.523805
C	4.215142	-0.872726	1.300268
C	4.126600	0.564845	-0.572980
C	5.618670	-0.659576	0.768377
H	4.081740	-0.627863	2.357428
H	3.873211	-1.906281	1.138439
C	5.349875	-0.318049	-0.691643
H	3.492500	0.570951	-1.465258
H	4.391453	1.603835	-0.327566
H	6.250805	-1.540968	0.905030
H	6.097906	0.187214	1.275382
H	5.102004	-1.225894	-1.257806
H	6.183702	0.183605	-1.190124

TSb_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.731150	1.621095	0.340904
C	-5.059114	1.995855	0.502836
C	-6.064734	1.035823	0.442247
C	-5.743677	-0.300504	0.214229
C	-4.420614	-0.678802	0.030391
C	-3.412145	0.282839	0.098435
H	-2.930579	2.355957	0.402969
H	-5.308226	3.038384	0.683042
H	-7.103127	1.328848	0.574846
H	-6.529203	-1.050514	0.175437
H	-4.156643	-1.718252	-0.153260
C	-1.998044	-0.063478	0.001587
N	-0.968277	0.118821	0.587060
Mg	1.134191	-0.232242	0.527833
C	1.013200	-1.423241	-1.493520
H	2.008210	-1.740978	-1.151903
H	1.117733	-0.443010	-1.988608
C	-1.474200	-3.462692	0.368096
H	-2.244076	-4.037064	-0.164956
H	-0.688793	-4.172306	0.657279
H	-1.936191	-3.113432	1.302743
H	0.812167	-2.108003	-2.329839
Zn	-0.804498	-1.938574	-0.678983
C	-2.043798	-0.858139	-2.055751
H	-1.489673	-1.458611	-2.797655
H	-3.101749	-1.109533	-2.152046
H	-1.899502	0.186233	-2.360396
O	1.318731	1.779122	-0.045354
C	1.851957	2.765524	0.867864
C	0.600220	2.431565	-1.115814
C	1.843556	4.052107	0.074577
H	1.194902	2.821177	1.747643
H	2.842440	2.423328	1.186377
C	0.559209	3.898253	-0.731973
H	1.160623	2.268420	-2.047570
H	-0.387245	1.964089	-1.205969
H	2.715089	4.091102	-0.592154
H	1.856502	4.938213	0.714158
H	0.508068	4.552581	-1.605957
H	-0.312655	4.102675	-0.097964
Cl	1.398471	-0.983730	2.742346
O	3.266507	-0.165731	0.205777
C	4.142011	-1.196377	0.724952
C	3.887952	0.480770	-0.925905
C	5.476022	-0.959583	0.048355
H	4.152951	-1.111360	1.814170
H	3.718777	-2.176499	0.457044
C	5.044238	-0.418793	-1.308485
H	3.140184	0.598436	-1.717179
H	4.229065	1.479044	-0.614653
H	6.075595	-1.871545	-0.013351
H	6.054932	-0.204413	0.594400
H	4.689191	-1.236383	-1.949804
H	5.832564	0.118743	-1.842165

PRb_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	2.577168	-0.418885	1.368173
C	3.373894	-1.499329	1.727026
C	4.484121	-1.837513	0.955318
C	4.802474	-1.074212	-0.163873
C	4.017173	0.023088	-0.507013
C	2.884456	0.353848	0.243647
H	1.707592	-0.148484	1.967859
H	3.130240	-2.078855	2.615144
H	5.104117	-2.687060	1.231570
H	5.669268	-1.328857	-0.769393
H	4.281673	0.615216	-1.381270
C	1.989656	1.494278	-0.137853
N	0.737338	1.446275	0.066313
Mg	-0.850234	0.154416	0.413577
C	-2.147612	1.562599	-1.128041
H	-3.061268	1.367453	-0.550272
H	-1.944371	0.659839	-1.729223
C	-0.553390	4.731909	-0.260978
H	-0.114072	5.182480	-1.162260
H	-1.532304	5.206199	-0.116733
H	0.080545	5.046829	0.578702
H	-2.461614	2.290274	-1.889406

Zn	-0.652652	2.776200	-0.414544
C	2.675150	2.672615	-0.789986
H	1.981377	3.517409	-0.843172
H	3.580555	2.972884	-0.249046
H	2.984408	2.425578	-1.814437
O	0.041090	-1.502367	-0.534864
C	0.251104	-2.779159	0.109495
C	0.734172	-1.459892	-1.800411
C	0.799246	-3.672108	-0.982776
H	0.977468	-2.639184	0.923353
H	-0.705965	-3.101578	0.534302
C	1.624838	-2.685376	-1.801505
H	-0.017005	-1.499568	-2.603863
H	1.275997	-0.509343	-1.862188
H	-0.019544	-4.082662	-1.588832
H	1.383226	-4.505415	-0.583093
H	1.847070	-3.034986	-2.813220
H	2.573342	-2.462917	-1.293385
Cl	-1.108629	0.260268	2.766855
O	-2.575642	-1.144908	0.226902
C	-3.761230	-0.983193	1.043655
C	-2.908785	-1.865208	-0.976432
C	-4.818061	-1.851978	0.391503
H	-3.506398	-1.259681	2.069945
H	-4.044390	0.079556	1.031844
C	-4.416252	-1.785613	-1.076260
H	-2.382449	-1.404508	-1.819394
H	-2.561450	-2.904838	-0.875187
H	-5.829837	-1.487201	0.587183
H	-4.749371	-2.883602	0.758666
H	-4.712494	-0.822313	-1.512061
H	-4.838947	-2.587154	-1.687894

RCc_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.051592	0.028698	-2.224045
C	-5.429104	0.175800	-2.282597
C	-6.159938	0.381215	-1.114295
C	-5.522076	0.441890	0.122591
C	-4.144961	0.299184	0.201140
C	-3.416068	0.092591	-0.978791
H	-3.466397	-0.135881	-3.124039
H	-5.935874	0.128069	-3.241905
H	-7.239489	0.493778	-1.168568
H	-6.100129	0.599968	1.028339
H	-3.621068	0.338702	1.154690
C	-2.005721	-0.056545	-0.872068
N	-0.864829	-0.178963	-0.701846
Mg	1.304576	-0.462479	-0.176567
C	1.456582	-1.543896	1.738360
H	2.134982	-0.806013	2.195282
H	2.091246	-2.327857	1.291005
C	-1.396746	0.065714	2.698648
H	-2.387701	-0.111913	3.141852
H	-0.734044	0.306994	3.544123
H	-1.485978	0.996012	2.113727
H	1.015569	-2.058569	2.607649
Zn	-0.734926	-1.453451	1.609093
C	-1.382368	-3.076075	0.688842
H	-1.360628	-3.982420	1.309955
H	-2.418488	-2.975558	0.333167
H	-0.773967	-3.299222	-0.200830
O	1.174688	1.593095	0.217984
C	1.260554	2.117864	1.563020
C	0.615987	2.596809	-0.642515
C	0.449825	3.413398	1.558211
H	0.842764	1.357871	2.232533
H	2.318500	2.272901	1.811923
C	-0.347909	3.335751	0.256476
H	1.424414	3.252177	-1.002882
H	0.162022	2.086400	-1.497749
H	1.114573	4.284482	1.541607
H	-0.187731	3.494173	2.443323
H	-0.630234	4.316774	-0.134637
H	-1.260237	2.738390	0.390572
O	3.427368	-0.034390	-0.031485
C	4.375944	-1.125097	-0.070520
C	3.944722	1.085966	-0.779912
C	5.411848	-0.724711	-1.101274
H	4.807301	-1.236237	0.933548
H	3.839474	-2.043658	-0.332494
C	5.418267	0.792482	-0.966446
H	3.418819	1.135512	-1.746034
H	3.734516	2.000502	-0.215212
H	5.073614	-1.015102	-2.103644
H	6.384697	-1.187900	-0.915653
H	5.836774	1.308003	-1.835131
H	5.985537	1.097908	-0.078228
Cl	1.681407	-1.346949	-2.351664

TSc_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.605585	0.481474	-1.804197
C	-4.942144	0.813182	-1.976644
C	-5.896512	0.349704	-1.074812
C	-5.511843	-0.447004	0.000302
C	-4.178019	-0.793735	0.169611
C	-3.220587	-0.334631	-0.733642
H	-2.844569	0.843401	-2.491899
H	-5.239629	1.436872	-2.815585
H	-6.942998	0.611784	-1.209096
H	-6.254975	-0.802441	0.709147
H	-3.863564	-1.413842	1.005240
C	-1.790304	-0.593894	-0.591967
N	-0.734186	-0.170234	-0.969453
Mg	1.318814	-0.383914	-0.398851
C	1.074411	-1.641433	1.535259
H	1.840297	-1.037599	2.040469
H	1.585432	-2.323709	0.832608
C	-1.754880	0.296838	2.628916
H	-2.634434	-0.118949	3.138949
H	-1.087631	0.679622	3.413650
H	-2.114920	1.171362	2.065602
H	0.741363	-2.350792	2.308218
Zn	-0.886285	-1.012038	1.432872
C	-1.688531	-2.624424	0.318639
H	-1.860440	-3.191077	1.251677
H	-2.554136	-2.838117	-0.312857
H	-0.797265	-3.027884	-0.177298
O	1.225530	1.677383	0.004268
C	1.039207	2.158543	1.357458
C	0.617768	2.600691	-0.917067
C	0.087570	3.346810	1.251331
H	0.612494	1.333057	1.942799
H	2.019564	2.422160	1.773519
C	-0.536898	3.178824	-0.132828
H	1.359604	3.365910	-1.191195
H	0.326268	2.037188	-1.808846
H	0.641963	4.290991	1.303670
H	-0.651367	3.343907	2.058198

H	-0.912154	4.116084	-0.552304
H	-1.357853	2.448598	-0.109285
O	3.363721	-0.073572	0.214091
C	4.250124	-1.205919	0.389016
C	4.081329	1.005353	-0.431071
C	5.488518	-0.879413	-0.418910
H	4.465944	-1.304654	1.461239
H	3.734286	-2.107604	0.042205
C	5.544207	0.638269	-0.307214
H	3.766189	1.050319	-1.484942
H	3.802709	1.941896	0.061041
H	5.342058	-1.179331	-1.464031
H	6.379704	-1.382962	-0.034807
H	6.155995	1.112896	-1.079107
H	5.933461	0.938477	0.673787
Cl	2.073511	-1.460690	-2.357911

PRc_MeMgClZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	2.291138	-2.109548	-0.656491
C	2.862916	-3.306318	-0.244538
C	4.080275	-3.305940	0.432918
C	4.725657	-2.099793	0.683904
C	4.160764	-0.902716	0.255183
C	2.929980	-0.889006	-0.411107
H	1.340844	-2.110092	-1.188080
H	2.357326	-4.245570	-0.457909
H	4.525983	-4.242838	0.758846
H	5.675962	-2.088892	1.212744
H	4.682575	0.030311	0.456884
C	2.282804	0.397769	-0.826913
N	1.020825	0.519780	-0.924987
Mg	-0.932035	-0.178277	-0.609856
C	-1.833541	1.753885	-1.636484
H	-2.640509	2.033307	-0.946721
H	-2.193873	0.882560	-2.210906
C	0.690262	3.982508	-0.327083
H	1.187133	4.612399	-1.077654
H	-0.124887	4.582165	0.099740
H	1.426900	3.829417	0.475249
H	-1.831517	2.537015	-2.409104
Zn	0.075491	2.266320	-1.061354
C	3.239171	1.542237	-1.085634
H	2.707307	2.371392	-1.559216
H	3.666839	1.918075	-0.145628
H	4.080073	1.236571	-1.719282
O	-0.638687	0.335091	1.428303
C	-1.071612	1.573107	2.033624
C	0.453847	-0.200262	2.192333
C	0.010831	1.947025	3.046535
H	-1.173907	2.312226	1.227878
H	-2.057184	1.420514	2.491530
C	1.179361	1.029891	2.684307
H	0.047144	-0.798878	3.022607
H	1.038340	-0.847920	1.529914
H	-0.330837	1.737569	4.066517
H	0.268160	3.008702	2.991288
H	1.844191	0.826346	3.527991
H	1.772927	1.454383	1.862820
O	-2.941747	-0.470232	0.207132
C	-4.084603	-0.639330	-0.663625
C	-3.029622	-1.405672	1.305243
C	-4.767165	-1.909959	-0.199986
H	-4.729436	0.242831	-0.552574
H	-3.727405	-0.695016	-1.697322
C	-4.458221	-1.906072	1.291286
H	-2.314526	-2.223467	1.122500
H	-2.742047	-0.885066	2.224009
H	-4.304670	-2.780060	-0.682183
H	-5.836528	-1.914263	-0.428011
H	-4.557703	-2.887591	1.762696
H	-5.114810	-1.202916	1.819075
Cl	-1.205761	-2.225392	-1.780484

RC_Me$_2$MgZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.533922	-0.627953	0.135523
C	-2.298554	0.737519	-0.076867
C	-3.355362	1.643421	-0.227219
C	-4.657388	1.171572	-0.165102
C	-4.898951	-0.184554	0.044291
C	-3.843149	-1.080837	0.194133
H	-1.692687	-1.310918	0.245330
H	-3.148421	2.697245	-0.389477
H	-5.487274	1.862451	-0.280318
H	-5.922374	-0.547092	0.090752
H	-4.041003	-2.136268	0.356087
C	-0.949971	1.186408	-0.132670
N	0.164193	1.509928	-0.167617
Mg	2.327364	1.186256	0.111038
C	2.579657	-0.322572	-1.639004
H	2.534286	-1.192896	-2.304124
H	2.068921	0.467395	-2.213785
H	3.647517	-0.054075	-1.608963
Zn	1.666679	-1.245583	-0.022651
C	1.767043	-0.303787	1.839156
H	0.723865	-0.387577	2.177588
H	2.331582	-1.075217	2.382623
H	2.129425	0.632985	2.300797
C	0.486333	-2.815777	-0.161073
H	-0.116693	-2.981358	0.743263
H	-0.214735	-2.724505	-1.002894
H	1.040465	-3.748692	-0.332750
C	3.614819	2.846506	0.163827
H	3.582964	3.414829	-0.778026
H	3.351687	3.560492	0.958748
H	4.671058	2.586436	0.325582

TS_Me$_2$MgZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.473359	-0.602496	0.400289
C	-1.782056	0.581432	0.145149
C	-2.480695	1.730089	-0.245840
C	-3.863160	1.691820	-0.360915
C	-4.550821	0.508750	-0.103849
C	-3.854649	-0.637563	0.270760
H	-1.916532	-1.490048	0.689710
H	-1.926974	2.642394	-0.452937
H	-4.404958	2.586685	-0.655335
H	-5.633456	0.479294	-0.197172
H	-4.390718	-1.562518	0.465081
C	-0.327953	0.687365	0.193947
N	0.567737	1.391913	-0.181669
Mg	2.644826	1.121578	-0.187979
C	2.990213	-1.072466	0.270873
H	3.432573	-0.641202	1.185758
H	2.934266	-2.143656	0.515674
H	3.759835	-1.041217	-0.515438
Zn	0.951148	-1.191468	-0.081317

C	0.246474	-0.709477	1.853515
H	-0.668807	-0.341044	2.322777
H	0.311347	-1.773391	2.144615
H	1.094430	-0.176837	2.300864
C	0.087739	-2.128685	-1.582275
H	-0.540692	-1.454437	-2.179812
H	0.807427	-2.589937	-2.270321
H	-0.573463	-2.932296	-1.230344
C	4.281574	2.432768	-0.137240
H	5.194937	1.954234	0.244302
H	4.534829	2.829550	-1.131073
H	4.099585	3.306920	0.504128

PR_Me_2MgZn

Atom	Coordinate (Å)		
	x	y	z
C	2.959543	1.502950	-0.243632
C	1.825275	0.741925	0.064312
C	2.013905	-0.574349	0.496166
C	3.283355	-1.122208	0.603827
C	4.401700	-0.356018	0.283752
C	4.234750	0.957829	-0.140367
H	2.854221	2.531469	-0.579241
H	1.138745	-1.171017	0.735362
H	3.401910	-2.149057	0.941976
H	5.398916	-0.781147	0.367907
H	5.101425	1.564169	-0.392562
C	0.441606	1.303803	-0.063523
N	-0.606236	0.582039	-0.034742
Mg	-2.631396	0.872411	0.061797
C	-3.007014	-1.309353	0.799236
H	-3.906200	-1.410111	0.172577
H	-2.866998	-2.313147	1.221622
H	-3.305919	-0.717688	1.683306
Zn	-1.124502	-1.343638	-0.089690
C	0.360361	2.804026	-0.237113
H	0.792468	3.112407	-1.197622
H	-0.683338	3.129778	-0.216877
H	0.914229	3.335535	0.546261
C	-0.222126	-2.793361	-1.055654
H	-0.912289	-3.433497	-1.618644
H	0.517059	-2.401936	-1.767267
H	0.333005	-3.450093	-0.371283
C	-4.019880	2.445314	-0.035539
H	-3.716029	3.271482	0.624598
H	-4.091606	2.871660	-1.046603
H	-5.042992	2.173795	0.260030

RCa_Me_2MgZn_{THF1}

Atom	Coordinate (Å)		
	X	y	z
C	-3.549914	0.138758	-0.258237
C	-2.698190	1.192281	0.102631
C	-3.194292	2.479180	0.343134
C	-4.556221	2.707037	0.219922
C	-5.408954	1.664488	-0.137133
C	-4.909207	0.386472	-0.375693
H	-3.130992	-0.848657	-0.445274
H	-2.515692	3.279655	0.623262
H	-4.955583	3.700006	0.403985
H	-6.475527	1.850872	-0.230481
H	-5.581070	-0.419961	-0.654346
C	-1.308804	0.916714	0.234634
N	-0.188150	0.634038	0.341334
Mg	1.630642	-0.565518	0.708210
C	1.749357	-2.128938	-0.906768
H	2.793270	-2.145114	-0.544286
H	1.565525	-3.191007	-1.133869
H	1.774102	-1.620489	-1.880818
Zn	-0.261566	-2.233168	-0.158972
C	-0.559868	-2.177333	1.810063
H	-1.587823	-1.842549	2.012472
H	-0.472584	-3.187435	2.234669
H	0.087356	-1.545905	2.437203
C	-1.419971	-2.375268	-1.758058
H	-2.431307	-2.766867	-1.579185
H	-1.549913	-1.394751	-2.242317
H	-0.969120	-3.025645	-2.521690
O	2.699908	0.830858	-0.511593
C	2.535164	2.236144	-0.223330
C	4.087279	0.554144	-0.810045
C	3.781871	2.896407	-0.771078
H	1.602287	2.567740	-0.688567
H	2.456442	2.364845	0.867488
C	4.835677	1.833251	-0.487848
H	4.415005	-0.301475	-0.206853
H	4.158400	0.284803	-1.871848
H	3.989315	3.856757	-0.291587
H	3.683120	3.063439	-1.850816
H	5.116540	1.851888	0.572893
H	5.744754	1.943670	-1.084911
C	2.600536	-0.223665	2.559173
H	2.049427	0.528904	3.148122
H	2.708806	-1.093726	3.223944
H	3.615526	0.189107	2.428650

TSa_Me_2MgZn_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	-3.240486	0.022123	-0.656024
C	-2.538984	0.024624	0.549210
C	-3.085323	0.649974	1.675812
C	-4.333614	1.251708	1.595317
C	-5.030273	1.251065	0.389981
C	-4.479496	0.642638	-0.735182
H	-2.797717	-0.458457	-1.525154
H	-2.522748	0.650982	2.606147
H	-4.762021	1.725116	2.474832
H	-6.005829	1.726531	0.326693
H	-5.020213	0.647988	-1.677788
C	-1.199470	-0.536086	0.696359
N	-0.219298	-0.425997	1.377265
Mg	1.787413	-1.035414	1.142935
C	1.783851	-2.147973	-0.888136
H	1.762945	-3.049893	-0.255241
H	1.673738	-2.549032	-1.907229
O	2.436424	0.855942	0.529296
C	1.695755	2.097681	0.626465
C	3.569575	1.020534	-0.349358
H	0.634824	1.879749	0.464141
H	1.829155	2.490038	1.642591
C	2.307851	3.002457	-0.423786
C	3.752974	2.518218	-0.462426
H	4.418520	0.486445	0.091326
H	3.327185	0.569219	-1.323287
H	2.207137	4.060362	-0.167426
H	1.823039	2.833602	-1.394315
H	4.286058	2.803814	-1.372952
H	4.311633	2.900849	0.400616
H	2.820668	-1.772608	-0.892293
Zn	0.088308	-1.014118	-1.168724
C	-1.322326	-2.434922	-0.492845

H	-2.394457	-2.447620	-0.285563
H	-1.207294	-2.919137	-1.480372
H	-0.809415	-3.063288	0.244266
C	-0.129379	0.581258	-2.307990
H	-0.819433	0.409930	-3.145522
H	-0.537768	1.434281	-1.745974
H	0.820965	0.916329	-2.746846
C	3.067320	-1.936196	2.553654
H	4.128451	-1.814141	2.284223
H	2.959175	-1.501679	3.558935
H	2.911064	-3.019043	2.671155

PRa_Me_2MgZn_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	4.001671	0.810192	-0.139752
C	2.692375	0.320186	-0.184934
C	2.504627	-1.054196	-0.368704
C	3.586832	-1.915347	-0.487747
C	4.885373	-1.416129	-0.417975
C	5.088951	-0.051490	-0.243035
H	4.179478	1.875060	-0.006892
H	1.490317	-1.442017	-0.445893
H	3.418226	-2.978360	-0.643116
H	5.735078	-2.088575	-0.507597
H	6.099476	0.346667	-0.189963
C	1.504410	1.224450	-0.055275
N	0.381099	0.792401	0.353968
Mg	-0.566477	-0.717074	1.353487
C	-2.567602	0.667722	1.727384
H	-2.367638	-0.062851	2.530694
H	-2.934971	1.535150	2.295600
O	-1.377548	-1.701871	-0.316857
C	-1.287119	-1.222343	-1.674156
C	-2.620970	-2.429377	-0.157405
H	-0.653723	-0.328736	-1.666476
H	-0.809461	-1.995361	-2.293538
C	-2.726507	-0.996091	-2.071655
C	-3.402437	-2.216282	-1.450841
H	-2.389966	-3.480825	0.044000
H	-3.136793	-2.010661	0.715871
H	-2.863339	-0.931293	-3.154370
H	-3.095302	-0.066100	-1.617791
H	-4.469755	-2.071143	-1.264205
H	-3.292091	-3.083746	-2.111851
H	-3.447427	0.279054	1.193635
Zn	-1.407906	1.683844	0.383879
C	1.729914	2.667154	-0.439856
H	2.266479	2.760991	-1.391522
H	0.767475	3.182656	-0.510080
H	2.335156	3.180325	0.318879
C	-1.991901	2.959063	-0.994874
H	-1.686888	3.994040	-0.788471
H	-1.552710	2.698927	-1.969260
H	-3.081029	2.973428	-1.132332
C	-0.191486	-2.145308	2.863323
H	0.767225	-2.666006	2.713286
H	-0.162640	-1.744979	3.887503
H	-0.964343	-2.931151	2.865775

RCb_Me_2MgZn_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	-3.446312	0.204304	-0.406115
C	-2.831471	-0.790578	0.366905
C	-3.525080	-1.941921	0.759119
C	-4.846571	-2.093557	0.368985
C	-5.464166	-1.109796	-0.400686
C	-4.768727	0.033919	-0.786478
H	-2.880321	1.091892	-0.684168
H	-3.027646	-2.697627	1.360142
H	-5.398107	-2.980591	0.666219
H	-6.500670	-1.235932	-0.701943
H	-5.259512	0.796022	-1.384496
C	-1.474445	-0.600793	0.745512
N	-0.365966	-0.395209	1.018702
Mg	1.648598	0.373360	1.421137
C	2.025554	2.368316	0.568622
H	3.086742	2.057888	0.583238
H	2.008935	3.114398	-0.241769
H	1.862744	2.958412	1.483664
Zn	0.243312	1.849917	-0.575625
C	0.446589	0.601871	-2.102285
H	-0.510327	0.432266	-2.617555
H	1.148667	0.944017	-2.876952
H	0.800719	-0.388140	-1.779033
C	-1.193425	3.010606	0.150832
H	-1.977489	3.277812	-0.573006
H	-1.713891	2.554286	1.007214
H	-0.789781	3.963628	0.524127
O	2.613966	-0.905871	0.091699
C	3.494396	-0.524250	-0.989414
C	2.382887	-2.329519	0.075794
C	3.586368	-1.755444	-1.867516
H	3.058091	0.347498	-1.487950
H	4.467182	-0.250565	-0.558952
C	3.444502	-2.883822	-0.851343
H	2.442237	-2.694212	1.107091
H	1.369346	-2.512706	-0.310318
H	4.520673	-1.792614	-2.433842
H	2.750422	-1.772712	-2.578989
H	4.386238	-3.032005	-0.308721
H	3.150169	-3.838292	-1.295614
C	2.245267	-0.121303	3.387101
H	3.290599	0.154566	3.596778
H	1.646323	0.339423	4.186926
H	2.183962	-1.209312	3.554325

TSb_Me_2MgZn_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	3.282259	0.078847	-0.470822
C	2.276226	0.661103	0.300457
C	2.540509	1.818732	1.038488
C	3.802446	2.397170	0.989074
C	4.806381	1.812273	0.222928
C	4.547053	0.649404	-0.498956
H	3.065802	-0.828855	-1.029711
H	1.748251	2.254221	1.643495
H	4.003344	3.303914	1.553672
H	5.795075	2.262905	0.188419
H	5.333576	0.187984	-1.090191
C	0.943569	0.075689	0.437895
N	0.096500	-0.061360	1.281659
Mg	-1.866094	-0.797565	1.094665
C	-1.720841	-2.392837	-0.573615
H	-2.556468	-1.759290	-0.918714
H	-1.518595	-3.005321	-1.464713
H	-2.132101	-3.112049	0.149026
Zn	0.274376	-1.893234	-0.492481
C	0.376023	-0.111254	-1.667982
H	1.289621	0.282966	-2.114901

H	-0.097127	-0.766119	-2.422807
H	-0.334092	0.705154	-1.492511
C	1.745926	-3.137672	-0.076930
H	2.429802	-3.284634	-0.924192
H	2.360328	-2.772108	0.757437
H	1.380419	-4.132349	0.208957
O	-2.417083	0.884597	-0.041173
C	-3.192401	0.960040	-1.256858
C	-2.141807	2.210057	0.462886
C	-3.157261	2.423163	-1.651231
H	-2.734841	0.293704	-1.997304
H	-4.211386	0.611252	-1.040559
C	-3.087628	3.116686	-0.295543
H	-2.296626	2.199272	1.547507
H	-1.087510	2.448511	0.257262
H	-4.025505	2.713118	-2.248458
H	-2.252143	2.636156	-2.234654
H	-4.074699	3.125621	0.182535
H	-2.722148	4.145411	-0.349740
C	-3.307071	-1.214980	2.576979
H	-4.274199	-1.510125	2.140687
H	-3.029945	-2.022836	3.270112
H	-3.516128	-0.334491	3.204941

PRb_Me_2MgZn_{THF1}

Atom	Coordinate (Å)		
	x	y	z
C	2.248349	-2.207133	-0.475610
C	1.290557	-1.593564	0.338424
C	1.728067	-0.883309	1.461838
C	3.080124	-0.772157	1.755825
C	4.026092	-1.369168	0.923708
C	3.605909	-2.087155	-0.191428
H	1.936530	-2.771686	-1.352038
H	0.986598	-0.427876	2.117276
H	3.398144	-0.223431	2.639751
H	5.085993	-1.281240	1.149655
H	4.337501	-2.558811	-0.843194
C	-0.171261	-1.635900	0.006801
N	-0.952407	-0.708530	0.383772
Mg	-0.834987	1.279337	0.869886
C	-2.826174	1.750995	-0.350186
H	-2.013367	2.370190	-0.771023
H	-3.570244	1.767559	-1.157562
H	-3.279826	2.341082	0.459090
Zn	-2.837942	-0.293291	-0.096408
C	-0.631882	-2.800253	-0.837277
H	-0.232666	-3.757216	-0.480874
H	-1.725357	-2.837738	-0.840297
H	-0.294904	-2.680580	-1.876428
C	-4.305779	-1.598888	-0.132348
H	-4.363194	-2.116034	-1.100364
H	-4.167138	-2.382263	0.624924
H	-5.293180	-1.154483	0.045274
O	0.608146	1.828513	-0.546957
C	0.724595	1.238962	-1.861057
C	1.879416	2.383870	-0.135335
C	2.084548	1.671154	-2.373705
H	0.658585	0.146587	-1.755736
H	-0.117652	1.587945	-2.468582
C	2.891393	1.778680	-1.084225
H	1.825314	3.476934	-0.228201
H	2.040712	2.124244	0.917006
H	2.018691	2.648742	-2.866838
H	2.499734	0.954724	-3.087991
H	3.788149	2.396333	-1.182706
H	3.192541	0.782886	-0.730641
C	-0.424984	2.381488	2.625204
H	-0.170501	3.426718	2.385184
H	-1.228676	2.428762	3.374151
H	0.454189	1.971229	3.149243

RCa_Me_2MgZn_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	3.563046	-0.632776	-1.864198
C	4.807255	-1.237745	-1.772338
C	5.070709	-2.136357	-0.740708
C	4.095534	-2.437450	0.207465
C	2.844758	-1.843392	0.132398
C	2.586558	-0.942145	-0.909699
H	3.339352	0.071368	-2.660871
H	5.574611	-1.007955	-2.505688
H	6.048470	-2.606151	-0.674196
H	4.311547	-3.137168	1.009486
H	2.064120	-2.052627	0.862601
C	1.302840	-0.330425	-0.976052
N	0.248685	0.156009	-1.000986
Mg	-1.685232	0.966325	-0.132226
C	-1.856150	0.830897	2.115821
H	-2.913988	0.564371	1.951773
H	-1.805843	1.930653	2.168574
C	-0.520757	-2.403157	1.474862
H	0.126724	-3.100417	2.029627
H	-1.553737	-2.727999	1.669586
H	-0.344972	-2.608724	0.407617
H	-1.681906	0.525873	3.161135
Zn	-0.189058	-0.497695	1.946445
C	1.489114	0.286255	2.696577
H	1.319597	1.142155	3.368120
H	2.034217	-0.462568	3.292105
H	2.213019	0.636103	1.943043
O	-0.473080	2.806160	-0.071457
C	-0.177015	3.428463	-1.338041
C	0.576122	3.100434	0.869225
C	1.087959	4.241296	-1.113981
H	-0.017900	2.633593	-2.081423
H	-1.041894	4.023263	-1.649404
C	1.766926	3.472446	0.013912
H	0.259913	3.944768	1.500473
H	0.721795	2.218415	1.498998
H	0.839782	5.256161	-0.778872
H	1.692913	4.323628	-2.021312
H	2.513231	4.057792	0.558308
H	2.254724	2.565566	-0.372001
O	-2.435187	-1.031862	-0.528739
C	-3.711719	-1.394829	0.023948
C	-2.226357	-1.709366	-1.774942
C	-4.406237	-2.202811	-1.056272
H	-3.533935	-1.984117	0.935328
H	-4.250381	-0.477756	0.293936
C	-3.223992	-2.848410	-1.767823
H	-2.416578	-1.005731	-2.601797
H	-1.179815	-2.030033	-1.816922
H	-4.942109	-1.535108	-1.743745
H	-5.122497	-2.920309	-0.646764
H	-3.457224	-3.212855	-2.772038
H	-2.831966	-3.685815	-1.175225
C	-3.153211	1.860636	-1.400860
H	-2.754418	1.918903	-2.430235
H	-4.093131	1.288963	-1.488350
H	-3.444143	2.892898	-1.145790

TSa_Me_2MgZn_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	3.317358	0.204935	-1.383693
C	4.577475	-0.249487	-1.753028
C	5.104755	-1.395254	-1.164777
C	4.371298	-2.087314	-0.204285
C	3.119860	-1.628559	0.184255
C	2.589887	-0.480512	-0.406603
H	2.886121	1.089905	-1.846684
H	5.146657	0.290540	-2.505283
H	6.089428	-1.751507	-1.456846
H	4.778828	-2.987424	0.248524
H	2.536797	-2.159496	0.932774
C	1.252557	0.011557	-0.087668
N	0.254635	0.403578	-0.620195
Mg	-1.782721	0.827946	-0.166951
C	-1.740890	0.397646	2.170118
H	-2.763040	0.008037	2.042345
H	-1.798985	1.496779	2.111937
C	0.003874	-2.751524	1.573444
H	0.774935	-3.146817	2.250800
H	-0.933962	-3.260689	1.836676
H	0.270349	-3.100842	0.563697
H	-1.539095	0.236866	3.240178
Zn	-0.161502	-0.783567	1.620439
C	1.615140	0.336545	2.089907
H	1.062711	0.696866	2.975599
H	2.374956	-0.378199	2.423194
H	2.143953	1.216822	1.703614
O	-1.112213	2.905961	0.101736
C	-0.977928	3.605581	-1.155757
C	-0.066270	3.325763	1.000143
C	0.097619	4.651689	-0.928808
H	-0.671784	2.879975	-1.924313
H	-1.954950	4.013236	-1.433032
C	0.975927	3.974442	0.116244
H	-0.488428	4.043228	1.718766
H	0.291850	2.446798	1.544134
H	-0.338639	5.570768	-0.517985
H	0.625819	4.908251	-1.851180
H	1.623597	4.664777	0.663603
H	1.604573	3.203200	-0.350578
O	-2.017985	-1.339386	-0.508408
C	-3.204641	-2.013909	-0.055334
C	-1.523367	-1.957838	-1.709807
C	-3.625058	-2.897767	-1.212533
H	-2.947730	-2.598287	0.840495
H	-3.951525	-1.256749	0.212834
C	-2.277522	-3.267602	-1.819927
H	-1.736707	-1.289527	-2.559179
H	-0.437462	-2.070701	-1.614379
H	-4.220656	-2.319960	-1.931691
H	-4.215601	-3.759559	-0.889747
H	-2.341943	-3.628144	-2.850228
H	-1.785902	-4.039776	-1.213661
C	-3.475628	1.355086	-1.343929
H	-3.144803	1.579557	-2.373303
H	-4.233515	0.560968	-1.447222
H	-4.015668	2.254269	-1.006664

PRa_Me_2MgZn_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	-2.039026	-0.709980	1.702267
C	-3.212531	-0.477506	2.406142
C	-4.400929	-1.083483	2.001104
C	-4.396506	-1.936368	0.902556
C	-3.214474	-2.174229	0.205430
C	-2.022010	-1.547855	0.581808
H	-1.108451	-0.239825	2.020015
H	-3.200346	0.175493	3.276570
H	-5.323050	-0.899200	2.547067
H	-5.317350	-2.419218	0.583571
H	-3.231153	-2.839587	-0.655318
C	-0.760646	-1.704552	-0.216606
N	0.142769	-0.815151	-0.200925
Mg	0.440306	1.194407	0.192772
C	1.596726	1.283854	-2.126214
H	1.351418	2.235939	-1.620351
H	0.917152	1.258576	-2.989803
C	3.101446	-2.033328	-1.655668
H	2.926396	-2.605835	-2.576808
H	4.131024	-1.652319	-1.717117
H	3.087176	-2.766639	-0.835143
H	2.598211	1.483399	-2.533637
Zn	1.785517	-0.597530	-1.346390
C	-0.669438	-2.941862	-1.081636
H	0.357647	-3.055909	-1.442485
H	-0.974491	-3.851918	-0.550889
H	-1.325608	-2.847567	-1.958499
O	-1.324662	1.855692	-0.828056
C	-2.317527	2.588417	-0.073422
C	-1.954588	1.172426	-1.931389
C	-3.581498	2.528372	-0.908310
H	-2.451826	2.089350	0.896463
H	-1.939755	3.600238	0.103005
C	-3.433157	1.180769	-1.603893
H	-1.738758	1.728235	-2.855141
H	-1.514203	0.171818	-2.007674
H	-3.597042	3.340020	-1.646584
H	-4.483185	2.607076	-0.294352
H	-4.059334	1.074591	-2.494137
H	-3.671703	0.362505	-0.909816
O	2.503554	0.341616	0.677142
C	3.683025	1.176134	0.630048
C	2.604721	-0.593336	1.772413
C	4.473598	0.826297	1.876722
H	4.231032	0.931120	-0.290506
H	3.362180	2.223570	0.586704
C	4.080391	-0.629320	2.102084
H	2.004507	-0.212877	2.613451
H	2.182722	-1.544223	1.432428
H	4.143721	1.442212	2.723235
H	5.548099	0.977356	1.742392
H	4.277404	-0.985561	3.116778
H	4.605896	-1.283843	1.393845
C	0.416793	2.542639	1.835010
H	1.322957	2.483374	2.460729
H	0.313155	3.602833	1.552214
H	-0.430373	2.334892	2.511341

RCb_Me_2MgZn_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	4.290229	1.597639	-0.723821
C	5.676060	1.548178	-0.734427
C	6.332244	0.329928	-0.572468
C	5.609861	-0.848282	-0.398942
C	4.223321	-0.818388	-0.387245
C	3.569536	0.410468	-0.551090

H	3.762409	2.539262	-0.847649
H	6.247402	2.462044	-0.868922
H	7.418566	0.299026	-0.581504
H	6.129176	-1.793832	-0.272980
H	3.633991	-1.724485	-0.257097
C	2.145940	0.418920	-0.527379
N	0.987548	0.352042	-0.483377
Mg	-1.270948	-0.260972	-0.662172
C	-1.584102	-1.710321	1.022319
H	-2.407948	-2.112021	0.408197
H	-2.030624	-1.000720	1.737683
C	1.254190	-3.030498	-0.574103
H	2.131457	-3.629283	-0.285689
H	0.506144	-3.751867	-0.934629
H	1.557789	-2.451157	-1.459568
H	-1.307818	-2.571137	1.653097
Zn	0.564894	-1.883689	0.893462
C	1.268776	-1.161121	2.606604
H	0.467688	-0.787757	3.263959
H	1.817581	-1.908627	3.198054
H	1.968282	-0.321441	2.472019
O	-1.411556	1.617552	0.320918
C	-1.422285	2.780958	-0.530202
C	-0.779205	1.928516	1.581234
C	-1.102324	3.940856	0.389793
H	-0.649684	2.657799	-1.305006
H	-2.403161	2.835837	-1.015074
C	-0.141207	3.287796	1.376908
H	-1.560027	1.954647	2.355103
H	-0.067151	1.130717	1.821999
H	-2.008580	4.281503	0.906057
H	-0.672053	4.791052	-0.146059
H	-0.028510	3.841201	2.312954
H	0.851849	3.173797	0.921850
O	-3.476580	0.037018	-0.658247
C	-4.273827	-0.841301	-1.476915
C	-4.254179	0.503190	0.458244
C	-5.689839	-0.716393	-0.946621
H	-4.152720	-0.544082	-2.523175
H	-3.892396	-1.868140	-1.363906
C	-5.442158	-0.432949	0.529802
H	-3.621365	0.492992	1.351606
H	-4.564806	1.541135	0.265397
H	-6.283112	-1.616448	-1.129647
H	-6.202997	0.132689	-1.415548
H	-5.160850	-1.355983	1.054286
H	-6.298829	0.009718	1.045447
C	-1.198332	-0.427042	-2.787881
H	-1.714366	-1.310015	-3.199514
H	-1.688357	0.442761	-3.261687
H	-0.176368	-0.458645	-3.198439

TSb_Me$_2$MgZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.703554	1.608129	0.099557
C	-5.035756	1.994454	0.187356
C	-6.033618	1.030707	0.294432
C	-5.700573	-0.322204	0.308135
C	-4.373422	-0.715216	0.200505
C	-3.372411	0.251984	0.102762
H	-2.909406	2.349104	0.028487
H	-5.294220	3.050222	0.176529
H	-7.075127	1.333557	0.367249
H	-6.480227	-1.074251	0.397072
H	-4.098826	-1.768381	0.198430
C	-1.957206	-0.103452	0.062709
N	-0.932752	0.121107	0.643197
Mg	1.206915	-0.262946	0.731026
C	1.065267	-1.482544	-1.359852
H	2.072880	-1.729551	-0.995615
H	1.113841	-0.494762	-1.848151
C	-1.343210	-3.453140	0.699803
H	-2.102183	-4.081110	0.213169
H	-0.545788	-4.124947	1.043354
H	-1.812581	-3.044039	1.606675
H	0.918829	-2.181581	-2.195860
Zn	-0.692680	-2.000026	-0.461518
C	-2.016910	-1.101287	-1.904889
H	-1.468146	-1.773209	-2.587822
H	-3.070893	-1.385150	-1.941444
H	-1.906052	-0.095016	-2.329286
O	1.381583	1.743569	0.050655
C	1.790811	2.741075	1.010039
C	0.662292	2.365600	-1.033969
C	1.685479	4.052449	0.263581
H	1.104382	2.706471	1.869832
H	2.799328	2.483802	1.351431
C	0.455144	3.803963	-0.601169
H	1.284753	2.296424	-1.937818
H	-0.268417	1.809699	-1.197202
H	2.573187	4.203067	-0.364690
H	1.585965	4.909845	0.934086
H	0.368182	4.485609	-1.451272
H	-0.455366	3.891584	0.005769
O	3.371018	-0.131573	0.304184
C	4.249488	-1.144105	0.836348
C	3.967652	0.476624	-0.857433
C	5.587324	-0.893873	0.171477
H	4.252905	-1.053416	1.926236
H	3.847996	-2.135291	0.572654
C	5.154295	-0.401024	-1.203620
H	3.214729	0.529004	-1.651667
H	4.273581	1.501448	-0.599365
H	6.212006	-1.790632	0.140656
H	6.139049	-0.108537	0.703465
H	4.828604	-1.246988	-1.823525
H	5.933503	0.141293	-1.746055
C	1.461743	-1.099599	2.671402
H	1.828681	-2.139427	2.633083
H	2.172408	-0.563802	3.323266
H	0.511296	-1.139866	3.227415

PRb_Me$_2$MgZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	2.577168	-0.418885	1.368173
C	3.373894	-1.499329	1.727026
C	4.484121	-1.837513	0.955318
C	4.802474	-1.074212	-0.163873
C	4.017173	0.023088	-0.507013
C	2.884456	0.353848	0.243647
H	1.707592	-0.148484	1.967859
H	3.130240	-2.078855	2.615144
H	5.104117	-2.687060	1.231570
H	5.669268	-1.328857	-0.769393
H	4.281673	0.615216	-1.381270
C	1.989656	1.494278	-0.137853
N	0.737338	1.446275	0.066313
Mg	-0.850234	0.154416	0.413577
C	-2.147612	1.562599	-1.128041
H	-3.061268	1.367453	-0.550272

H	-1.944371	0.659839	-1.729223
C	-0.553390	4.731909	-0.260978
H	-0.114072	5.182480	-1.162260
H	-1.532304	5.206199	-0.116733
H	0.080545	5.046829	0.578702
H	-2.461614	2.290274	-1.889406
Zn	-0.652652	2.776200	-0.414544
C	2.675150	2.672615	-0.789986
H	1.981377	3.517409	-0.843172
H	3.580555	2.972884	-0.249046
H	2.984408	2.425578	-1.814437
O	0.041090	-1.502367	-0.534864
C	0.251104	-2.779159	0.109495
C	0.734172	-1.459892	-1.800411
C	0.799246	-3.672108	-0.982776
H	0.977468	-2.639184	0.923353
H	-0.705965	-3.101578	0.534302
C	1.624838	-2.685376	-1.801505
H	-0.017005	-1.499568	-2.603863
H	1.275997	-0.509343	-1.862188
H	-0.019544	-4.082662	-1.588832
H	1.383226	-4.505415	-0.583093
H	1.847070	-3.034986	-2.813220
H	2.573342	-2.462917	-1.293385
O	-2.575642	-1.144908	0.226902
C	-3.761230	-0.983193	1.043655
C	-2.908785	-1.865208	-0.976432
C	-4.818061	-1.851978	0.391503
H	-3.506398	-1.259681	2.069945
H	-4.044390	0.079556	1.031844
C	-4.416252	-1.785613	-1.076260
H	-2.382449	-1.404508	-1.819394
H	-2.561450	-2.904838	-0.875187
H	-5.829837	-1.487201	0.587183
H	-4.749371	-2.883602	0.758666
H	-4.712494	-0.822313	-1.512061
H	-4.838947	-2.587154	-1.687894
C	-1.082483	0.249557	2.528739
H	-2.054697	0.629452	2.764068
H	-0.972314	-0.730368	2.944082
H	-0.337108	0.897382	2.940612

RCc_Me$_2$MgZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	4.135627	0.502950	2.145554
C	5.517151	0.623057	2.134485
C	6.216971	0.526482	0.933712
C	5.543065	0.310091	-0.265980
C	4.161466	0.189847	-0.274550
C	3.463504	0.287044	0.937271
H	3.574767	0.571483	3.073228
H	6.051234	0.790110	3.065328
H	7.299799	0.619400	0.933591
H	6.096545	0.233815	-1.197384
H	3.608939	0.017311	-1.196671
C	2.046671	0.152017	0.901086
N	0.898920	0.021099	0.786094
Mg	-1.380682	-0.491961	0.483632
C	-1.507397	-1.858056	-1.291752
H	-2.221933	-1.197058	-1.805954
H	-2.101180	-2.566381	-0.689051
C	1.319689	-0.435846	-2.581656
H	2.299780	-0.716417	-2.996530
H	0.646129	-0.356482	-3.449498
H	1.434651	0.592609	-2.200208
H	-1.114425	-2.494167	-2.102431
Zn	0.644204	-1.689965	-1.191750
C	1.380316	-3.106993	-0.015951
H	1.319645	-4.119727	-0.439470
H	2.439666	-2.946454	0.235362
H	0.843119	-3.145788	0.944641
O	-1.320739	1.457384	-0.363248
C	-1.415981	1.687338	-1.786288
C	-0.767805	2.618960	0.267226
C	-0.665127	2.990514	-2.051923
H	-0.956164	0.826414	-2.284824
H	-2.477226	1.735983	-2.063353
C	0.159379	3.190492	-0.781382
H	-1.581831	3.318896	0.515675
H	-0.279299	2.296407	1.192452
H	-1.366616	3.823072	-2.180694
H	-0.050169	2.926173	-2.954446
H	0.422661	4.235555	-0.596829
H	1.083801	2.597950	-0.819054
O	-3.566789	-0.111395	0.156806
C	-4.472205	-1.200802	0.423484
C	-4.075210	1.095849	0.750245
C	-5.507954	-0.652833	1.388541
H	-4.918132	-1.516299	-0.529741
H	-3.899665	-2.039267	0.838356
C	-5.541548	0.822693	1.011037
H	-3.529177	1.288429	1.688701
H	-3.884092	1.923652	0.058767
H	-5.160630	-0.769154	2.423248
H	-6.474368	-1.155501	1.293553
H	-5.955232	1.466532	1.792199
H	-6.126656	0.972681	0.094884
C	-1.643264	-0.870608	2.567340
H	-2.617090	-1.302933	2.851986
H	-0.877349	-1.531719	3.004173
H	-1.563731	0.074588	3.134788

TSc_Me$_2$MgZn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.601677	0.804077	-1.677595
C	-4.931255	1.199509	-1.727806
C	-5.863663	0.616936	-0.873202
C	-5.463434	-0.362611	0.031561
C	-4.137195	-0.771629	0.076042
C	-3.201532	-0.193520	-0.780551
H	-2.856971	1.257054	-2.328380
H	-5.240237	1.966435	-2.433418
H	-6.904365	0.929160	-0.910757
H	-6.188696	-0.811895	0.704888
H	-3.809646	-1.533660	0.778473
C	-1.776671	-0.514122	-0.750637
N	-0.719326	-0.073562	-1.101866
Mg	1.402098	-0.425629	-0.728969
C	1.120435	-2.001368	1.048383
H	1.956838	-1.488170	1.542038
H	1.519604	-2.567506	0.188589
C	-1.590633	-0.142171	2.537901
H	-2.474543	-0.607107	2.996113
H	-0.896605	0.087832	3.358858
H	-1.931407	0.824279	2.134828
H	0.854699	-2.810414	1.745933
Zn	-0.779726	-1.265122	1.122883
C	-1.716262	-2.673795	-0.169728
H	-1.869352	-3.374332	0.670750
H	-2.612816	-2.761426	-0.789075

H	-0.859939	-3.021465	-0.761482
O	1.290325	1.527562	0.129141
C	1.233454	1.780065	1.549386
C	0.672950	2.620932	-0.564078
C	0.262848	2.947379	1.733192
H	0.881926	0.859400	2.031058
H	2.245632	2.005215	1.909999
C	-0.426741	3.062463	0.373815
H	1.422643	3.411900	-0.725803
H	0.322590	2.244276	-1.530486
H	0.808629	3.870151	1.961194
H	-0.440774	2.760463	2.550258
H	-0.793444	4.070402	0.161178
H	-1.266593	2.358128	0.298474
O	3.471865	-0.136046	0.085191
C	4.371417	-1.264613	0.095017
C	4.148381	1.013227	-0.464479
C	5.577223	-0.837023	-0.718032
H	4.636079	-1.484732	1.138612
H	3.848600	-2.131172	-0.325421
C	5.620879	0.660349	-0.443233
H	3.789022	1.174439	-1.493740
H	3.884044	1.889152	0.136666
H	5.397665	-1.021538	-1.785214
H	6.487580	-1.367287	-0.425268
H	6.195504	1.226658	-1.181381
H	6.047375	0.856128	0.548712
C	2.125572	-1.074767	-2.620594
H	3.104498	-1.581673	-2.583098
H	1.443699	-1.770034	-3.136627
H	2.258534	-0.230555	-3.319088

PRc_Me_2MgZn_{THF2}

Atom	Coordinate (Å)		
	x	y	z
C	2.367869	-2.036795	-0.445101
C	3.018261	-3.215185	-0.105334
C	4.350247	-3.188965	0.302701
C	5.024584	-1.974329	0.358053
C	4.373843	-0.795900	0.004962
C	3.032423	-0.805230	-0.394638
H	1.329649	-2.057775	-0.772371
H	2.484208	-4.161379	-0.164180
H	4.860070	-4.111261	0.571390
H	6.064666	-1.941347	0.674574
H	4.923427	0.141146	0.051900
C	2.301816	0.459649	-0.747015
N	1.034552	0.509856	-0.824280
Mg	-0.888976	-0.392303	-0.743192
C	-1.823373	1.622420	-1.797837
H	-2.707855	1.803374	-1.173074
H	-2.044413	0.727985	-2.405957
C	0.440882	3.904656	-0.150563
H	0.917145	4.597855	-0.858253
H	-0.426851	4.432627	0.268397
H	1.160347	3.772790	0.671407
H	-1.833155	2.419958	-2.555775
Zn	-0.031904	2.180668	-0.978935
C	3.180528	1.672528	-0.973450
H	2.570981	2.496673	-1.353279
H	3.647700	2.004530	-0.035646
H	3.992441	1.467711	-1.681829
O	-0.838250	0.209205	1.331403
C	-1.425625	1.393219	1.907352
C	0.225098	-0.240138	2.182205
C	-0.452985	1.868664	2.988329
H	-1.551789	2.121962	1.096399
H	-2.418182	1.144190	2.305224
C	0.807408	1.039783	2.736502
H	-0.197036	-0.878391	2.975262
H	0.915966	-0.829657	1.569286
H	-0.854883	1.656066	3.985460
H	-0.270575	2.945383	2.922374
H	1.405608	0.882910	3.638226
H	1.440085	1.510065	1.971710
O	-3.036107	-0.661017	-0.028805
C	-4.073378	-0.907870	-0.997313
C	-3.146330	-1.612920	1.047728
C	-4.656831	-2.259483	-0.637728
H	-4.820094	-0.104783	-0.920324
H	-3.628289	-0.877236	-1.998287
C	-4.504249	-2.264251	0.877544
H	-2.332237	-2.349054	0.949586
H	-3.018690	-1.081213	1.996988
H	-4.052174	-3.060618	-1.082748
H	-5.689318	-2.375078	-0.978897
H	-4.545631	-3.262818	1.321400
H	-5.285351	-1.649405	1.342431
C	-0.978535	-2.313335	-1.678173
H	-0.885263	-3.134916	-0.945096
H	-1.942317	-2.486638	-2.186858
H	-0.200302	-2.509673	-2.433242

RC_$MgCl_2Zn$

Atom	Coordinate (Å)		
	x	y	z
C	-3.057270	-0.517845	-0.657811
C	-2.596832	0.653400	-0.039202
C	-3.480846	1.562159	0.557035
C	-4.839072	1.289559	0.528005
C	-5.304591	0.129282	-0.087414
C	-4.419720	-0.771145	-0.677118
H	-2.345418	-1.203506	-1.113047
H	-3.098552	2.461969	1.029810
H	-5.537812	1.983721	0.984957
H	-6.371536	-0.075380	-0.108127
H	-4.793920	-1.671559	-1.154639
C	-1.201860	0.909785	-0.032188
N	-0.056945	1.089006	-0.045188
Mg	2.063538	1.208762	-0.155214
Cl	2.661448	3.420487	-0.117419
Zn	0.986062	-1.887609	0.289650
C	1.211337	-1.601997	2.186758
H	0.364808	-1.977699	2.774849
H	2.113052	-2.099433	2.566003
H	1.317453	-0.536501	2.437932
C	0.338826	-2.180064	-1.506995
H	-0.577112	-2.784795	-1.544455
H	0.119367	-1.232162	-2.018930
H	1.079874	-2.696663	-2.130333
Cl	3.449390	-0.626765	-0.462643

TS_$MgCl_2Zn$

Atom	Coordinate (Å)		
	x	y	z
C	-2.899941	-0.200094	0.330119
C	-1.967844	0.815880	0.119682
C	-2.402689	2.092407	-0.252240
C	-3.760016	2.348468	-0.388380
C	-4.687023	1.330978	-0.177558
C	-4.255093	0.055379	0.174403
H	-2.559956	-1.195386	0.606609

H	-1.665765	2.874306	-0.417178
H	-4.096461	3.345774	-0.658807
H	-5.749552	1.532734	-0.286260
H	-4.975552	-0.742470	0.332526
C	-0.520371	0.607653	0.241082
N	0.487645	1.154025	-0.132076
Mg	2.522102	0.919519	-0.158613
Cl	4.504131	2.096339	-0.138087
Zn	0.025696	-1.599768	0.017439
C	-0.299497	-0.673856	1.859262
H	-0.936193	0.059625	2.358286
H	-0.685873	-1.644749	2.220647
H	0.726767	-0.531178	2.212607
C	-0.816467	-2.516151	-1.469368
H	-1.207414	-1.788634	-2.191653
H	-0.116870	-3.169394	-2.001823
H	-1.662944	-3.130667	-1.141584
Cl	2.444918	-1.501827	0.058636
C	-2.899941	-0.200094	0.330119
C	-1.967844	0.815880	0.119682
C	-2.402689	2.092407	-0.252240

PR_$MgCl_2Zn$

Atom	Coordinate (Å)		
	x	y	z
C	-2.854750	1.827036	0.522546
C	-1.892084	0.994700	-0.058998
C	-2.325308	-0.129661	-0.770030
C	-3.675712	-0.430390	-0.880587
C	-4.620983	0.390481	-0.272731
C	-4.206689	1.518951	0.428184
H	-2.548583	2.713058	1.073444
H	-1.597218	-0.760576	-1.273962
H	-3.989717	-1.302251	-1.448965
H	-5.679373	0.156671	-0.354093
H	-4.940436	2.165693	0.902323
C	-0.434363	1.290982	0.060626
N	0.452914	0.368364	0.112678
Mg	2.502119	0.425915	0.045911
Cl	3.902118	2.238171	-0.182136
Zn	0.077760	-1.499620	0.225905
C	-0.071042	2.750035	0.117617
H	-0.366890	3.175190	1.085048
H	1.007065	2.900126	0.005349
H	-0.598812	3.322248	-0.653269
C	-0.868052	-3.158953	0.399387
H	-0.259054	-3.950250	0.849066
H	-1.766410	-3.036569	1.016180
H	-1.199364	-3.516182	-0.583324
Cl	2.692239	-1.937417	-0.171436
C	-2.854750	1.827036	0.522546
C	-1.892084	0.994700	-0.058998
C	-2.325308	-0.129661	-0.770030

RCa_$MgCl_2Zn_{THF1}$

Atom	Coordinate (Å)		
	X	y	z
C	-3.488225	0.572825	-0.018647
C	-2.557548	1.617328	0.074795
C	-2.962808	2.956978	0.093752
C	-4.316304	3.246087	0.015805
C	-5.247079	2.213250	-0.077904
C	-4.836408	0.882058	-0.095044
H	-3.131370	-0.454765	-0.035722
H	-2.222985	3.748338	0.168950
H	-4.648222	4.279872	0.028788
H	-6.306101	2.449254	-0.137962
H	-5.568981	0.083960	-0.168263
C	-1.183393	1.265693	0.157854
N	-0.082732	0.905275	0.223235
Mg	1.629051	-0.352321	0.534538
Zn	-1.364014	-2.299029	-0.202725
C	-1.327796	-2.359886	1.733018
H	-1.850100	-1.498693	2.173359
H	-1.815977	-3.255597	2.137956
H	-0.306799	-2.353281	2.138605
C	-1.949177	-1.966529	-2.015967
H	-3.039092	-2.000430	-2.142681
H	-1.622220	-0.971719	-2.351885
H	-1.519784	-2.685215	-2.725716
O	2.863255	0.750833	-0.680912
C	2.942991	2.192230	-0.520886
C	4.154212	0.228479	-1.087108
C	4.311317	2.575135	-1.048739
H	2.107183	2.639702	-1.066883
H	2.838529	2.418573	0.549424
C	5.132131	1.328199	-0.741572
H	4.329773	-0.713880	-0.557136
H	4.117341	0.025940	-2.164978
H	4.695919	3.479684	-0.570854
H	4.271938	2.748612	-2.130928
H	5.383644	1.286694	0.325924
H	6.057240	1.259742	-1.319612
Cl	2.485909	0.060953	2.639178
Cl	1.351944	-2.304644	-0.722388

TSa_$MgCl_2Zn_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.494061	-0.360313	-0.179597
C	-2.511313	-0.140582	0.785308
C	-2.760476	0.746564	1.839366
C	-3.988418	1.385304	1.933785
C	-4.968204	1.158946	0.969937
C	-4.717322	0.290754	-0.088285
H	-3.296943	-1.037084	-1.007795
H	-1.980708	0.917052	2.577768
H	-4.181509	2.063743	2.760605
H	-5.928899	1.662184	1.043348
H	-5.477495	0.118040	-0.845226
C	-1.172402	-0.740968	0.727957
N	-0.114063	-0.559335	1.276608
Mg	1.919460	-0.651644	1.001816
Cl	3.538859	-1.015511	2.601944
O	2.044596	1.216015	0.157262
C	1.144324	2.326881	0.398068
C	2.940494	1.524124	-0.939437
H	0.128874	1.926945	0.500770
H	1.438295	2.803094	1.341909
C	1.339320	3.244961	-0.790523
C	2.808246	3.019097	-1.131252
H	3.943357	1.184570	-0.659328
H	2.605737	0.962334	-1.822440
H	1.100749	4.284651	-0.552002
H	0.700923	2.924719	-1.624552
H	3.072696	3.329091	-2.145523
H	3.454477	3.555735	-0.426036
Zn	-0.447897	-1.027550	-1.393544
C	-1.371433	-2.533307	-0.277888
H	-2.222255	-2.706247	0.384596
H	-1.701911	-2.947002	-1.250363
H	-0.519247	-3.110386	0.091984

C	-0.738807	0.544771	-2.495640
H	-1.512960	0.383629	-3.254840
H	-1.073090	1.384700	-1.871220
H	0.174522	0.855589	-3.017883
Cl	1.817656	-1.838564	-1.139849

PRa_$MgCl_2Zn_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.911316	1.169672	-0.025995
C	-2.655818	0.682700	0.352821
C	-2.577250	-0.584373	0.940046
C	-3.716609	-1.357537	1.120854
C	-4.955985	-0.874106	0.711747
C	-5.050191	0.390154	0.137965
H	-3.999864	2.156153	-0.475742
H	-1.614225	-0.953517	1.291916
H	-3.637529	-2.335663	1.588257
H	-5.848671	-1.479472	0.846923
H	-6.016107	0.773052	-0.181583
C	-1.419069	1.492256	0.153989
N	-0.308951	0.937241	-0.153145
Mg	0.235475	-0.921777	-0.869224
Cl	-0.836353	-2.640621	-1.994116
O	1.162075	-1.699503	0.814416
C	1.415464	-0.903153	1.994129
C	2.288423	-2.600992	0.612034
H	0.862300	0.036406	1.885605
H	1.035964	-1.442885	2.872850
C	2.918891	-0.769216	2.016488
C	3.347997	-2.180836	1.625254
H	1.935559	-3.628396	0.743618
H	2.627893	-2.466841	-0.422351
H	3.302943	-0.454074	2.990293
H	3.235697	-0.037252	1.260232
H	4.354319	-2.222918	1.201019
H	3.323667	-2.837778	2.502311
Zn	1.375427	1.845429	-0.327594
C	-1.576908	2.979104	0.333168
H	-2.217383	3.222773	1.187329
H	-0.601684	3.457964	0.464929
H	-2.045302	3.419697	-0.556238
C	2.805997	2.927706	0.381053
H	2.667813	4.000198	0.204319
H	2.894356	2.787766	1.465648
H	3.766147	2.640497	-0.063441
Cl	2.205171	0.044727	-1.894826

RCb_$MgCl_2Zn_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	3.190540	-0.170195	0.379529
C	2.616167	-1.277886	-0.259543
C	3.350955	-2.445497	-0.495959
C	4.674430	-2.495859	-0.086304
C	5.252049	-1.398017	0.548414
C	4.514579	-0.239221	0.780917
H	2.586491	0.721215	0.533645
H	2.885299	-3.291114	-0.993242
H	5.259411	-3.393416	-0.263102
H	6.290601	-1.445966	0.864546
H	4.973522	0.612340	1.274179
C	1.256327	-1.173168	-0.659773
N	0.146226	-1.013668	-0.954640
Mg	-1.858682	-0.303466	-1.252203
Zn	0.724624	2.251813	0.240738
C	0.112439	1.486569	1.911382
H	0.919923	1.333503	2.638942
H	-0.648391	2.104173	2.407643
H	-0.348227	0.504132	1.728527
C	1.856959	2.772535	-1.238100
H	2.889982	3.000108	-0.945118
H	1.908724	1.962181	-1.979767
H	1.469897	3.650267	-1.770910
O	-2.479943	-0.718534	0.654038
C	-3.193623	0.198519	1.524344
C	-2.223974	-1.968403	1.340057
C	-3.074269	-0.416096	2.901717
H	-2.725345	1.182634	1.422468
H	-4.235025	0.251964	1.182198
C	-3.081178	-1.908168	2.586831
H	-2.470238	-2.788065	0.656820
H	-1.152848	-2.010712	1.582490
H	-3.887339	-0.107236	3.563687
H	-2.121191	-0.123043	3.361236
H	-4.100038	-2.249855	2.368367
H	-2.677347	-2.526175	3.392920
Cl	-2.912279	-1.693660	-2.768759
Cl	-1.613889	2.032103	-1.182542

TSb_$MgCl_2Zn_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	3.412247	0.507310	-0.633502
C	2.454104	0.857286	0.317440
C	2.805030	1.700262	1.377799
C	4.096029	2.200946	1.467769
C	5.048972	1.849537	0.514966
C	4.707088	0.997791	-0.531377
H	3.143306	-0.156775	-1.451847
H	2.051168	1.958152	2.117256
H	4.360554	2.867194	2.284619
H	6.060641	2.240447	0.587927
H	5.449994	0.716164	-1.272687
C	1.074917	0.351505	0.294734
N	0.148054	0.294743	1.066717
Mg	-1.780384	-0.433670	1.086404
Zn	0.945597	-1.677721	-0.708558
C	0.588813	0.139901	-1.698790
H	1.029744	1.130630	-1.830594
H	0.897603	-0.411254	-2.607621
H	-0.501859	0.237109	-1.689422
C	2.348768	-2.936433	-0.251294
H	3.138900	-2.953696	-1.011055
H	2.819391	-2.653931	0.698441
H	1.968893	-3.957919	-0.142258
O	-2.561688	0.882588	-0.282470
C	-3.523999	0.577924	-1.319936
C	-2.256157	2.299509	-0.275426
C	-3.495899	1.791717	-2.222390
H	-3.211860	-0.356440	-1.798460
H	-4.506288	0.433464	-0.851007
C	-3.265606	2.918701	-1.221016
H	-2.321143	2.657880	0.757634
H	-1.225170	2.423793	-0.634170
H	-4.417598	1.901795	-2.799249
H	-2.654512	1.722971	-2.924005
H	-4.196008	3.153728	-0.690569
H	-2.890002	3.837588	-1.678323
Cl	-3.141423	-0.508688	2.943922
Cl	-1.359034	-2.309833	-0.412500

PRb_$MgCl_2Zn_{THF1}$

Atom	Coordinate (Å)		
	x	y	z
C	-2.096837	2.502684	-0.422074
C	-1.193930	1.763592	0.350734
C	-1.687600	0.999174	1.413208
C	-3.048714	0.958570	1.687355
C	-3.940992	1.678446	0.895736
C	-3.461662	2.448352	-0.160427
H	-1.736723	3.112117	-1.248335
H	-0.991176	0.451466	2.047653
H	-3.411665	0.369820	2.526769
H	-5.006736	1.647162	1.108016
H	-4.152500	3.014562	-0.779996
C	0.270527	1.775069	0.064008
N	0.985476	0.735026	0.263220
Mg	0.542880	-1.278545	0.452422
Zn	2.860393	0.655380	-0.081774
C	0.825906	3.064983	-0.477035
H	0.479623	3.932076	0.095904
H	1.919722	3.036801	-0.470199
H	0.503519	3.216344	-1.515060
C	4.729412	1.094391	-0.092888
H	4.906869	2.175704	-0.104836
H	5.229425	0.690475	0.794671
H	5.229177	0.669590	-0.970822
O	-1.121264	-1.565996	-0.699646
C	-1.288511	-0.975953	-2.012852
C	-2.385522	-2.099311	-0.225051
C	-2.646330	-1.454562	-2.479883
H	-1.262941	0.118185	-1.901632
H	-0.448648	-1.297798	-2.636461
C	-3.418403	-1.521839	-1.167478
H	-2.333549	-3.193904	-0.279326
H	-2.510573	-1.798121	0.820256
H	-2.568242	-2.450886	-2.931702
H	-3.090662	-0.777321	-3.213874
H	-4.319641	-2.138083	-1.220353
H	-3.704069	-0.512759	-0.838279
Cl	0.055951	-2.253007	2.494758
Cl	2.477588	-1.782467	-0.891448

RCa_$MgCl_2Zn_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	3.439809	0.236072	-2.437629
C	4.781901	-0.097010	-2.538939
C	5.412127	-0.782220	-1.502158
C	4.708763	-1.140597	-0.354363
C	3.366885	-0.816763	-0.235352
C	2.738876	-0.127451	-1.281978
H	2.933018	0.769347	-3.236650
H	5.339938	0.178444	-3.428854
H	6.464475	-1.038784	-1.589567
H	5.207868	-1.672620	0.450012
H	2.788864	-1.069828	0.651073
C	1.358540	0.186075	-1.134620
N	0.233837	0.402997	-0.949596
Mg	-1.798757	0.524244	-0.110564
Cl	-3.717661	0.969800	-1.411277
C	0.547474	-2.730193	1.476941
H	1.439156	-3.364700	1.390465
H	-0.181698	-3.283445	2.084047
H	0.109634	-2.636976	0.472322
Zn	0.913004	-0.975371	2.208881
C	1.915291	0.603001	2.729393
H	1.374893	1.219672	3.459107
H	2.887187	0.355972	3.177194
H	2.134095	1.254002	1.869263
O	-1.310238	2.582253	0.104648
C	-1.265790	3.436103	-1.063096
C	-0.367681	3.059423	1.092527
C	-0.363471	4.595469	-0.683653
H	-0.844785	2.854358	-1.896590
H	-2.290025	3.719733	-1.320863
C	0.581970	3.946137	0.319579
H	-0.922011	3.621903	1.856290
H	0.098504	2.192265	1.568435
H	-0.942139	5.390482	-0.197469
H	0.141435	5.025377	-1.552970
H	1.102965	4.661823	0.961315
H	1.334155	3.333837	-0.197565
O	-1.880057	-1.535116	-0.578333
C	-2.890231	-2.363696	0.040700
C	-1.547683	-2.054792	-1.882724
C	-3.429304	-3.224248	-1.081623
H	-2.404500	-2.958486	0.826718
H	-3.638632	-1.710495	0.501011
C	-2.183430	-3.429008	-1.933809
H	-1.967789	-1.378279	-2.641570
H	-0.456329	-2.068380	-1.977100
H	-4.192087	-2.673656	-1.647181
H	-3.871625	-4.155510	-0.717688
H	-2.395260	-3.751250	-2.956807
H	-1.520979	-4.170139	-1.467494
Cl	-1.604229	0.050768	2.227921

TSa_$MgCl_2Zn_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	3.078325	1.097422	-1.602054
C	4.334963	1.012968	-2.186715
C	5.279021	0.121954	-1.683263
C	4.966449	-0.682390	-0.590903
C	3.718567	-0.586408	0.011227
C	2.770131	0.303199	-0.493684
H	2.323969	1.778075	-1.991245
H	4.576727	1.640855	-3.040329
H	6.260674	0.052826	-2.144986
H	5.698997	-1.385507	-0.203631
H	3.469592	-1.216106	0.862984
C	1.405943	0.395785	0.040179
N	0.298040	0.523863	-0.416541
Mg	-1.764042	0.355028	-0.153209
Cl	-3.527559	0.376544	-1.708424
C	1.059525	-2.892807	1.400174
H	1.900220	-3.241444	2.011876
H	0.192036	-3.516623	1.646028
H	1.321605	-3.089061	0.351387
Zn	0.677363	-1.005690	1.656805
C	1.789383	0.735900	2.047297
H	1.146606	0.767838	2.944770
H	2.797346	0.425053	2.332628
H	1.838507	1.777648	1.715808
O	-1.845830	2.448043	0.173055
C	-1.885007	3.304324	-0.998008
C	-1.053200	3.080223	1.203520
C	-1.218301	4.598878	-0.574507
H	-1.323547	2.811151	-1.804979
H	-2.926824	3.406536	-1.312966
C	-0.224615	4.111909	0.472954
H	-1.734461	3.545345	1.929046

H	-0.476043	2.303938	1.714205
H	-1.948006	5.278521	-0.117320
H	-0.753094	5.115534	-1.418198
H	0.143683	4.901254	1.133736
H	0.636978	3.630174	-0.011580
O	-1.433580	-1.731612	-0.483613
C	-2.427583	-2.691647	-0.058139
C	-0.793072	-2.189888	-1.695365
C	-2.582005	-3.645368	-1.224592
H	-2.050003	-3.191692	0.844342
H	-3.347228	-2.151703	0.193365
C	-1.176079	-3.649952	-1.811628
H	-1.181492	-1.597702	-2.537203
H	0.283394	-2.009940	-1.598448
H	-3.296461	-3.238095	-1.951301
H	-2.931848	-4.632666	-0.911031
H	-1.131480	-4.010266	-2.842857
H	-0.507074	-4.268569	-1.199112
Cl	-1.545429	-0.254082	2.261405

PRa_MgCl$_2$Zn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	2.056242	0.299437	1.835452
C	3.245839	-0.181098	2.367175
C	4.448650	0.457461	2.072938
C	4.448621	1.589906	1.264152
C	3.253274	2.078100	0.745043
C	2.043998	1.425372	1.006243
H	1.114559	-0.190929	2.080147
H	3.233026	-1.053742	3.016238
H	5.381902	0.079839	2.483259
H	5.382682	2.097622	1.036417
H	3.270173	2.961876	0.110583
C	0.760292	1.886339	0.397661
N	-0.150922	1.048917	0.094871
Mg	-0.316008	-0.997561	-0.304864
Cl	-0.326669	-2.934028	1.023318
C	-3.525389	2.361682	-0.992941
H	-3.408208	3.422527	-1.240271
H	-4.085782	1.896184	-1.813030
H	-4.155311	2.304872	-0.095206
Zn	-1.848572	1.451895	-0.698289
C	0.637606	3.366291	0.144406
H	-0.391420	3.612763	-0.135708
H	0.933772	3.960134	1.016512
H	1.289325	3.668272	-0.685889
O	1.583546	-1.269984	-1.137547
C	2.564386	-2.255880	-0.734860
C	2.176841	-0.328040	-2.059183
C	3.724982	-2.062466	-1.688160
H	2.853709	-2.045608	0.304711
H	2.093656	-3.241671	-0.778145
C	3.668009	-0.561993	-1.945950
H	1.796551	-0.543932	-3.066439
H	1.857749	0.680544	-1.770636
H	3.555985	-2.617526	-2.619414
H	4.672144	-2.397143	-1.256349
H	4.207244	-0.248099	-2.843859
H	4.072198	-0.010725	-1.085148
O	-2.394451	-0.449471	0.499846
C	-3.570498	-1.198383	0.082603
C	-2.473130	-0.183991	1.926051
C	-4.254865	-1.611110	1.368002
H	-4.192964	-0.525669	-0.523020
H	-3.237582	-2.032005	-0.542540
C	-3.916403	-0.448422	2.292500
H	-1.790152	-0.877397	2.436322
H	-2.137985	0.844366	2.098776
H	-3.815494	-2.540730	1.750687
H	-5.328462	-1.766269	1.231692
H	-4.037087	-0.681704	3.353713
H	-4.538977	0.424544	2.057212
Cl	-1.410567	-0.486709	-2.432898

RCb_MgCl$_2$Zn$_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.952609	1.794993	0.606977
C	-5.335699	1.890223	0.626247
C	-6.112162	0.740240	0.750724
C	-5.514067	-0.513172	0.857927
C	-4.132229	-0.627774	0.841026
C	-3.356665	0.532340	0.715543
H	-3.331389	2.681880	0.513745
H	-5.810360	2.863518	0.544010
H	-7.195678	0.822143	0.765172
H	-6.126981	-1.404179	0.956765
H	-3.642420	-1.595758	0.925821
C	-1.937963	0.417115	0.688207
N	-0.783015	0.316150	0.664138
Mg	1.432904	0.017933	0.700074
C	-1.526461	-3.204920	0.479915
H	-2.532901	-3.618774	0.629479
H	-0.839155	-4.060934	0.456141
H	-1.272524	-2.639513	1.389009
Zn	-1.333776	-2.095621	-1.092914
C	-1.725586	-0.944982	-2.601601
H	-0.889130	-0.894301	-3.311462
H	-2.602697	-1.275233	-3.172975
H	-1.935782	0.088800	-2.289465
O	1.381635	1.753175	-0.465293
C	1.215749	3.041762	0.169227
C	0.800937	1.774175	-1.791464
C	0.700611	3.959617	-0.922701
H	0.484616	2.931684	0.984248
H	2.180834	3.336992	0.595298
C	-0.091956	2.994153	-1.797452
H	1.618591	1.863337	-2.520766
H	0.281437	0.823904	-1.954857
H	1.535410	4.387735	-1.490832
H	0.102808	4.782258	-0.521994
H	-0.278776	3.369515	-2.806925
H	-1.059010	2.755795	-1.333451
Cl	1.473659	-0.130673	3.049831
O	3.528802	0.194263	0.544103
C	4.383387	-0.697531	1.297846
C	4.144538	0.505061	-0.727708
C	5.740622	-0.575071	0.641694
H	4.342245	-0.390264	2.345891
H	3.983730	-1.719409	1.212095
C	5.353330	-0.405127	-0.821813
H	3.410888	0.332267	-1.522104
H	4.418750	1.568593	-0.718804
H	6.372665	-1.447217	0.829150
H	6.264571	0.316377	1.008889
H	5.061472	-1.372916	-1.249670
H	6.146201	0.019864	-1.443284
Cl	1.373751	-1.737087	-0.919689

TSb_MgCl$_2$Zn$_{THF2}$

Atom	Coordinate (Å)

	x	y	z
C	-3.557915	1.800451	0.533040
C	-4.840688	2.274740	0.772840
C	-5.942461	1.462027	0.520834
C	-5.758072	0.174507	0.024885
C	-4.477686	-0.294226	-0.239464
C	-3.370724	0.516032	0.013821
H	-2.686784	2.417767	0.741672
H	-4.980709	3.280154	1.161452
H	-6.946573	1.831987	0.712148
H	-6.615640	-0.465975	-0.163587
H	-4.336309	-1.297887	-0.635115
C	-1.982336	0.066541	-0.172495
N	-0.937618	0.255139	0.405527
Mg	1.138589	-0.033872	0.644478
C	-1.812378	-3.427944	0.685327
H	-1.737201	-4.427507	0.243583
H	-1.129936	-3.394782	1.543476
H	-2.830953	-3.309406	1.072573
Zn	-1.341131	-2.024562	-0.565351
C	-2.021004	-0.709390	-2.060022
H	-1.582039	-1.551122	-2.627795
H	-3.067990	-0.632985	-2.348698
H	-1.463755	0.168899	-2.398410
O	1.398499	1.961527	0.066002
C	2.291119	2.899509	0.704668
C	0.742361	2.581797	-1.062684
C	2.545705	3.950910	-0.352854
H	1.788934	3.319517	1.586675
H	3.176124	2.343219	1.030513
C	1.183190	4.034462	-1.032520
H	1.076881	2.063946	-1.973341
H	-0.339005	2.440957	-0.955768
H	3.308699	3.603112	-1.061661
H	2.879058	4.900713	0.073135
H	1.220241	4.474175	-2.032503
H	0.492804	4.630170	-0.423439
Cl	1.248540	-0.711545	2.890683
O	3.238155	-0.134017	0.338361
C	4.016169	-1.208582	0.925131
C	3.809703	0.242812	-0.933612
C	5.289565	-1.261352	0.108284
H	4.155621	-0.982092	1.985082
H	3.438006	-2.138893	0.835899
C	4.786410	-0.862808	-1.273378
H	2.998697	0.355838	-1.662041
H	4.318015	1.210482	-0.810384
H	5.755845	-2.249715	0.136548
H	6.016577	-0.527598	0.478444
H	4.255006	-1.700730	-1.742136
H	5.575641	-0.527981	-1.951755
Cl	0.980633	-1.790448	-1.163165

PRb_$MgCl_2Zn_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	2.550019	-0.443066	1.368881
C	3.362718	-1.519651	1.704121
C	4.461874	-1.840923	0.911396
C	4.754509	-1.066156	-0.207470
C	3.954703	0.026403	-0.528114
C	2.831511	0.339761	0.245506
H	1.693151	-0.187912	1.992795
H	3.139343	-2.107268	2.591949
H	5.095015	-2.686014	1.170500
H	5.613338	-1.307103	-0.829353
H	4.199345	0.627354	-1.401913
C	1.947990	1.497293	-0.091571
N	0.681701	1.444193	0.066246
Mg	-0.789049	-0.036517	0.462198
C	-0.770912	4.876412	-0.273066
H	0.139827	5.471049	-0.413410
H	-1.470281	5.160265	-1.068049
H	-1.217955	5.187452	0.678349
Zn	-0.408694	2.983063	-0.277290
C	2.668573	2.710218	-0.627210
H	1.992458	3.570467	-0.656852
H	3.548537	2.960517	-0.024198
H	3.022153	2.529877	-1.650544
O	0.217374	-1.578878	-0.538095
C	0.413401	-2.911700	-0.012029
C	0.808883	-1.464467	-1.848567
C	0.923798	-3.722011	-1.186195
H	1.155638	-2.850515	0.795801
H	-0.540721	-3.253548	0.403430
C	1.707099	-2.676354	-1.972084
H	0.001171	-1.473732	-2.596094
H	1.334778	-0.504911	-1.901842
H	0.086330	-4.102117	-1.786005
H	1.529831	-4.574032	-0.867000
H	1.888676	-2.955953	-3.013193
H	2.673799	-2.476270	-1.489270
Cl	-0.889696	-0.033217	2.832739
O	-2.403611	-1.440660	0.297602
C	-3.571283	-1.337473	1.143549
C	-2.786433	-1.935018	-1.004869
C	-4.613547	-2.200968	0.467835
H	-3.283455	-1.655482	2.148729
H	-3.884181	-0.283447	1.181181
C	-4.302674	-1.952717	-1.002813
H	-2.362458	-1.274691	-1.770270
H	-2.363606	-2.943005	-1.126977
H	-5.631745	-1.922928	0.752902
H	-4.460351	-3.257481	0.721927
H	-4.690467	-0.973664	-1.311430
H	-4.709957	-2.712176	-1.675749
Cl	-2.292198	1.486807	-0.900189

RCc_$MgCl_2Zn_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.852981	-1.104284	-1.993817
C	-5.228837	-1.054850	-2.159068
C	-5.973235	-0.065375	-1.520885
C	-5.350620	0.881928	-0.711043
C	-3.975827	0.848225	-0.534533
C	-3.231689	-0.146373	-1.183477
H	-3.256269	-1.871702	-2.478570
H	-5.723025	-1.791672	-2.785276
H	-7.051327	-0.033781	-1.653776
H	-5.939339	1.647300	-0.214071
H	-3.471169	1.570674	0.103325
C	-1.821964	-0.198327	-0.991684
N	-0.672750	-0.232789	-0.839427
Mg	1.471175	-0.460832	-0.322304
C	-1.657934	1.310921	2.248843
H	-2.635167	1.749013	2.491955
H	-0.972743	1.613806	3.052919
H	-1.301699	1.811863	1.336162
Zn	-1.720320	-0.612940	2.009467
C	-2.375053	-2.388148	1.610980
H	-2.139332	-3.113525	2.400371

H	-3.461286	-2.427888	1.455256
H	-1.906238	-2.768655	0.692510
O	1.507492	1.618972	-0.305801
C	1.550589	2.388422	0.919224
C	1.103286	2.475492	-1.384492
C	0.822757	3.698120	0.614643
H	1.058400	1.786773	1.691933
H	2.600340	2.538257	1.201532
C	0.139516	3.437003	-0.728626
H	1.990890	2.988743	-1.785517
H	0.670750	1.844015	-2.167794
H	1.537803	4.522945	0.522073
H	0.111750	3.956601	1.405071
H	-0.019999	4.346631	-1.313498
H	-0.830549	2.942113	-0.585770
O	3.527203	-0.264320	0.121008
C	4.277510	-1.443519	0.497630
C	4.331507	0.574053	-0.740146
C	5.459559	-1.475513	-0.447208
H	4.585024	-1.332211	1.545681
H	3.619723	-2.315732	0.414702
C	5.734745	0.009619	-0.648140
H	3.932320	0.501156	-1.762981
H	4.238244	1.609335	-0.394839
H	5.166911	-1.940866	-1.396626
H	6.308224	-2.027728	-0.034763
H	6.326773	0.228850	-1.540776
H	6.259302	0.423306	0.222177
Cl	1.931815	-1.686956	-2.287303
Cl	0.949414	-1.150191	1.900675

TSc_$MgCl_2Zn_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	3.346645	1.372274	1.470778
C	4.626805	1.905066	1.523484
C	5.703564	1.185496	1.010723
C	5.495973	-0.069891	0.447470
C	4.217608	-0.612082	0.405888
C	3.136462	0.103203	0.919707
H	2.492832	1.923004	1.859126
H	4.785757	2.885583	1.964780
H	6.705911	1.604394	1.049903
H	6.332769	-0.631550	0.040811
H	4.055926	-1.594164	-0.033086
C	1.747161	-0.375328	0.855187
N	0.653065	0.121114	0.967466
Mg	-1.427829	-0.017296	0.647934
C	1.996249	-0.971170	-2.605362
H	2.848844	-1.560055	-2.963712
H	1.232816	-0.985737	-3.392842
H	2.346426	0.064863	-2.499773
Zn	1.297565	-1.632158	-0.913213
C	1.837042	-2.422824	0.955839
H	2.220478	-3.290431	0.385739
H	2.561662	-2.289189	1.761528
H	0.866883	-2.675556	1.393858
O	-1.199742	1.606798	-0.676811
C	-1.148018	1.374649	-2.107558
C	-0.342803	2.719579	-0.354398
C	-0.012888	2.248144	-2.637900
H	-0.968283	0.302606	-2.258980
H	-2.123531	1.628290	-2.539321
C	0.762749	2.632349	-1.379374
H	-0.920420	3.650314	-0.448109
H	-0.013786	2.592871	0.681567
H	-0.412549	3.144419	-3.125717
H	0.601592	1.711824	-3.367578
H	1.320280	3.566832	-1.485844
H	1.463219	1.836515	-1.090471
O	-3.415822	-0.004909	-0.095170
C	-4.284409	-1.140284	0.136955
C	-4.179760	1.220361	0.002678
C	-5.576613	-0.552963	0.665264
H	-4.423327	-1.661384	-0.819178
H	-3.792345	-1.819315	0.841244
C	-5.628916	0.787691	-0.055923
H	-3.941312	1.701063	0.962973
H	-3.867874	1.880253	-0.812287
H	-5.505068	-0.398444	1.749190
H	-6.437802	-1.195531	0.463377
H	-6.295729	1.513819	0.416805
H	-5.948441	0.652903	-1.096859
Cl	-2.182281	0.094288	2.876384
Cl	-1.041601	-2.063373	-0.766568

PRc_$MgCl_2Zn_{THF2}$

Atom	Coordinate (Å)		
	x	y	z
C	2.231602	-1.970726	-1.223379
C	2.671232	-3.279384	-1.069272
C	3.729180	-3.564369	-0.210329
C	4.354289	-2.530097	0.480300
C	3.923391	-1.218598	0.313956
C	2.839985	-0.926343	-0.523544
H	1.399600	-1.750973	-1.887423
H	2.182871	-4.077455	-1.624164
H	4.070448	-4.588984	-0.083660
H	5.182949	-2.744449	1.150966
H	4.420231	-0.422125	0.864707
C	2.311797	0.464750	-0.645809
N	1.059870	0.706703	-0.739135
Mg	-0.885667	-0.192677	-0.516888
C	0.721486	4.364841	-0.097195
H	1.742286	4.737341	-0.243662
H	0.043819	5.056554	-0.610812
H	0.501796	4.439534	0.975647
Zn	0.500507	2.550665	-0.720498
C	3.370730	1.543197	-0.616576
H	2.951644	2.507591	-0.916386
H	3.779448	1.661517	0.396031
H	4.213180	1.298459	-1.272943
O	-0.512349	-0.137051	1.572290
C	-0.908410	0.955761	2.429599
C	0.590838	-0.821555	2.185814
C	0.234627	1.143869	3.429919
H	-1.076402	1.834004	1.793730
H	-1.859598	0.700734	2.913913
C	1.364886	0.290916	2.853425
H	0.198859	-1.545522	2.917032
H	1.134514	-1.361013	1.401964
H	-0.057236	0.767582	4.416724
H	0.510071	2.196002	3.543693
H	2.066970	-0.067343	3.611042
H	1.925222	0.850666	2.091490
O	-2.891493	-0.506656	0.296750
C	-4.038212	-0.397836	-0.579844
C	-3.077788	-1.621307	1.197415
C	-4.819070	-1.680290	-0.383919
H	-4.613318	0.488190	-0.278932
H	-3.679806	-0.250325	-1.603305
C	-4.541399	-1.992493	1.080594

H	-2.427420	-2.445992	0.868070
H	-2.771420	-1.308536	2.200965
H	-4.408648	-2.469947	-1.025592
H	-5.881057	-1.560438	-0.615473
H	-4.725988	-3.035972	1.350586
H	-5.153186	-1.355437	1.731942
Cl	-1.177689	-2.164633	-1.792550
Cl	-1.763510	1.922235	-1.487089

RC_{gm}_MeMg(μ-Cl)$_2$MeMg

Atom	Coordinate (Å)		
	x	y	z
C	-3.749766	-0.135083	-1.154969
C	-5.071160	-0.550953	-1.202781
C	-5.731875	-0.909621	-0.030111
C	-5.078726	-0.855614	1.199059
C	-3.757321	-0.441834	1.266188
C	-3.097210	-0.082340	0.084131
H	-3.218930	0.148960	-2.059034
H	-5.587813	-0.595069	-2.156884
H	-6.767833	-1.234577	-0.074532
H	-5.601819	-1.136802	2.108174
H	-3.233634	-0.393258	2.216513
C	-1.742139	0.348026	0.135657
N	-0.638158	0.700845	0.162636
Mg	1.362401	1.523342	-0.034986
Cl	2.532090	0.183559	1.717746
C	1.442620	3.621088	-0.157312
H	0.791047	4.089191	0.595587
H	2.446292	4.037672	0.008725
H	1.109743	4.004864	-1.132542
Mg	3.538484	-1.222518	-0.032572
Cl	2.121353	-0.156366	-1.728699
C	5.151038	-2.563146	-0.053338
H	5.385208	-2.922819	-1.064614
H	6.070177	-2.104925	0.336799
H	4.962741	-3.454469	0.561113

TS_{gm}_MeMg(μ-Cl)$_2$MeMg

Atom	Coordinate (Å)		
	x	y	z
C	-3.720046	-1.240782	-0.376597
C	-5.100312	-1.120078	-0.274509
C	-5.677021	0.130009	-0.072608
C	-4.872685	1.262678	0.025750
C	-3.491814	1.149309	-0.061727
C	-2.912606	-0.105327	-0.262051
H	-3.256792	-2.209834	-0.545957
H	-5.726388	-2.004577	-0.356804
H	-6.757162	0.223599	0.005305
H	-5.323577	2.240464	0.172921
H	-2.862064	2.031645	0.010840
C	-1.473848	-0.293539	-0.433539
N	-0.648261	-0.781467	-1.160000
Mg	0.785721	-0.162722	0.179648
Cl	2.306870	1.708652	-0.105576
C	-0.837283	0.614770	1.475898
H	-1.608331	0.094623	2.049236
H	0.048221	0.650071	2.147676
H	-1.136551	1.658745	1.340375
Mg	4.192177	0.097878	-0.066461
Cl	2.597727	-1.689096	0.662020
C	6.155444	0.094225	-0.800335
H	6.611924	-0.904118	-0.764893
H	6.202001	0.423941	-1.847021
H	6.814630	0.763783	-0.231173

PR_{gm}_MeMg(μ-Cl)$_2$MeMg

Atom	Coordinate (Å)		
	x	y	z
C	3.319918	-1.233286	0.070506
C	4.558726	-1.801089	0.328341
C	5.666201	-0.986507	0.560594
C	5.517008	0.395261	0.532907
C	4.269949	0.960049	0.277435
C	3.150564	0.155055	0.040674
H	2.441702	-1.848004	-0.115168
H	4.666121	-2.883711	0.350092
H	6.639347	-1.428337	0.762758
H	6.374620	1.040297	0.711751
H	4.178640	2.043649	0.262148
C	1.778848	0.719888	-0.243004
N	0.805551	-0.037194	-0.523050
Mg	-1.102848	0.019818	-0.902472
Cl	-2.803666	1.678256	-0.186988
C	1.686709	2.235837	-0.161985
H	2.326950	2.720447	-0.911332
H	0.654165	2.554687	-0.332581
H	2.008794	2.612219	0.817886
Mg	-4.328347	-0.187151	0.375291
Cl	-2.780323	-1.760634	-0.749818
C	-5.950608	-0.409425	1.683523
H	-6.224399	-1.462642	1.832464
H	-5.733578	0.002413	2.678415
H	-6.852942	0.103056	1.322841

RC_{vi}_MeMg(μ-Cl)$_2$MeMg

Atom	Coordinate (Å)		
	x	y	z
C	2.685011	-0.653821	0.031202
C	4.025776	-0.983246	0.158052
C	4.997919	0.012803	0.100861
C	4.640593	1.346557	-0.084708
C	3.305369	1.695981	-0.212814
C	2.332326	0.690238	-0.153585
H	1.911311	-1.419100	0.072888
H	4.313281	-2.020395	0.302834
H	6.046660	-0.253124	0.202663
H	5.405595	2.116070	-0.127393
H	3.008018	2.730908	-0.354811
C	0.954732	1.026652	-0.261446
N	-0.176172	1.274358	-0.334283
Mg	-2.333619	1.291561	-0.014168
Cl	-2.063171	-0.417538	1.841154
C	-3.383419	3.106204	0.121860
H	-3.110882	3.801075	-0.685860
H	-4.474003	2.982274	0.065461
H	-3.182009	3.634398	1.064815
Mg	-1.585027	-2.055377	0.093592
Cl	-2.668344	-0.631730	-1.580425
C	0.050958	-3.349394	-0.178641
H	0.735819	-3.366727	0.681656
H	-0.270950	-4.389217	-0.333023
H	0.654284	-3.085166	-1.059413

TS_{vi}_MeMg(μ-Cl)$_2$MeMg

Atom	Coordinate (Å)		
	x	y	z
C	3.106387	-0.576662	-0.997119
C	4.453772	-0.254605	-0.909793

C	4.891157	0.692127	0.013014
C	3.976520	1.334599	0.841530
C	2.624704	1.029230	0.752356
C	2.188674	0.064747	-0.162667
H	2.767201	-1.309496	-1.723637
H	5.166754	-0.747673	-1.564818
H	5.948861	0.932129	0.083162
H	4.314283	2.078875	1.557525
H	1.897929	1.530830	1.386787
C	0.747372	-0.165989	-0.219063
N	-0.296690	0.411399	-0.316148
Mg	-2.321125	1.133965	-0.454043
Cl	-2.355990	0.117978	2.009814
C	-3.107390	2.935164	-1.184020
H	-2.862063	3.079580	-2.245969
H	-4.201994	2.989264	-1.107649
H	-2.711962	3.811358	-0.651525
Mg	-1.167236	-1.437422	0.613821
Cl	-2.795901	-1.292003	-1.179782
C	0.810444	-2.322035	0.189222
H	1.569283	-2.345745	0.976152
H	0.188464	-3.234765	0.311320
H	1.292717	-2.483699	-0.776975

PR_{vi}_MeMg(μ-Cl)$_2$MeMg

Atom	Coordinate (Å)		
	x	y	z
C	2.796366	-1.190519	-0.985901
C	4.114030	-0.794767	-0.783946
C	4.476756	-0.143096	0.391687
C	3.515858	0.115971	1.364112
C	2.192667	-0.252405	1.149037
C	1.817586	-0.902752	-0.030102
H	2.522089	-1.701797	-1.907012
H	4.861642	-0.997659	-1.546945
H	5.509038	0.158321	0.551010
H	3.795359	0.612218	2.290316
H	1.440155	-0.058160	1.913068
C	0.376531	-1.234067	-0.270775
N	-0.531167	-0.348632	-0.131733
Mg	-0.113355	1.704620	0.032415
Cl	-4.156589	-1.418227	0.877534
C	1.475038	3.071479	0.178988
H	2.328615	2.730336	-0.426023
H	1.240576	4.093757	-0.148171
H	1.846345	3.145929	1.211560
Mg	-2.560417	-0.356244	-0.404946
Cl	-2.506286	2.083557	-0.645214
C	0.122431	-2.659921	-0.691039
H	0.701413	-3.361630	-0.079891
H	-0.938392	-2.916976	-0.617148
H	0.441889	-2.814569	-1.730064

RC_{gm}_MeMg(μ-Cl)(μ-Me)MgCl

Atom	Coordinate (Å)		
	x	y	z
C	-2.731399	0.640209	0.059770
C	-4.088988	0.920756	0.020331
C	-5.018045	-0.116906	0.027125
C	-4.600832	-1.445633	0.074227
C	-3.248608	-1.746839	0.114864
C	-2.319390	-0.698346	0.107263
H	-1.985718	1.434290	0.049313
H	-4.423606	1.953252	-0.017581
H	-6.079988	0.111820	-0.005776
H	-5.332503	-2.248114	0.077961
H	-2.904836	-2.776560	0.150040
C	-0.927356	-0.991064	0.132880
N	0.209525	-1.222206	0.145125
Mg	2.370983	-1.341514	-0.170100
C	3.205985	-3.251027	-0.430117
H	2.938839	-3.695393	-1.400423
H	4.304204	-3.264568	-0.380464
H	2.856817	-3.958214	0.336803
Mg	2.084353	1.614561	-0.277133
Cl	2.870789	0.345578	1.629162
C	2.392107	0.171893	-1.901116
H	3.361705	-0.276218	-2.170516
H	1.609722	-0.479297	-2.322770
H	2.341115	1.052980	-2.560709
Cl	0.211722	2.979519	-0.254828

TS_{gm}_MeMg(μ-Cl)(μ-Me)MgCl

Atom	Coordinate (Å)		
	x	y	z
C	3.560634	-1.287141	0.157387
C	4.891511	-1.462465	-0.198026
C	5.702025	-0.355857	-0.438377
C	5.183541	0.930223	-0.317549
C	3.854908	1.115183	0.044925
C	3.045068	0.003800	0.285342
H	2.916584	-2.144600	0.340548
H	5.297099	-2.466455	-0.290736
H	6.741665	-0.497063	-0.722437
H	5.815985	1.793769	-0.505837
H	3.438924	2.115310	0.143117
C	1.658524	0.207151	0.699050
N	0.938383	0.488301	1.620701
Mg	-0.655933	0.265991	0.327076
Cl	-2.371967	1.893718	-0.178771
C	0.815674	-0.181649	-1.288600
H	1.188563	-1.203292	-1.418391
H	-0.140465	-0.129677	-1.852071
H	1.494493	0.507942	-1.797627
Mg	-3.561819	-0.244110	0.098492
Cl	-5.775178	-0.688591	-0.291940
C	-1.866761	-1.624255	0.420904
H	-1.010771	-1.829028	1.086766
H	-2.634929	-2.250649	0.901720
H	-1.632069	-2.134037	-0.525021

PR_{gm}_MeMg(μ-Cl)(μ-Me)MgCl

Atom	Coordinate (Å)		
	x	y	z
C	-3.337385	-1.246308	0.255354
C	-4.571295	-1.865695	0.122354
C	-5.666769	-1.146556	-0.353781
C	-5.510599	0.191967	-0.694587
C	-4.268193	0.807343	-0.564060
C	-3.160966	0.098924	-0.084994
H	-2.469383	-1.787169	0.626063
H	-4.684132	-2.914726	0.388581
H	-6.635923	-1.628952	-0.459166
H	-6.358772	0.763007	-1.066161
H	-4.170522	1.855058	-0.838928
C	-1.795435	0.724049	0.075734
N	-0.839513	0.084618	0.602682
Mg	1.059339	0.289171	1.005177
Cl	2.790102	1.891112	0.233440
C	-1.686799	2.150572	-0.440713

H	-2.337271	2.833965	0.121625
H	-0.654925	2.501325	-0.345546
H	-1.984645	2.228173	-1.494609
Mg	3.853191	-0.318105	0.255428
Cl	5.122069	-1.196450	-1.450412
C	2.424315	-1.444210	1.533910
H	1.423606	-1.907289	1.555780
H	3.017960	-2.299331	1.171880
H	2.712085	-1.318958	2.587675

RC_{vi}_MgCl(μ-Cl)(μ-Me)MeMg

Atom	Coordinate (Å)		
	x	y	z
C	-3.191937	-1.778676	-0.157018
C	-2.370971	-0.643952	-0.126461
C	-2.908716	0.639398	0.043469
C	-4.280976	0.777279	0.184664
C	-5.102290	-0.347444	0.156778
C	-4.561508	-1.619942	-0.014669
H	-2.752475	-2.763274	-0.287658
H	-2.250460	1.506008	0.059677
H	-4.711532	1.765194	0.318236
H	-6.176745	-0.231165	0.270500
H	-5.209880	-2.490762	-0.035012
C	-0.961718	-0.788658	-0.246396
N	0.190527	-0.895189	-0.328307
Mg	2.317722	-0.578473	-0.098385
Cl	2.002022	0.925737	1.828184
Mg	1.534375	2.267378	-0.227481
C	-0.262830	3.277199	-0.643314
H	-0.891113	3.391859	0.252937
H	-0.134285	4.287901	-1.055587
H	-0.864968	2.725057	-1.381622
C	2.679055	0.981382	-1.662987
H	3.344730	0.165721	-1.994902
H	1.959480	1.079588	-2.490537
H	3.359889	1.847084	-1.742698
Cl	3.441498	-2.588282	-0.116959

TS_{vi}_MgCl(μ-Cl)(μ-Me)MeMg

Atom	Coordinate (Å)		
	x	y	z
C	-2.664139	1.459410	0.365304
C	-2.260199	0.169757	0.004081
C	-3.182957	-0.730146	-0.531332
C	-4.504805	-0.339739	-0.699260
C	-4.912215	0.937186	-0.322313
C	-3.991556	1.835645	0.208546
H	-1.931550	2.155032	0.767203
H	-2.861258	-1.723598	-0.830628
H	-5.221253	-1.037177	-1.124753
H	-5.950421	1.233829	-0.446754
H	-4.305672	2.834984	0.497615
C	-0.837647	-0.131333	0.146564
N	0.237791	0.344072	-0.078499
Mg	2.358332	0.498082	-0.026436
Cl	2.312908	-1.454832	-1.628490
Mg	0.967997	-1.810440	0.423355
C	-1.046727	-1.961742	1.335542
H	-1.801531	-2.587020	0.852380
H	-0.435473	-2.637690	1.969332
H	-1.546868	-1.319039	2.065040
C	2.414178	-0.856704	1.817376
H	2.584572	0.141239	2.258543
H	1.815207	-1.329429	2.614162
H	3.391668	-1.358427	1.850831
Cl	3.604651	2.435603	-0.055836

PR_{vi}_MgCl(μ-Cl)(μ-Me)MeMg

Atom	Coordinate (Å)		
	x	y	z
C	2.093881	-0.306831	1.086124
C	1.729313	-1.056207	-0.037514
C	2.740386	-1.582073	-0.848609
C	4.077741	-1.328026	-0.565687
C	4.426010	-0.574189	0.550860
C	3.429933	-0.069962	1.382413
H	1.313343	0.066956	1.747684
H	2.484592	-2.176088	-1.723377
H	4.851669	-1.723682	-1.218797
H	5.472527	-0.385866	0.777149
H	3.694890	0.502243	2.268022
C	0.280158	-1.290847	-0.329056
N	-0.603017	-0.395380	-0.120124
Mg	-0.594476	1.651628	-0.013058
Cl	-4.356078	-1.548453	0.655988
Mg	-2.645916	-0.266027	-0.216639
C	-0.047487	-2.657963	-0.877126
H	0.412511	-3.453035	-0.279114
H	-1.129257	-2.815048	-0.919556
H	0.346982	-2.764766	-1.895853
C	-2.762759	2.002042	-0.416770
H	-2.810311	2.751523	0.389356
H	-2.528744	2.563858	-1.335415
H	-3.825171	1.743370	-0.553262
Cl	0.769003	3.490530	-0.263483

RC_{gm}_MeMg(μ-Cl)$_2$MeMg$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	5.118964	0.287637	-2.013290
C	6.438152	-0.011319	-2.319429
C	7.271696	-0.564605	-1.350140
C	6.794490	-0.823408	-0.067272
C	5.478452	-0.529168	0.255342
C	4.643532	0.027138	-0.722591
H	4.455336	0.717534	-2.758106
H	6.818053	0.186747	-3.317413
H	8.304215	-0.796708	-1.597230
H	7.450332	-1.254985	0.683122
H	5.086604	-0.722107	1.250992
C	3.289752	0.317391	-0.384449
N	2.189256	0.529285	-0.081522
Mg	0.276666	0.496482	1.183143
Cl	-2.194017	0.126172	1.973965
C	1.468966	0.264618	2.937595
H	2.080638	1.168019	3.110162
H	0.931948	0.083624	3.882983
H	2.195762	-0.563269	2.840693
Mg	-2.312888	-1.085176	-0.169002
Cl	-0.928745	0.514006	-1.393787
O	-4.129415	-0.118340	-0.711562
C	-4.475551	-0.096932	-2.112944
C	-5.305312	-0.395775	0.081234
C	-5.985611	0.012156	-2.142238
H	-3.945701	0.740140	-2.576975
H	-4.129855	-1.035800	-2.573593
C	-6.374003	-0.802571	-0.914118
H	-5.059166	-1.177793	0.809112
H	-5.571491	0.518681	0.626998

H	-6.412417	-0.369074	-3.073823
H	-6.296012	1.057690	-2.023238
H	-6.302327	-1.875769	-1.132927
H	-7.383239	-0.594337	-0.548731
O	-0.011687	2.582901	0.965310
C	-1.289876	3.233553	0.767448
C	1.048625	3.422440	0.465373
C	-0.992067	4.420850	-0.124210
H	-1.978592	2.504877	0.329045
H	-1.669520	3.538826	1.751525
C	0.422097	4.791042	0.305672
H	1.880672	3.378859	1.176447
H	1.388106	3.022505	-0.501474
H	-1.717504	5.229136	0.002558
H	-0.998844	4.110954	-1.177582
H	0.405772	5.321748	1.265837
H	0.955895	5.409514	-0.421161
C	-2.796441	-3.099715	-0.633597
H	-2.549135	-3.341896	-1.680950
H	-2.288290	-3.866769	-0.026961
H	-3.875672	-3.304302	-0.533185
O	-0.086079	-1.680920	0.621320
C	-0.102038	-2.562172	1.788003
C	0.697376	-2.322167	-0.417952
C	0.861996	-3.699194	1.472698
H	0.216239	-1.955669	2.641943
H	-1.131185	-2.902058	1.946014
C	1.717084	-3.132144	0.344367
H	0.025749	-2.962785	-1.008710
H	1.099326	-1.533985	-1.058533
H	0.313015	-4.580017	1.117611
H	1.442520	-3.995286	2.350897
H	2.189595	-3.902499	-0.271440
H	2.501753	-2.472500	0.740495

TS_{gm}_MeMg(μ-Cl)$_2$MeMg$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	5.176801	0.998786	-0.410351
C	6.529420	0.823840	-0.142810
C	6.982708	-0.372991	0.403202
C	6.082898	-1.398018	0.687333
C	4.729033	-1.226342	0.435058
C	4.275579	-0.028149	-0.120568
H	4.809447	1.925176	-0.847061
H	7.230968	1.623673	-0.364790
H	8.041237	-0.508674	0.609582
H	6.438138	-2.333159	1.111984
H	4.016113	-2.015975	0.666846
C	2.875806	0.173120	-0.465688
N	2.066855	0.365287	-1.321918
Mg	0.519177	0.376367	0.176622
Cl	-1.379502	-0.037811	1.890381
C	2.198758	0.288349	1.712291
H	2.851724	1.157881	1.869194
H	1.323629	0.444526	2.371301
H	2.723451	-0.590285	2.104220
Mg	-2.412680	-1.077772	-0.099368
Cl	-1.430401	0.555723	-1.635476
O	-4.210465	-0.004405	0.130110
C	-5.075163	0.126698	-1.020819
C	-5.004434	-0.180870	1.325681
C	-6.455757	0.372550	-0.449174
H	-4.686059	0.937738	-1.643441
H	-5.037313	-0.812715	-1.594042
C	-6.410059	-0.453758	0.830570
H	-4.573198	-0.999240	1.912962
H	-4.942965	0.742913	1.915437
H	-7.249399	0.070460	-1.137583
H	-6.589412	1.435763	-0.214542
H	-6.532025	-1.519863	0.599486
H	-7.171031	-0.172485	1.563375
O	0.357300	2.461205	0.318493
C	-0.866904	3.161213	0.654323
C	1.186743	3.296393	-0.521149
C	-0.888738	4.369798	-0.256776
H	-1.705429	2.473287	0.506852
H	-0.815096	3.440713	1.714837
C	0.595196	4.684236	-0.399308
H	2.220957	3.209261	-0.169700
H	1.129819	2.918104	-1.551707
H	-1.475001	5.193379	0.159754
H	-1.315452	4.098349	-1.231095
H	0.969949	5.185102	0.502048
H	0.830577	5.310602	-1.263997
C	-3.017260	-3.079802	-0.407018
H	-3.120507	-3.325078	-1.476359
H	-2.333442	-3.837808	0.007150
H	-4.003418	-3.286409	0.041208
O	0.093560	-1.746349	-0.213013
C	0.484848	-2.705240	0.815528
C	0.393871	-2.310389	-1.520715
C	1.037379	-3.909965	0.072843
H	1.240702	-2.216461	1.442924
H	-0.394967	-2.929298	1.426899
C	1.491642	-3.309945	-1.252375
H	-0.518318	-2.794598	-1.897562
H	0.671262	-1.484834	-2.179973
H	0.245124	-4.648553	-0.102111
H	1.840463	-4.399547	0.631418
H	1.590592	-4.047378	-2.053576
H	2.453943	-2.789915	-1.142127

PR_{gm}_MeMg(μ-Cl)$_2$MeMg$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	4.656805	-0.465504	-1.138312
C	5.883098	-0.839566	-1.667931
C	7.028890	-0.799660	-0.874338
C	6.929580	-0.382794	0.448146
C	5.695409	-0.008753	0.974796
C	4.537411	-0.042918	0.190742
H	3.747704	-0.486543	-1.737501
H	5.951007	-1.164357	-2.704424
H	7.992325	-1.092309	-1.285844
H	7.817012	-0.347716	1.076770
H	5.643515	0.312935	2.012635
C	3.173386	0.342937	0.716649
N	2.147976	0.308674	-0.019829
Mg	0.199272	0.572573	0.160920
Cl	-1.553211	0.191339	1.897212
C	3.149019	0.759507	2.182406
H	3.796080	1.626833	2.373905
H	2.125163	1.025756	2.467858
H	3.496186	-0.044718	2.846154
Mg	-2.407586	-1.188876	-0.027386
Cl	-1.490023	0.495920	-1.676515
O	-4.271637	-0.186367	-0.011316
C	-5.043488	-0.167398	-1.234468
C	-5.149518	-0.388517	1.120586
C	-6.482413	-0.013313	-0.788893
H	-4.665887	0.648509	-1.857714

H	-4.885490	-1.121655	-1.761065
C	-6.482189	-0.789751	0.522318
H	-4.711165	-1.153332	1.772359
H	-5.209816	0.555461	1.677404
H	-7.188675	-0.401202	-1.527680
H	-6.716837	1.043189	-0.609461
H	-6.499592	-1.869377	0.324503
H	-7.322667	-0.547021	1.177916
O	0.089264	2.644341	0.336018
C	-1.152934	3.386888	0.385905
C	1.095827	3.410927	-0.370557
C	-0.987826	4.480444	-0.646364
H	-1.972960	2.691258	0.179862
H	-1.270106	3.789036	1.400840
C	0.498946	4.794375	-0.528501
H	2.021902	3.372796	0.211127
H	1.273117	2.931667	-1.344497
H	-1.635545	5.339592	-0.452285
H	-1.218595	4.090248	-1.646500
H	0.691238	5.400628	0.365425
H	0.906716	5.322580	-1.394426
C	-2.991072	-3.216978	-0.133777
H	-3.002505	-3.594464	-1.168989
H	-2.334817	-3.903676	0.424148
H	-4.009005	-3.384075	0.255049
O	-0.087287	-1.656175	-0.029448
C	0.429088	-2.408038	1.111539
C	0.424107	-2.254633	-1.260273
C	1.059959	-3.649332	0.520470
H	1.172613	-1.773182	1.612767
H	-0.402774	-2.603419	1.794301
C	1.569628	-3.134029	-0.818423
H	-0.394950	-2.834371	-1.709221
H	0.710169	-1.443150	-1.934432
H	0.301254	-4.427996	0.367964
H	1.844884	-4.054539	1.164781
H	1.784549	-3.926071	-1.540901
H	2.471883	-2.523561	-0.678625

RC_{vi}_MeMg(μ-Cl)$_2$MeMg$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	1.831333	-0.834048	-1.570326
Mg	0.489786	2.328667	0.530652
O	0.474936	-2.521293	-1.726524
C	-0.848926	-2.607901	-1.152257
C	1.137553	-3.802618	-1.609177
C	-0.842520	-3.878106	-0.329459
H	-1.038927	-1.690027	-0.582033
H	-1.577713	-2.669859	-1.974084
C	0.061026	-4.774217	-1.167914
H	1.598062	-4.041493	-2.572582
H	1.932770	-3.713560	-0.855166
H	-1.847202	-4.282982	-0.180291
H	-0.394569	-3.694627	0.656475
H	-0.488471	-5.162168	-2.034721
H	0.473429	-5.623785	-0.616947
O	0.071125	3.996301	-0.663191
C	0.272886	3.941481	-2.096109
C	-1.139585	4.731549	-0.370355
C	-0.795965	4.837790	-2.692027
H	1.299749	4.254035	-2.311129
H	0.151336	2.894742	-2.411281
C	-1.918060	4.720009	-1.666995
H	-1.648638	4.237001	0.464076
H	-0.862841	5.749207	-0.064357
H	-1.085982	4.517110	-3.697609
H	-0.442453	5.874174	-2.754350
H	-2.442547	3.762021	-1.778200
H	-2.651067	5.529117	-1.723349
N	1.498025	-1.247494	0.612357
C	1.079323	-1.148381	1.689879
C	0.510505	-0.987955	2.984799
C	-0.871721	-0.777320	3.077988
C	1.322361	-0.998875	4.124567
C	-1.438562	-0.583117	4.328643
H	-1.469315	-0.739861	2.168952
C	0.738604	-0.799373	5.366475
H	2.392742	-1.155817	4.027066
C	-0.635680	-0.593635	5.467061
H	-2.508016	-0.415291	4.415876
H	1.357120	-0.801501	6.259205
H	-1.085070	-0.436104	6.443983
C	0.625130	2.793499	2.589819
H	-0.044511	2.165884	3.200068
H	1.634195	2.645994	3.005395
H	0.356161	3.837803	2.816307
Cl	2.426521	1.555514	-0.751788
Cl	-1.317005	0.956962	-0.257661
O	0.759570	0.012846	-3.181019
C	1.396924	0.919260	-4.107315
C	-0.604424	-0.220455	-3.571737
C	0.319546	1.313882	-5.110491
H	1.773302	1.769868	-3.524575
H	2.252143	0.409287	-4.566349
C	-0.979734	1.007202	-4.370136
H	-0.655078	-1.137733	-4.176964
H	-1.192459	-0.344583	-2.656772
H	0.390945	0.697722	-6.014396
H	0.407127	2.362256	-5.412624
H	-1.825788	0.830664	-5.040075
H	-1.252453	1.822811	-3.685804
C	3.641801	-1.631861	-2.324270
H	4.123572	-2.360894	-1.652214
H	3.504312	-2.161548	-3.282644
H	4.403928	-0.859695	-2.518324

TS_{vi}_MeMg(μ-Cl)$_2$MeMg$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	2.129675	-1.118118	-1.611632
Mg	0.627234	1.771476	-0.481190
O	0.821477	-2.753395	-1.227723
C	-0.261810	-2.868679	-0.277466
C	0.893658	-3.935033	-2.046614
C	-0.799609	-4.278162	-0.451432
H	0.131852	-2.664570	0.723769
H	-1.007838	-2.096433	-0.517986
C	-0.469914	-4.578274	-1.909268
H	1.151418	-3.622224	-3.064911
H	1.693501	-4.585762	-1.664923
H	-1.866551	-4.343843	-0.222035
H	-0.266819	-4.975685	0.206517
H	-1.191259	-4.087562	-2.575923
H	-0.456390	-5.645936	-2.144432
O	0.043437	3.678277	-1.124159
C	-0.100609	3.927952	-2.542887
C	-0.998809	4.374982	-0.395759
C	-1.010068	5.133316	-2.632324
H	0.900067	4.068936	-2.961007
H	-0.561346	3.041059	-3.006484
C	-1.948652	4.893575	-1.456162

H	-1.467251	3.670941	0.301265
H	-0.525828	5.184687	0.174482
H	-1.523295	5.193757	-3.595686
H	-0.437058	6.057533	-2.487390
H	-2.685868	4.121499	-1.710374
H	-2.484391	5.788931	-1.129985
N	1.452954	-0.337777	0.271672
C	1.110487	0.134128	1.308987
C	0.585953	-0.152628	2.638934
C	-0.795290	-0.310717	2.779121
C	1.436253	-0.302168	3.734187
C	-1.321107	-0.631658	4.023887
H	-1.437224	-0.173537	1.909049
C	0.898335	-0.625414	4.974294
H	2.508474	-0.169400	3.609368
C	-0.476374	-0.789580	5.119885
H	-2.394432	-0.758042	4.139047
H	1.556135	-0.748327	5.830600
H	-0.891850	-1.039608	6.092740
C	1.098448	2.344965	1.617945
H	0.191332	2.539014	2.204254
H	1.917617	2.149862	2.316724
H	1.385209	3.285809	1.106726
Cl	2.442818	1.574691	-2.042528
Cl	-1.507661	0.822375	-0.923564
O	1.082703	-1.042601	-3.462698
C	1.634702	-0.483866	-4.663276
C	-0.326905	-1.162022	-3.703903
C	0.631942	0.577612	-5.090250
H	2.629696	-0.095830	-4.427788
H	1.725404	-1.288765	-5.408450
C	-0.703657	0.083953	-4.499431
H	-0.502354	-2.084341	-4.280524
H	-0.828492	-1.232800	-2.733513
H	0.602090	0.688688	-6.177932
H	0.912491	1.544351	-4.657424
H	-1.444283	-0.149064	-5.270109
H	-1.141205	0.832319	-3.828468
C	4.018934	-2.011987	-1.927898
H	4.074633	-2.452358	-2.938536
H	4.886132	-1.339279	-1.847343
H	4.214594	-2.843533	-1.231574

PR_{vi}_MeMg(μ-Cl)$_2$MeMg$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	1.175322	-1.479420	-0.919667
Mg	0.337592	1.537942	-2.168560
O	-0.701191	-2.356081	-0.948719
C	-1.983065	-1.697318	-0.805179
C	-0.828089	-3.766644	-0.642552
C	-2.825302	-2.675082	-0.015115
H	-1.811560	-0.732852	-0.312439
H	-2.386475	-1.501158	-1.807033
C	-2.319720	-4.013174	-0.542136
H	-0.326465	-4.335178	-1.432517
H	-0.314249	-3.958005	0.310664
H	-3.896222	-2.520067	-0.169160
H	-2.615365	-2.583810	1.059486
H	-2.743195	-4.215913	-1.533334
H	-2.554845	-4.858284	0.109958
O	-0.616395	3.230043	-1.345692
C	-0.902508	4.372890	-2.188096
C	-1.699501	3.026705	-0.410108
C	-2.034160	5.096647	-1.490475
H	0.019392	4.951657	-2.292501
H	-1.207798	4.003085	-3.177738
C	-2.814257	3.935363	-0.886058
H	-1.966775	1.963641	-0.412170
H	-1.339383	3.302451	0.591041
H	-2.622904	5.705956	-2.181315
H	-1.643898	5.750618	-0.700680
H	-3.406133	3.431537	-1.660513
H	-3.484993	4.230299	-0.074582
N	0.823315	0.510624	-0.440436
C	1.222224	0.924608	0.698645
C	1.454965	-0.043981	1.822428
C	0.538115	-1.078922	2.036726
C	2.583559	0.030520	2.643757
C	0.747573	-2.026292	3.032205
H	-0.362919	-1.121109	1.424909
C	2.808584	-0.931279	3.622784
H	3.306022	0.831776	2.501615
C	1.892055	-1.960428	3.821190
H	0.014009	-2.813670	3.193370
H	3.703999	-0.875696	4.237101
H	2.066337	-2.704134	4.594652
C	1.517638	2.366616	1.035114
H	1.109502	2.645099	2.014488
H	2.603206	2.521306	1.091768
H	1.123431	3.038245	0.267381
Cl	2.084384	2.628124	-3.297761
Cl	-1.622452	0.855789	-3.305656
O	1.310622	-0.896702	-2.965576
C	0.588495	-1.675848	-3.944229
C	2.661718	-0.810280	-3.485444
C	1.041806	-1.088529	-5.264927
H	0.886458	-2.731801	-3.830603
H	-0.477036	-1.557266	-3.731263
C	2.499794	-0.669135	-4.997022
H	3.137104	0.048551	-3.002132
H	3.190701	-1.733480	-3.207781
H	0.424792	-0.212913	-5.496528
H	0.944518	-1.802726	-6.087181
H	2.674253	0.364825	-5.308619
H	3.216786	-1.307538	-5.521639
C	2.667724	-2.920229	-0.536954
H	2.637085	-3.755086	-1.257325
H	3.691356	-2.517994	-0.586614
H	2.569244	-3.373865	0.462235

RC_{gm}_MeMg(μ-Cl)(μ-Me)MgCl $_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	5.049940	0.356943	-1.927728
C	6.373782	0.099247	-2.250869
C	7.223109	-0.477157	-1.309167
C	6.757226	-0.800886	-0.036868
C	5.436725	-0.548936	0.302449
C	4.585978	0.031091	-0.647627
H	4.374142	0.804437	-2.650945
H	6.745029	0.347827	-3.240772
H	8.259187	-0.676246	-1.569765
H	7.425413	-1.250146	0.691939
H	5.053122	-0.792926	1.290054
C	3.229200	0.279741	-0.289229
N	2.127853	0.457446	0.031519
Mg	0.244591	0.441985	1.332476
C	1.462552	0.131247	3.062072
H	2.090265	1.017903	3.262587
H	0.947279	-0.087227	4.012295
H	2.177495	-0.699038	2.912103

Mg	-2.129342	-0.722305	-0.050094
O	-3.995905	0.194868	-0.445026
C	-4.401061	0.501582	-1.799071
C	-5.149278	-0.190521	0.337827
C	-5.907689	0.636966	-1.735182
H	-3.869378	1.405038	-2.112107
H	-4.098276	-0.330676	-2.451336
C	-6.262280	-0.392587	-0.669213
H	-4.899572	-1.097259	0.900527
H	-5.370486	0.621884	1.043368
H	-6.381343	0.447244	-2.702109
H	-6.190239	1.644493	-1.404852
H	-6.210691	-1.406039	-1.087336
H	-7.253131	-0.249673	-0.229703
O	0.034693	2.529009	1.044924
C	-1.185759	3.215608	0.677179
C	1.172547	3.366298	0.755669
C	-0.733512	4.462248	-0.056316
H	-1.788989	2.538894	0.062084
H	-1.729674	3.453925	1.601107
C	0.601883	4.760006	0.614195
H	1.896997	3.243109	1.567593
H	1.630477	3.025550	-0.184349
H	-1.458747	5.276715	0.022645
H	-0.580935	4.237681	-1.120281
H	0.445796	5.214501	1.600613
H	1.250663	5.417792	0.029405
O	-0.120143	-1.674106	0.550650
C	-0.210580	-2.585177	1.695194
C	0.658945	-2.326990	-0.487357
C	0.702717	-3.758517	1.366763
H	0.120226	-2.018225	2.572903
H	-1.257914	-2.881431	1.813907
C	1.618223	-3.199472	0.282712
H	-0.029752	-2.920872	-1.105320
H	1.108397	-1.540098	-1.095863
H	0.116365	-4.593398	0.963873
H	1.240064	-4.115522	2.249632
H	2.076223	-3.973705	-0.338951
H	2.417108	-2.584938	0.721430
Cl	-2.956814	-2.900564	-0.522385
C	-2.022846	0.266374	1.936249
H	-2.616669	-0.566688	2.358246
H	-1.442522	0.587728	2.816053
H	-2.741808	1.082145	1.768079
Cl	-0.871430	0.560455	-1.637053

TS_{gm}_MeMg(μ-Cl)(μ-Me)$MgCl_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	5.192023	0.854163	-0.331402
C	6.541653	0.607410	-0.109097
C	6.954812	-0.635680	0.359972
C	6.017518	-1.635168	0.611458
C	4.666769	-1.392309	0.403724
C	4.252996	-0.147146	-0.074095
H	4.856036	1.817856	-0.708714
H	7.272227	1.387500	-0.306372
H	8.010918	-0.827647	0.531075
H	6.340856	-2.606851	0.975307
H	3.927017	-2.164006	0.610318
C	2.854612	0.133550	-0.371646
N	2.040754	0.394432	-1.205147
Mg	0.515124	0.463690	0.321241
C	2.242857	0.198377	1.810768
H	2.945487	1.022482	1.996972
H	1.400773	0.358256	2.509470
H	2.733694	-0.725290	2.138075
Mg	-2.150181	-0.696816	0.147010
O	-4.033656	0.251326	0.298120
C	-4.786402	0.486219	-0.917303
C	-4.940031	-0.087613	1.375995
C	-6.223597	0.632696	-0.466232
H	-4.364704	1.367625	-1.407944
H	-4.657259	-0.384012	-1.578466
C	-6.277301	-0.334614	0.709488
H	-4.545632	-0.966149	1.899810
H	-4.974345	0.762746	2.070055
H	-6.932590	0.392863	-1.263075
H	-6.417790	1.658736	-0.129596
H	-6.332295	-1.369513	0.348723
H	-7.117518	-0.159432	1.386725
O	0.486681	2.566635	0.434110
C	-0.725993	3.324216	0.666271
C	1.414598	3.354970	-0.347482
C	-0.626277	4.518948	-0.257890
H	-1.582419	2.674130	0.456348
H	-0.743942	3.621598	1.723579
C	0.876511	4.768280	-0.286229
H	2.413489	3.228129	0.084628
H	1.420969	2.964287	-1.374637
H	-1.207855	5.372126	0.101603
H	-0.986646	4.249817	-1.259222
H	1.200791	5.265326	0.636608
H	1.205311	5.372277	-1.136148
O	-0.025036	-1.657557	-0.239620
C	0.389819	-2.668036	0.733571
C	0.230661	-2.164367	-1.583601
C	0.870543	-3.854024	-0.082361
H	1.189756	-2.222659	1.339134
H	-0.467604	-2.901815	1.372323
C	1.303299	-3.207526	-1.392301
H	-0.704348	-2.601951	-1.960114
H	0.517790	-1.312001	-2.202683
H	0.042880	-4.551103	-0.261929
H	1.672333	-4.398620	0.424820
H	1.353793	-3.910044	-2.228569
H	2.284450	-2.722903	-1.289228
Cl	-3.092964	-2.855253	0.094762
Cl	-1.406729	0.772638	-1.627199
C	-1.167872	0.181791	1.931183
H	-2.214789	0.371463	2.230338
H	-0.820018	-0.611053	2.612646
H	-0.679728	1.100713	2.288968

PR_{gm}_MeMg(μ-Cl)(μ-Me)$MgCl_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.606169	-0.368003	1.106069
C	-5.816912	-0.741204	1.671281
C	-6.975556	-0.757378	0.895677
C	-6.904632	-0.397560	-0.445135
C	-5.686258	-0.023769	-1.007280
C	-4.515510	-0.001040	-0.241632
H	-3.688428	-0.347464	1.691663
H	-5.862234	-1.021601	2.721848
H	-7.926604	-1.049542	1.335349
H	-7.801991	-0.407139	-1.060427
H	-5.657149	0.252304	-2.058989
C	-3.168657	0.387558	-0.808934
N	-2.127286	0.403483	-0.095479
Mg	-0.171379	0.647385	-0.256938

C	-3.181232	0.739853	-2.291662
H	-3.863054	1.572601	-2.512871
H	-2.172765	1.033262	-2.600405
H	-3.504639	-0.106160	-2.914316
Mg	2.179872	-0.910638	-0.092670
O	4.057353	0.013723	-0.166834
C	4.788894	0.280531	1.055534
C	4.981559	-0.325821	-1.228844
C	6.235976	0.404276	0.628152
H	4.365708	1.180954	1.510408
H	4.639333	-0.567198	1.740556
C	6.302204	-0.579266	-0.533529
H	4.593216	-1.202078	-1.760180
H	5.031355	0.524966	-1.921366
H	6.927035	0.168011	1.441529
H	6.448419	1.423134	0.281222
H	6.336361	-1.610310	-0.158982
H	7.158230	-0.422511	-1.195114
O	-0.002589	2.718910	-0.435578
C	1.251367	3.437558	-0.356401
C	-1.064111	3.513951	0.150254
C	0.992922	4.558920	0.625957
H	2.028812	2.734026	-0.037741
H	1.493434	3.815562	-1.358872
C	-0.465413	4.892611	0.335362
H	-1.927923	3.471490	-0.520202
H	-1.343591	3.061794	1.112811
H	1.674348	5.402216	0.485629
H	1.103264	4.189684	1.654143
H	-0.547012	5.476014	-0.590238
H	-0.956438	5.450782	1.136805
O	0.064906	-1.632710	0.061834
C	-0.427504	-2.390662	-1.083407
C	-0.468947	-2.214229	1.289162
C	-1.093999	-3.614386	-0.493026
H	-1.141878	-1.749757	-1.619016
H	0.423371	-2.619728	-1.732814
C	-1.619668	-3.079616	0.832580
H	0.334720	-2.801208	1.755066
H	-0.751612	-1.390258	1.949184
H	-0.350021	-4.402423	-0.319937
H	-1.873610	-4.012334	-1.148148
H	-1.860151	-3.863451	1.555899
H	-2.510577	-2.457514	0.671896
Cl	3.011161	-3.105776	-0.023292
Cl	1.391050	0.571018	1.739582
C	1.398392	0.253278	-1.863972
H	1.935915	1.203631	-2.000814
H	1.996958	-0.482774	-2.431313
H	0.502875	0.325562	-2.508172

RC_{vi}_MgCl(μ-Cl)(μ-Me)$MeMg_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	0.772296	-0.574471	-1.130299
Mg	0.445825	2.166497	0.319176
O	-0.694060	-2.165583	-1.562005
C	-1.484736	-2.778884	-0.535322
C	-0.465793	-3.205182	-2.528424
C	-0.815644	-4.122416	-0.315890
H	-1.487314	-2.116694	0.335041
H	-2.516700	-2.890688	-0.903610
C	-0.324164	-4.500741	-1.724255
H	-1.335315	-3.238626	-3.202283
H	0.432292	-2.936615	-3.091761
H	-1.497003	-4.860706	0.116434
H	0.033184	-4.000983	0.367168
H	-0.925629	-5.300496	-2.167428
H	0.717275	-4.834048	-1.701647
O	0.158096	3.768572	-1.022603
C	0.546604	3.638746	-2.409899
C	-0.996494	4.629359	-0.912835
C	-0.269425	4.678988	-3.150654
H	1.630238	3.776803	-2.477699
H	0.303684	2.614643	-2.732295
C	-1.547069	4.722455	-2.320904
H	-1.690851	4.189762	-0.187541
H	-0.667562	5.606570	-0.534958
H	-0.435304	4.407800	-4.198331
H	0.234544	5.652898	-3.128289
H	-2.175799	3.848826	-2.542104
H	-2.144779	5.624189	-2.477641
N	0.787522	-1.130214	1.039399
C	0.737776	-1.154407	2.198233
C	0.651201	-1.168224	3.619934
C	1.225713	-2.218465	4.346324
C	-0.021245	-0.122897	4.266278
C	1.121877	-2.216635	5.729018
H	1.744386	-3.017648	3.824474
C	-0.114259	-0.136765	5.649970
H	-0.448055	0.687921	3.679004
C	0.454170	-1.179909	6.377228
H	1.563849	-3.025145	6.303890
H	-0.630161	0.669630	6.162974
H	0.377638	-1.184370	7.461329
C	-1.072258	0.788923	-0.533184
H	-1.489046	1.652490	-1.086785
H	-1.525299	-0.066395	-1.051203
H	-1.583364	0.782040	0.447695
C	0.122611	2.943547	2.269156
H	-0.884503	2.731606	2.666198
H	0.831903	2.591990	3.034275
H	0.211627	4.042707	2.262810
Cl	2.506474	1.350753	-0.646229
O	0.499311	0.082942	-3.146297
C	1.568083	0.362815	-4.067751
C	-0.685440	-0.052526	-3.938474
C	0.932461	1.184177	-5.195850
H	2.346775	0.886230	-3.504390
H	1.975145	-0.591179	-4.431211
C	-0.581373	1.079219	-4.941986
H	-0.677187	-1.035564	-4.436794
H	-1.548137	0.001885	-3.269079
H	1.206699	0.772173	-6.171530
H	1.271349	2.225355	-5.178489
H	-1.155913	0.881391	-5.850941
H	-0.972512	2.003523	-4.496933
Cl	2.566170	-2.131253	-1.660158

TS_{vi}_MgCl(μ-Cl)(μ-Me)$MeMg_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	1.029702	-0.691036	0.633007
Mg	-0.698910	1.625852	0.479828
O	0.972848	-2.285524	-0.770245
C	-0.013362	-2.465103	-1.809627
C	1.791074	-3.471267	-0.654901
C	0.058028	-3.933860	-2.174324
H	-0.985066	-2.137380	-1.422062
H	0.262047	-1.824121	-2.660390
C	1.531523	-4.239188	-1.932746
H	2.831338	-3.154193	-0.514500

H	1.477342	-4.025058	0.238834
H	-0.268543	-4.122001	-3.200609
H	-0.568776	-4.528554	-1.498659
H	2.143988	-3.839713	-2.752504
H	1.748912	-5.305520	-1.829178
O	-0.539054	3.635222	-0.104430
C	0.691554	4.385934	0.032635
C	-1.287294	4.114566	-1.244787
C	0.531366	5.570315	-0.897806
H	0.812487	4.647267	1.087481
H	1.526949	3.737702	-0.267695
C	-0.311127	4.974840	-2.019370
H	-1.658535	3.249099	-1.806794
H	-2.146998	4.690090	-0.876306
H	1.494001	5.962930	-1.235514
H	-0.014182	6.380625	-0.398862
H	0.309721	4.348016	-2.672542
H	-0.814865	5.723054	-2.636840
N	-1.118051	-0.663547	0.867047
C	-2.253067	-0.335148	0.712693
C	-3.591337	-0.823045	0.394000
C	-4.087540	-0.661658	-0.901086
C	-4.340372	-1.494389	1.360530
C	-5.330797	-1.184583	-1.230558
H	-3.490538	-0.127675	-1.639668
C	-5.588685	-2.006152	1.024304
H	-3.940151	-1.613579	2.364505
C	-6.082978	-1.853428	-0.267604
H	-5.716153	-1.067647	-2.240075
H	-6.175741	-2.529043	1.774738
H	-7.058769	-2.256660	-0.526020
C	0.421983	0.876894	-1.242732
H	1.028790	1.755468	-1.521279
H	0.977665	0.025309	-1.655608
H	-0.472245	0.911101	-1.898652
C	-2.896242	1.779527	0.899798
H	-3.507530	1.969664	0.008714
H	-3.559890	1.421982	1.692397
H	-2.525729	2.758195	1.264992
Cl	0.979856	1.549559	2.196012
O	3.043655	-0.368064	0.093134
C	3.583121	-0.381655	-1.243757
C	4.118135	-0.312007	1.062739
C	5.057350	-0.680078	-1.066898
H	3.035508	-1.132604	-1.827547
H	3.417358	0.604305	-1.699617
C	5.354394	0.020078	0.253843
H	3.849798	0.434332	1.817444
H	4.187805	-1.293977	1.548942
H	5.658782	-0.316824	-1.904591
H	5.220203	-1.761631	-0.969670
H	5.436863	1.103393	0.100520
H	6.270688	-0.328195	0.737841
Cl	1.556400	-2.141780	2.481733

PR_{vi}_MgCl(μ-Cl)(μ-Me)$MeMg_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	0.984367	-0.465902	-0.765080
Mg	-1.951862	-1.401859	0.277706
O	2.734604	0.074271	0.384001
C	3.127944	1.453802	0.568673
C	3.913793	-0.740077	0.178463
C	4.563387	1.524073	0.095511
H	2.438478	2.090344	0.003344
H	3.035605	1.698516	1.636365
C	5.088505	0.156714	0.513257
H	3.835970	-1.630750	0.812751
H	3.933168	-1.053406	-0.875400
H	5.109271	2.360261	0.540963
H	4.594391	1.628157	-0.996389
H	5.293563	0.138588	1.591086
H	5.998323	-0.144388	-0.013055
O	-3.620366	-0.220413	-0.118799
C	-3.685175	0.849403	-1.087776
C	-4.904529	-0.406305	0.513790
C	-5.010995	1.534174	-0.823028
H	-2.808653	1.492575	-0.944767
H	-3.637055	0.409277	-2.092165
C	-5.876516	0.372149	-0.348496
H	-5.106449	-1.480437	0.569812
H	-4.850339	-0.002845	1.535793
H	-5.401651	2.036417	-1.711799
H	-4.905871	2.281953	-0.026311
H	-6.200900	-0.236161	-1.201598
H	-6.764426	0.686282	0.206373
N	-0.536252	0.149877	0.497121
C	-0.842758	1.234776	1.086153
C	-0.180714	2.541458	0.758061
C	0.275334	3.418127	1.746810
C	-0.017913	2.900617	-0.584005
C	0.921967	4.600112	1.400407
H	0.155319	3.162066	2.798066
C	0.606947	4.092687	-0.932800
H	-0.393331	2.234297	-1.361124
C	1.087961	4.941218	0.060862
H	1.295564	5.259800	2.180076
H	0.718783	4.357639	-1.981360
H	1.584901	5.870118	-0.208026
C	-2.542337	-2.920503	1.633763
H	-3.317349	-3.572793	1.200397
H	-1.744989	-3.596309	1.981881
H	-2.988612	-2.490119	2.546018
C	-1.950058	1.350934	2.111888
H	-1.602945	1.846569	3.026147
H	-2.770132	1.968716	1.718831
H	-2.345388	0.367378	2.387372
Cl	-1.097276	-1.732678	-1.982753
O	1.351612	-2.318205	0.131813
C	1.270749	-2.556518	1.558710
C	1.567322	-3.560488	-0.571467
C	1.610218	-4.024834	1.732404
H	1.958362	-1.867364	2.061294
H	0.245387	-2.334799	1.885257
C	1.134310	-4.622920	0.412839
H	0.978741	-3.523397	-1.493990
H	2.636557	-3.641058	-0.818847
H	1.120442	-4.456087	2.610162
H	2.694145	-4.161699	1.841997
H	0.039636	-4.714532	0.405469
H	1.567805	-5.602159	0.193572
Cl	2.055860	0.136591	-2.779588

TS_MgCl(μ-Cl)(μ-Me)$MeMg_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	1.412091	-0.880202	-1.055446
Mg	0.352109	2.367661	0.619096
O	-0.077766	-2.352859	-1.316011
C	-1.311903	-2.532593	-0.580030
C	0.093732	-3.434940	-2.259122
C	-1.876402	-3.859992	-1.053280

H	-1.083650	-2.504676	0.490789
H	-1.968761	-1.683236	-0.814216
C	-1.302120	-3.978584	-2.460255
H	0.568489	-3.026734	-3.157806
H	0.769602	-4.181684	-1.821958
H	-2.969008	-3.875017	-1.023266
H	-1.507300	-4.680136	-0.425724
H	-1.861909	-3.345900	-3.161773
H	-1.299774	-5.001340	-2.846075
O	0.213932	3.903964	-0.855600
C	0.483748	3.611025	-2.243114
C	-0.996090	4.683114	-0.748167
C	-0.492287	4.463182	-3.031516
H	1.538618	3.827706	-2.442180
H	0.312573	2.534812	-2.403977
C	-1.685883	4.521403	-2.085911
H	-1.575912	4.303801	0.101851
H	-0.723263	5.728261	-0.548984
H	-0.727871	4.032265	-4.010259
H	-0.084339	5.468395	-3.193915
H	-2.241284	3.573667	-2.111698
H	-2.381771	5.336379	-2.301994
N	1.187441	-1.244813	1.080275
C	1.136616	-1.145103	2.234134
C	1.065044	-0.930144	3.638145
C	1.041770	-2.001877	4.538245
C	1.014977	0.397178	4.083502
C	0.966602	-1.732583	5.896339
H	1.083751	-3.023140	4.170909
C	0.937756	0.646637	5.445171
H	1.032930	1.213620	3.361721
C	0.914238	-0.414440	6.347081
H	0.949016	-2.552947	6.607866
H	0.897772	1.673483	5.798916
H	0.855165	-0.214166	7.413674
C	-1.227716	1.039109	-0.000171
H	-2.228710	1.500417	0.039795
H	-1.109963	0.719552	-1.053412
H	-1.310751	0.116010	0.596662
C	0.707092	3.449667	2.438627
H	1.706728	3.321295	2.885791
H	0.621734	4.530110	2.229552
H	-0.010861	3.251030	3.252124
Cl	2.402094	1.305376	-0.454308
O	0.714847	-0.104958	-2.889011
C	1.633711	0.448567	-3.857014
C	-0.511141	-0.373855	-3.583282
C	0.761920	1.128001	-4.920024
H	2.297113	1.126214	-3.310360
H	2.232309	-0.372576	-4.273337
C	-0.678653	0.830945	-4.482103
H	-0.404227	-1.301834	-4.168454
H	-1.299834	-0.504796	-2.836379
H	0.965973	0.702090	-5.907203
H	0.959007	2.202858	-4.984268
H	-1.350143	0.636183	-5.322447
H	-1.098605	1.662538	-3.900535
Cl	3.256347	-2.159107	-1.723516

RC_{vi}_$MgCl(\mu\text{-}Cl)Me_2Mg_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
Mg	1.463918	-0.971806	-1.072114
Mg	0.240424	2.364009	0.596523
O	-0.067015	-2.396075	-1.310439
C	-1.316478	-2.494512	-0.587564
C	0.057168	-3.497716	-2.238599
C	-1.914581	-3.826055	-1.001061
H	-1.102502	-2.414286	0.483322
H	-1.945292	-1.640430	-0.877779
C	-1.355907	-4.009060	-2.407195
H	0.523002	-3.116974	-3.153792
H	0.720802	-4.254315	-1.799754
H	-3.006919	-3.815942	-0.961505
H	-1.556405	-4.628445	-0.344641
H	-1.905652	-3.385601	-3.124641
H	-1.384834	-5.043862	-2.758195
O	0.188324	3.972812	-0.833400
C	0.522418	3.724351	-2.214859
C	-1.035779	4.732875	-0.759975
C	-0.456008	4.550659	-3.028342
H	1.574575	3.986008	-2.370429
H	0.400965	2.646902	-2.403501
C	-1.679688	4.567397	-2.119700
H	-1.635782	4.337472	0.068233
H	-0.786751	5.781398	-0.546891
H	-0.646090	4.115816	-4.015289
H	-0.075485	5.568997	-3.174534
H	-2.208231	3.605400	-2.168379
H	-2.389650	5.366131	-2.350357
N	1.219942	-1.322081	1.077875
C	1.177574	-1.209831	2.231088
C	1.119339	-0.985949	3.634579
C	1.170061	-2.049777	4.542810
C	1.011010	0.340623	4.071226
C	1.110416	-1.773230	5.900232
H	1.256766	-3.070591	4.182134
C	0.951029	0.597523	5.432374
H	0.972159	1.150602	3.343176
C	1.001058	-0.455672	6.342424
H	1.150062	-2.587388	6.617969
H	0.867008	1.624191	5.778935
H	0.955295	-0.249585	7.408572
C	-1.396665	1.164599	-0.123895
H	-2.370366	1.681270	-0.154265
H	-1.203513	0.841769	-1.164651
H	-1.571160	0.239793	0.450894
C	0.605905	3.384455	2.450579
H	1.614438	3.257747	2.877905
H	0.502233	4.469201	2.273759
H	-0.096792	3.153893	3.268864
Cl	2.313791	1.275307	-0.433539
O	0.801541	-0.236598	-2.934524
C	1.676275	0.521896	-3.806956
C	-0.473141	-0.415447	-3.573681
C	0.803174	0.997212	-4.965300
H	2.089281	1.341106	-3.206899
H	2.499983	-0.127636	-4.124113
C	-0.620936	0.808346	-4.446800
H	-0.456260	-1.339217	-4.173512
H	-1.232462	-0.506538	-2.790103
H	0.965538	0.372464	-5.850782
H	1.023625	2.032240	-5.244572
H	-1.354741	0.669307	-5.245173
H	-0.941435	1.662099	-3.833581
Cl	3.326369	-2.238966	-1.686033

RC_{gm}_$MeMg(\mu\text{-}Cl)_2MeMgZn$

Atom	Coordinate (Å)		
	x	y	z
C	3.191151	-2.812445	-0.169851
C	2.752697	-1.528661	0.177660

C	3.659021	-0.481281	0.398722
C	5.015886	-0.731913	0.264758
C	5.458717	-2.006715	-0.080723
C	4.552105	-3.042869	-0.295523
H	2.469926	-3.606875	-0.337525
H	3.286418	0.504999	0.671497
H	5.730296	0.068927	0.430361
H	6.523883	-2.195383	-0.184205
H	4.908609	-4.032749	-0.564069
C	1.365701	-1.246306	0.298232
N	0.242217	-0.970518	0.398085
Mg	-1.339687	0.498665	0.231788
C	-1.430176	2.626875	0.023949
H	-1.721712	2.828583	-1.017145
H	-0.875055	3.507774	0.377516
Cl	-3.007372	-0.389841	1.825526
Cl	-2.565820	-0.512473	-1.656710
Mg	-4.302914	-1.279420	-0.065830
C	-6.120027	-2.308908	-0.218935
H	-6.074190	-3.296741	0.259939
H	-6.944929	-1.765815	0.262052
H	-6.418027	-2.477668	-1.262579
H	-2.362495	2.686456	0.614122
Zn	0.901931	2.304194	-0.173712
C	1.613243	2.361370	1.652344
H	2.690691	2.565687	1.714226
H	1.114994	3.135349	2.252057
H	1.447555	1.411841	2.183969
C	1.058798	2.030331	-2.101156
H	0.509111	2.791377	-2.671423
H	2.090961	2.032378	-2.473149
H	0.623306	1.061164	-2.389124

TS_{gm}_MeMg(μ-Cl)$_2$MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	2.855228	2.396456	-0.353617
C	2.745776	1.047573	0.002444
C	3.893399	0.276892	0.185828
C	5.144684	0.851479	0.012600
C	5.254624	2.198414	-0.324420
C	4.110139	2.970096	-0.504562
H	1.951011	2.981524	-0.501573
H	3.792586	-0.772519	0.453311
H	6.038193	0.247770	0.146137
H	6.236701	2.648057	-0.446771
H	4.194532	4.021525	-0.766024
C	1.395167	0.502006	0.094217
N	0.289052	0.713024	-0.324347
Mg	-1.422305	-0.424353	-0.118094
C	-0.879226	-2.458740	0.610924
H	-1.430255	-2.148602	1.515222
H	-0.345902	-3.356785	0.953105
Cl	-3.261680	-0.396004	-1.701822
Cl	-2.788700	0.681021	1.594944
Mg	-4.628374	0.888900	-0.031411
C	-6.264037	2.189621	-0.160645
H	-5.971340	3.231994	0.024400
H	-6.746693	2.167791	-1.146855
H	-7.040664	1.946892	0.577930
H	-1.607482	-2.868331	-0.106532
Zn	1.041215	-1.787154	0.096934
C	2.132835	-2.468552	-1.387342
H	3.054322	-2.949084	-1.032950
H	1.601577	-3.208244	-1.998863
H	2.444315	-1.659309	-2.061435
C	1.510064	-0.786256	1.899469
H	1.720628	-1.794883	2.302462
H	2.337647	-0.164505	2.244771
H	0.583693	-0.433634	2.367665

PR_{gm}_MeMg(μ-Cl)$_2$MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	0.419281	3.627764	0.572498
C	0.175538	2.420399	-0.089201
C	1.226812	1.818705	-0.789582
C	2.492802	2.388724	-0.805590
C	2.730959	3.575415	-0.114614
C	1.690535	4.193255	0.571097
H	-0.383057	4.124964	1.113088
H	1.035777	0.906366	-1.351650
H	3.292170	1.915281	-1.372415
H	3.721878	4.022633	-0.121497
H	1.867158	5.122722	1.106850
C	-1.166549	1.760890	-0.054494
N	-1.280338	0.496208	-0.145883
Mg	-0.296837	-1.254638	-0.047486
C	-2.089975	-2.616193	0.030654
H	-1.304969	-3.212920	-0.471711
H	-2.990057	-2.982602	-0.479233
Cl	1.211166	-1.809098	1.802796
Cl	1.439456	-1.829841	-1.675060
Mg	3.089029	-1.877901	0.191078
C	5.178596	-1.854987	0.223641
H	5.608918	-1.426800	-0.691537
H	5.578079	-1.272089	1.064511
H	5.587263	-2.870261	0.320613
H	-2.144934	-3.014434	1.053199
Zn	-2.895133	-0.661661	-0.036368
C	-4.808549	-0.271501	-0.030884
H	-5.084913	0.368587	-0.879372
H	-5.423121	-1.177820	-0.101901
H	-5.123131	0.259493	0.876697
C	-2.352591	2.677736	0.101791
H	-3.278954	2.125792	-0.080384
H	-2.395670	3.084494	1.120315
H	-2.294092	3.534161	-0.579866

RC_{vi}_MeMg(μ-Cl)$_2$MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.075814	-1.863261	-1.069184
C	-1.574519	-2.053129	0.226235
C	-2.429287	-2.115458	1.334128
C	-3.796115	-1.998487	1.133902
C	-4.300794	-1.818894	-0.152699
C	-3.445311	-1.747234	-1.249563
H	-1.390481	-1.806134	-1.910762
H	-2.017291	-2.254260	2.329896
H	-4.471239	-2.048566	1.982927
H	-5.373517	-1.729393	-0.301240
H	-3.846614	-1.596877	-2.247356
C	-0.166537	-2.156234	0.395656
N	0.989420	-2.209633	0.490912
Mg	2.936710	-1.472329	-0.200173
C	4.433386	-2.781256	-0.864152
H	4.036628	-3.552308	-1.540214
H	5.233071	-2.268933	-1.417328
H	4.923263	-3.316117	-0.037843
Cl	3.177821	0.436240	1.436838

Cl	1.618775	0.138597	-1.647848
Mg	1.347827	1.572688	0.316912
C	-0.336603	1.161844	1.773256
H	-1.333443	1.318626	2.206975
H	0.347880	1.583144	2.528453
H	-0.193054	0.072739	1.804596
Zn	-1.051216	2.162301	0.045691
C	-2.829073	1.838909	-0.707165
H	-3.479616	2.722785	-0.695183
H	-2.761651	1.511893	-1.753182
H	-3.354384	1.042729	-0.161763
C	0.443022	3.344761	-0.844123
H	0.274892	3.203173	-1.919155
H	-0.002313	4.313401	-0.575650
H	1.527727	3.556610	-0.771738

TS_{vi}_MeMg(μ-Cl)$_2$MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	1.953865	-2.201519	0.037107
C	1.920950	-0.891644	0.537153
C	3.103798	-0.160934	0.646009
C	4.309578	-0.734376	0.265133
C	4.340830	-2.036324	-0.226316
C	3.162066	-2.769487	-0.339285
H	1.022135	-2.755913	-0.051765
H	3.075962	0.854142	1.032458
H	5.228739	-0.161722	0.352774
H	5.287054	-2.480831	-0.523818
H	3.183944	-3.785515	-0.723723
C	0.593256	-0.370998	0.854887
N	-0.550189	-0.721774	0.848803
Mg	-2.557431	-1.380769	0.777738
C	-3.715441	-2.554918	2.079407
H	-4.078315	-1.979749	2.942890
H	-4.602798	-2.983268	1.593496
H	-3.143181	-3.400619	2.486378
Cl	-1.859236	-1.976236	-1.709390
Cl	-3.041687	0.993538	-0.215798
Mg	-1.085723	0.276392	-1.375743
C	0.886018	1.144141	-1.821151
H	1.865643	1.596670	-1.605035
H	0.542748	1.689187	-2.713417
H	1.179847	0.129140	-2.140441
Zn	0.493097	2.062509	0.047981
C	0.897173	1.428553	2.009880
H	1.551155	2.301286	2.174958
H	-0.106900	1.653699	2.397129
H	1.308404	0.645110	2.656011
C	-0.065447	3.946666	0.039510
H	-0.941756	4.101212	0.682671
H	0.728146	4.599115	0.427150
H	-0.328749	4.318622	-0.958503

PR_{vi}_MeMg(μ-Cl)$_2$MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	2.105618	-0.277834	-1.279464
C	1.783737	-1.160097	-0.240247
C	2.810703	-1.683018	0.549517
C	4.124715	-1.285590	0.341437
C	4.434769	-0.390608	-0.679851
C	3.426419	0.101969	-1.500179
H	1.317489	0.074424	-1.945158
H	2.571968	-2.367837	1.361219
H	4.913023	-1.673248	0.981523
H	5.465644	-0.087190	-0.842346
H	3.665894	0.774674	-2.320038
C	0.345836	-1.459883	0.040043
N	-0.480163	-0.495554	0.212391
Mg	-2.596669	-0.980281	0.419619
C	-3.569308	-2.664190	1.146941
H	-3.107992	-3.050643	2.066891
H	-4.620147	-2.459007	1.388651
H	-3.570528	-3.490171	0.422008
Cl	-2.499011	-0.213098	-2.168528
Cl	-2.914624	1.455128	0.935645
Mg	-1.335340	1.224361	-0.782591
C	0.313154	2.660672	-0.805924
H	1.389264	2.863685	-0.882483
H	-0.125204	3.563028	-0.360674
H	0.019808	2.664034	-1.876121
Zn	0.784792	1.180252	0.622856
C	-0.028980	-2.913300	0.049614
H	0.735095	-3.530836	0.534196
H	-0.994872	-3.093480	0.534227
H	-0.095860	-3.260483	-0.990845
C	1.816595	1.275926	2.258622
H	1.694230	0.358880	2.847107
H	2.888403	1.389776	2.054572
H	1.507523	2.117934	2.886455

RC_{gm}_MeMg(μ-Cl)(μ-Me)MgClZn

Atom	Coordinate (Å)		
	x	y	z
C	2.667749	2.929459	0.069779
C	2.548628	1.582716	-0.295779
C	3.678068	0.776294	-0.498526
C	4.935778	1.334201	-0.329998
C	5.061297	2.673315	0.033622
C	3.934190	3.468401	0.231845
H	1.777412	3.531681	0.225162
H	3.550106	-0.267207	-0.780826
H	5.821024	0.723760	-0.480640
H	6.050554	3.103092	0.165935
H	4.044188	4.510395	0.516749
C	1.269308	0.985788	-0.439731
N	0.252042	0.437995	-0.545763
Mg	-1.362113	-0.920418	-0.176079
C	-1.042644	-3.034981	-0.332517
H	-2.056506	-3.198512	0.078900
H	-0.473869	-3.860272	0.121559
Mg	-3.805845	0.738626	-0.107993
H	-1.106129	-3.272698	-1.404465
Zn	1.057178	-2.308331	0.199297
C	2.003601	-2.534523	-1.505969
H	3.097396	-2.585491	-1.414494
H	1.695285	-3.452225	-2.026543
H	1.788137	-1.707760	-2.199877
C	1.180368	-1.782523	2.088537
H	0.326278	-2.125090	2.688974
H	2.079787	-2.194837	2.565182
H	1.238233	-0.692706	2.222361
Cl	-5.348637	2.436959	-0.342840
Cl	-2.309480	0.281284	1.744995
C	-2.932781	-0.485952	-1.739798
H	-3.594029	0.131648	-2.369337
H	-2.004344	-0.455929	-2.337097
H	-3.331034	-1.505663	-1.846678

TS_{gm}_MeMg(μ-Cl)(μ-Me)MgClZn

Atom	Coordinate (Å)		
	x	y	z
C	2.851112	2.460984	-0.132559
C	2.769850	1.083835	0.102480
C	3.932138	0.315340	0.162836
C	5.169367	0.919132	-0.009569
C	5.251748	2.292368	-0.226253
C	4.093068	3.061870	-0.285543
H	1.936210	3.045751	-0.185280
H	3.852586	-0.755237	0.336129
H	6.073115	0.317208	0.030340
H	6.223293	2.764212	-0.349038
H	4.156503	4.133647	-0.453350
C	1.431810	0.510992	0.211359
N	0.292206	0.751194	-0.085813
Mg	-1.344988	-0.500693	0.046323
C	-0.693455	-2.591858	0.401858
H	-1.250028	-2.426285	1.341461
H	-0.104029	-3.487132	0.647322
Cl	-2.854958	0.242829	1.811846
Mg	-4.112027	0.432857	-0.276379
H	-1.406090	-2.956680	-0.352450
Zn	1.154335	-1.760978	-0.123634
C	2.155470	-2.117194	-1.775017
H	3.131814	-2.575449	-1.569321
H	1.623586	-2.791232	-2.457808
H	2.357206	-1.190915	-2.329438
C	1.680714	-1.035515	1.786325
H	2.068369	-2.047751	2.006784
H	2.413906	-0.353161	2.220644
H	0.732087	-0.912618	2.322691
Cl	-5.993983	1.734127	-0.560914
C	-2.725540	-0.552314	-1.720760
H	-1.732473	-0.438812	-2.189712
H	-2.988600	-1.612844	-1.843064
H	-3.344451	-0.021762	-2.462303

PR_{gm}_MeMg(μ-Cl)(μ-Me)MgClZn

Atom	Coordinate (Å)		
	x	y	z
C	-0.851146	3.374503	-0.493498
C	-0.407460	2.221686	0.162225
C	-1.326660	1.498173	0.931553
C	-2.653388	1.897657	1.023636
C	-3.088829	3.030934	0.339176
C	-2.183493	3.768267	-0.416051
H	-0.157636	3.965549	-1.087282
H	-0.981479	0.627933	1.487825
H	-3.347516	1.329793	1.639734
H	-4.128055	3.342952	0.405221
H	-2.513996	4.657629	-0.946969
C	1.008842	1.752185	0.055102
N	1.307893	0.521054	0.187164
Mg	0.594694	-1.363643	0.018111
C	2.572049	-2.395251	-0.394022
H	1.814354	-3.197313	-0.475852
H	3.297549	-2.820791	0.312023
Mg	-2.292895	-1.863890	-0.448021
H	3.055135	-2.421847	-1.382333
Zn	3.062782	-0.354881	-0.011966
C	4.946685	0.150685	-0.004898
H	5.229712	0.674673	0.916831
H	5.608995	-0.719439	-0.096567
H	5.185562	0.825932	-0.836703
C	2.040361	2.815787	-0.222845
H	1.939032	3.198173	-1.246500
H	1.928667	3.674337	0.449528
H	3.045080	2.396112	-0.117756
Cl	-4.583822	-1.621163	-0.608930
Cl	-1.032629	-2.234607	1.637651
C	-0.652709	-1.457721	-1.874233
H	-0.484585	-0.397553	-2.119383
H	0.261968	-1.997922	-2.173436
H	-1.358929	-1.802116	-2.645772

RC_{vi}_MgCl(μ-Cl)(μ-Me)MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	-2.384337	-1.080315	-0.120363
C	-1.652872	-2.250112	0.133651
C	-2.280587	-3.499522	0.208381
C	-3.653167	-3.572298	0.029088
C	-4.386145	-2.414831	-0.224381
C	-3.755491	-1.174811	-0.299610
H	-1.882356	-0.114550	-0.167179
H	-1.692634	-4.391809	0.402345
H	-4.153197	-4.534569	0.084853
H	-5.461555	-2.480468	-0.365809
H	-4.330543	-0.274885	-0.500814
C	-0.245514	-2.143372	0.297836
N	0.900498	-2.003510	0.419298
Mg	2.728750	-0.916380	0.013911
Cl	1.646503	0.417067	-1.768577
Mg	1.277735	1.650995	0.347795
C	-0.492497	1.209775	1.769133
H	-1.518894	1.157321	2.155401
H	0.092622	1.656608	2.589628
H	-0.181789	0.155574	1.714811
Zn	-1.073443	2.466316	0.191330
C	-2.873227	2.493391	-0.590489
H	-3.232907	3.499415	-0.838870
H	-2.907107	1.911595	-1.522454
H	-3.614516	2.048476	0.088625
C	0.544608	3.590774	-0.572172
H	0.492163	3.537898	-1.666559
H	0.085505	4.546021	-0.280755
H	1.613480	3.775459	-0.345659
C	2.875980	0.683831	1.567902
H	3.964950	0.634131	1.403807
H	2.773773	1.652874	2.084708
H	2.647534	-0.033757	2.373706
Cl	4.526847	-2.333578	-0.197253

TS_{vi}_MgCl(μ-Cl)(μ-Me)MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	-1.780264	-2.395372	0.048761
C	-1.929318	-1.108921	-0.488705
C	-3.202084	-0.549829	-0.595564
C	-4.314047	-1.269738	-0.176682
C	-4.162976	-2.548611	0.351064
C	-2.893594	-3.110599	0.463879
H	-0.781518	-2.818507	0.132190
H	-3.315477	0.449905	-1.006021
H	-5.303651	-0.829489	-0.263782
H	-5.035782	-3.108566	0.676932
H	-2.770816	-4.108344	0.876701
C	-0.685619	-0.433724	-0.860737
N	0.487605	-0.654109	-0.895282
Mg	2.412974	-1.028841	-0.257359
Cl	2.883397	1.424387	-0.003074

Mg	1.087659	0.764468	1.521363
C	-1.080659	1.099054	1.789401
H	-2.122161	1.385005	1.576101
H	-0.868329	1.642153	2.724755
H	-1.174705	0.028665	2.031426
Zn	-0.789790	2.028479	-0.083379
C	-1.246614	1.290314	-2.002981
H	-2.006023	2.081306	-2.133474
H	-0.300958	1.625861	-2.451662
H	-1.604769	0.465772	-2.629172
C	-0.249919	3.915648	-0.196205
H	0.444662	4.070138	-1.032347
H	-1.108692	4.577007	-0.373069
H	0.250845	4.283113	0.708569
C	1.752408	-1.270370	1.966140
H	2.607560	-1.194507	2.654188
H	0.860775	-1.387968	2.605947
H	1.829568	-2.285903	1.542053
Cl	4.024159	-2.582380	-0.810413

PR_{vi}_MgCl(μ-Cl)(μ-Me)MeMgZn

Atom	Coordinate (Å)		
	x	y	z
C	2.330444	0.410502	1.281518
C	1.813198	1.263814	0.300699
C	2.691263	1.876902	-0.597600
C	4.049970	1.589138	-0.555095
C	4.552995	0.713583	0.404797
C	3.693681	0.135488	1.333458
H	1.656884	-0.023306	2.018955
H	2.303869	2.546951	-1.362837
H	4.720782	2.046400	-1.277992
H	5.616550	0.491451	0.434497
H	4.083219	-0.525804	2.103572
C	0.331870	1.442510	0.187710
N	-0.424560	0.414535	0.082741
Mg	-2.532652	0.462922	-0.027681
Cl	-2.410852	-1.872538	-0.942887
Mg	-1.113003	-1.519498	1.163262
C	0.814979	-2.642763	0.933477
H	1.884478	-2.804214	0.747353
H	0.342530	-3.607799	0.702987
H	0.796995	-2.517894	2.031914
Zn	0.829732	-1.178075	-0.537761
C	-0.139544	2.869071	0.188161
H	0.253280	3.404771	-0.685356
H	-1.231770	2.950157	0.172454
H	0.246792	3.393944	1.070201
C	1.554539	-1.011145	-2.340720
H	1.237169	-0.061218	-2.790222
H	2.651933	-1.017734	-2.351775
H	1.213173	-1.818849	-2.998828
Cl	-4.023346	2.178542	-0.423465
C	-2.659791	-0.311221	2.163505
H	-3.740022	-0.318919	1.940057
H	-2.607845	-0.936522	3.068900
H	-2.420466	0.700667	2.531313

RC_{gm}_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	-4.571604	2.544933	0.429547
C	-3.992436	1.345913	-0.001759
C	-4.697761	0.442199	-0.809601
C	-5.996189	0.752902	-1.183571
C	-6.579301	1.943845	-0.756951
C	-5.871566	2.836257	0.045804
H	-4.004594	3.230203	1.053070
H	-4.210128	-0.476818	-1.134378
H	-6.554689	0.064680	-1.811102
H	-7.597338	2.180591	-1.054645
H	-6.335091	3.762698	0.371654
C	-2.660729	1.005013	0.363700
N	-1.582249	0.668198	0.632525
Mg	0.123341	-0.640053	0.166546
C	0.302544	-2.288189	-1.311417
H	0.571956	-1.950479	-2.321603
H	-0.059421	-3.327620	-1.393265
Cl	1.863396	0.052497	1.871968
Cl	1.024335	1.166144	-1.385933
Mg	3.122017	1.171004	0.015944
C	5.103646	1.757280	-0.482348
H	5.517856	2.540476	0.172434
H	5.825554	0.923898	-0.463892
H	5.155596	2.167466	-1.505295
O	3.367120	-0.901698	-0.720173
C	4.165751	-1.828672	0.041412
C	3.621253	-1.080348	-2.128027
H	4.700501	-1.277581	0.824194
H	3.486543	-2.546362	0.524884
C	5.083116	-2.501676	-0.963179
C	4.245986	-2.454160	-2.235673
H	2.667010	-0.966881	-2.652067
H	4.312804	-0.292008	-2.464281
H	5.366080	-3.512418	-0.656173
H	6.000572	-1.913351	-1.093482
H	4.830524	-2.580047	-3.151172
H	3.464660	-3.225840	-2.213428
H	1.278083	-2.429046	-0.806223
Zn	-1.912592	-1.973083	-1.454093
C	-2.956194	-2.940162	-0.084494
H	-3.938042	-3.278255	-0.445886
H	-2.438242	-3.833545	0.294159
H	-3.154007	-2.309379	0.795819
C	-2.173738	-0.881064	-3.074119
H	-1.453528	-1.141774	-3.863187
H	-3.175524	-0.969344	-3.517711
H	-2.020644	0.190714	-2.875965
O	-0.555238	-1.901350	1.720656
C	0.087842	-3.173371	1.937208
C	-1.271045	-1.498814	2.903365
C	-0.044650	-3.435638	3.423711
H	-0.434342	-3.925988	1.330356
H	1.128353	-3.102022	1.598094
C	-1.370765	-2.756307	3.739960
H	-0.695434	-0.709983	3.410521
H	-2.238546	-1.090879	2.592198
H	0.772262	-2.944379	3.968368
H	-0.026266	-4.502439	3.662152
H	-1.514060	-2.542217	4.802429
H	-2.209381	-3.373733	3.392146
O	2.469230	3.107549	0.766832
C	1.210516	3.370210	1.422852
C	2.844703	4.244909	-0.039148
C	0.976858	4.857899	1.254459
H	0.429178	2.780520	0.921737
H	1.292758	3.036673	2.461639
C	1.603140	5.109535	-0.111289
H	3.676921	4.763082	0.457276
H	3.195743	3.883538	-1.012256
H	1.508676	5.424609	2.029355

H	-0.083939	5.119388	1.306310
H	1.836791	6.160119	-0.305084
H	0.937419	4.749577	-0.906245

TS_{gm}_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	4.004877	-1.072236	2.220130
C	3.833410	-1.377246	0.864370
C	4.917737	-1.811494	0.103336
C	6.166331	-1.944763	0.695795
C	6.333576	-1.657407	2.047921
C	5.252183	-1.222231	2.809735
H	3.149302	-0.724864	2.796007
H	4.769609	-2.029188	-0.951500
H	7.012442	-2.276792	0.100238
H	7.311236	-1.771133	2.509420
H	5.381889	-0.996211	3.864845
C	2.508011	-1.131801	0.311373
N	1.503528	-0.524546	0.538967
Mg	-0.206729	0.139523	-0.505401
C	0.281126	-0.700813	-2.644967
H	-0.538350	-1.361058	-2.318709
H	0.659530	-1.227641	-3.536024
Cl	-2.408274	1.148894	-1.298104
Cl	-1.623825	-1.906119	0.265480
Mg	-3.221607	-0.087522	0.693907
C	-4.227189	0.483218	2.466486
H	-3.858907	1.375258	2.996801
H	-5.297604	0.666282	2.272950
H	-4.197904	-0.333168	3.207368
O	-4.797051	-0.995141	-0.378312
C	-5.877362	-0.170113	-0.870323
C	-5.320968	-2.243042	0.128020
H	-5.747445	0.846242	-0.479557
H	-5.809026	-0.137072	-1.965210
C	-7.145440	-0.848871	-0.392607
C	-6.737371	-2.317289	-0.401774
H	-4.662005	-3.047196	-0.212123
H	-5.303207	-2.208110	1.228636
H	-8.002884	-0.626448	-1.033319
H	-7.386474	-0.528280	0.629194
H	-7.378088	-2.953526	0.214573
H	-6.742642	-2.710996	-1.425565
H	-0.164440	0.215966	-3.055907
Zn	2.202016	-0.753361	-1.916863
C	3.655892	0.505782	-2.374757
H	4.462539	0.027178	-2.947391
H	3.301817	1.352219	-2.980722
H	4.132134	0.932709	-1.479440
C	2.273750	-2.758691	-1.275129
H	2.546547	-3.080927	-2.296453
H	2.891144	-3.359466	-0.603103
H	1.221480	-3.014539	-1.103157
O	0.810240	2.001553	-0.781685
C	0.603892	2.837708	-1.945577
C	1.889445	2.539061	0.021134
C	1.295042	4.140011	-1.609257
H	1.066085	2.342676	-2.812008
H	-0.475499	2.919000	-2.108179
C	2.497071	3.648371	-0.812966
H	1.456821	2.927097	0.956128
H	2.582845	1.727516	0.265438
H	0.645848	4.765484	-0.981906
H	1.563305	4.710663	-2.502301
H	2.961906	4.420985	-0.194694
H	3.258667	3.236751	-1.487600
O	-1.084509	0.903082	1.437335
C	-1.258413	2.334443	1.662956
C	-0.619206	0.304666	2.677615
C	-0.634023	2.629496	3.024156
H	-0.767894	2.851194	0.831024
H	-2.330726	2.557856	1.633395
C	0.212724	1.391948	3.309259
H	-1.499204	0.049775	3.285963
H	-0.071790	-0.604057	2.417253
H	-1.416576	2.729199	3.785772
H	-0.056210	3.558685	3.017258
H	0.385181	1.225151	4.376073
H	1.187056	1.446054	2.803914

PR_{gm}_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.273791	3.154973	-0.001278
C	-2.508339	2.476451	-0.953038
C	-1.424550	3.130538	-1.543494
C	-1.103340	4.433660	-1.179126
C	-1.853558	5.092853	-0.207757
C	-2.937637	4.449744	0.382959
H	-4.123612	2.654856	0.463506
H	-0.823150	2.598219	-2.278101
H	-0.259137	4.933404	-1.648764
H	-1.596031	6.107934	0.085006
H	-3.525921	4.958980	1.143080
C	-2.820511	1.055456	-1.317325
N	-1.986464	0.119820	-1.130171
Mg	-0.201185	-0.528886	-0.317061
C	-0.287306	-2.308825	-2.158568
H	0.565249	-1.614988	-2.249128
H	-0.483059	-2.575607	-3.208456
Cl	1.850900	-1.876772	0.530015
Cl	1.549294	1.028582	-1.397333
Mg	3.009493	0.271640	0.409737
C	3.689962	1.420043	2.050262
H	3.098701	1.325111	2.974591
H	4.722904	1.146734	2.323566
H	3.716139	2.496867	1.820230
O	4.681377	-0.312240	-0.686334
C	5.569219	-1.330937	-0.167133
C	5.449016	0.712315	-1.366037
H	5.238866	-1.599669	0.842754
H	5.487805	-2.216295	-0.810406
C	6.947102	-0.707308	-0.222076
C	6.849486	0.145812	-1.481347
H	4.961919	0.920485	-2.323278
H	5.429324	1.622554	-0.747940
H	7.742179	-1.456491	-0.260489
H	7.111898	-0.072461	0.658275
H	7.608087	0.930736	-1.538224
H	6.936594	-0.482309	-2.376160
H	0.108611	-3.217155	-1.686573
Zn	-2.183703	-1.835390	-1.626110
C	-3.892379	-2.812250	-1.578276
H	-4.396538	-2.826448	-2.554873
H	-3.780274	-3.862194	-1.273174
H	-4.606175	-2.353435	-0.877495
C	-4.198790	0.862615	-1.904105
H	-4.366328	-0.185707	-2.169082
H	-4.972965	1.174176	-1.189833
H	-4.332741	1.490623	-2.794064
O	-1.569701	-1.858180	0.829186

C	-1.307774	-3.230309	1.232181
C	-2.763247	-1.372147	1.495107
C	-2.215834	-3.472138	2.419110
H	-1.558956	-3.884657	0.386098
H	-0.238324	-3.316589	1.446590
C	-3.421173	-2.606187	2.073773
H	-2.458217	-0.664450	2.280902
H	-3.366364	-0.839264	0.752998
H	-1.743091	-3.122039	3.346326
H	-2.458405	-4.531101	2.541820
H	-4.054863	-2.372697	2.933562
H	-4.036965	-3.096369	1.308791
O	0.135437	0.576584	1.482336
C	0.194679	0.016032	2.815863
C	-0.075398	1.998870	1.613204
C	-0.431578	1.060811	3.744451
H	-0.347132	-0.935112	2.788849
H	1.242574	-0.192464	3.062423
C	-1.017405	2.099801	2.787558
H	0.894077	2.478550	1.819028
H	-0.470586	2.367398	0.663698
H	0.341775	1.519206	4.371550
H	-1.181319	0.622760	4.410313
H	-1.060053	3.106800	3.212427
H	-2.031188	1.822676	2.465489

RC_{vi}_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	3.111304	-2.839817	-0.345329
C	2.547956	-1.896205	-1.214374
C	2.568391	-2.078484	-2.602865
C	3.154161	-3.226149	-3.117592
C	3.711365	-4.172239	-2.259401
C	3.693508	-3.980120	-0.879174
H	3.088344	-2.661719	0.728037
H	2.118440	-1.327648	-3.250408
H	3.177518	-3.383652	-4.191970
H	4.167417	-5.068740	-2.670923
H	4.134795	-4.720399	-0.218417
C	1.901996	-0.756629	-0.659480
N	1.340331	0.143348	-0.187295
Mg	-1.021573	0.229735	-1.599793
Mg	0.265870	1.671451	1.205736
C	2.302243	2.383436	1.765173
H	1.825648	3.323736	1.428763
H	3.065643	2.158550	1.008828
O	-0.750593	2.994318	2.460335
C	-0.181399	3.597789	3.643940
C	-2.188627	3.157449	2.459834
H	0.551922	2.901267	4.063670
H	0.330626	4.523174	3.346825
C	-1.365185	3.868717	4.547984
C	-2.462133	4.184312	3.538018
H	-2.491131	3.455309	1.450991
H	-2.643633	2.184488	2.692386
H	-1.171087	4.678784	5.256077
H	-1.619072	2.964616	5.117411
H	-3.472515	4.095601	3.946066
H	-2.337799	5.200485	3.143502
H	2.842387	2.706199	2.670743
Zn	2.060804	0.491092	2.805392
C	3.773846	-0.441452	2.509893
H	4.064796	-0.388654	1.449582
H	4.597637	0.027272	3.067813
H	3.781001	-1.502931	2.794081
C	0.389200	0.198452	3.850139
H	0.096362	-0.860068	3.845768
H	0.613849	0.454743	4.897398
H	-0.515194	0.765691	3.591651
O	-0.865315	-1.957216	-1.443385
C	-0.810330	-2.830773	-0.291417
C	-0.948996	-2.748000	-2.649775
C	-0.489013	-4.198012	-0.854961
H	-0.065956	-2.433846	0.408250
H	-1.787902	-2.814114	0.210488
C	-1.236998	-4.159223	-2.181483
H	-1.726666	-2.319342	-3.293468
H	0.012096	-2.681429	-3.178720
H	-0.807752	-5.006241	-0.191389
H	0.592406	-4.297971	-1.027096
H	-2.314532	-4.296365	-2.015677
H	-0.903335	-4.911493	-2.901278
Cl	-1.631742	0.098359	0.897799
O	-3.076732	0.209960	-2.070666
C	-3.930789	-0.917862	-1.786953
C	-3.538979	0.813873	-3.290314
C	-4.597562	-1.293105	-3.116777
H	-3.291446	-1.708056	-1.377401
H	-4.656979	-0.626503	-1.019112
C	-3.929009	-0.372316	-4.142265
H	-4.400413	1.459213	-3.065301
H	-2.721661	1.423331	-3.686850
H	-5.673938	-1.096410	-3.071822
H	-4.467059	-2.353379	-3.355942
H	-4.589537	-0.104569	-4.971291
H	-3.023956	-0.832001	-4.561202
Cl	-0.469406	2.762123	-0.871217
C	-0.011105	0.412986	-3.468282
H	1.050369	0.669329	-3.301108
H	-0.012697	-0.461446	-4.140884
H	-0.401422	1.251924	-4.069572

TS_{vi}_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	2.654624	-3.006291	0.653171
C	2.261635	-1.978598	-0.207192
C	2.226357	-2.184139	-1.589435
C	2.596065	-3.421027	-2.105738
C	2.979528	-4.449846	-1.250354
C	3.001005	-4.243775	0.128302
H	2.672437	-2.827425	1.726553
H	1.892932	-1.380195	-2.243384
H	2.579266	-3.580388	-3.181016
H	3.264552	-5.416403	-1.657859
H	3.296998	-5.048426	0.795817
C	1.768735	-0.707686	0.300048
N	0.861758	0.066778	0.213941
Mg	-0.996966	-0.004211	-1.164410
Mg	-0.096206	1.701946	1.429369
C	1.930339	2.234651	2.353903
H	1.279652	3.002080	2.796978
H	2.299742	2.623985	1.391566
O	-1.101209	3.011009	2.722746
C	-1.153272	2.676888	4.131099
C	-2.336861	3.658710	2.325035
H	-0.798909	1.647327	4.259447
H	-0.475548	3.354271	4.667999
C	-2.599015	2.879334	4.531895
C	-3.013013	4.032932	3.626457
H	-2.078739	4.504610	1.682283

H	-2.929164	2.935774	1.747794
H	-2.707088	3.094366	5.598276
H	-3.184929	1.982018	4.296531
H	-4.095865	4.132286	3.514080
H	-2.617640	4.982255	4.008833
H	2.806898	2.256492	3.015942
Zn	1.978723	0.163242	2.508108
C	3.710372	-0.073959	1.349017
H	3.871663	0.482761	0.418988
H	4.206068	0.516594	2.140341
H	4.222343	-1.035838	1.288806
C	1.209335	-1.174002	3.727067
H	0.525515	-1.854706	3.199768
H	1.985452	-1.803247	4.183889
H	0.630235	-0.734168	4.549438
O	-1.141845	-2.123358	-0.874065
C	-1.091746	-2.918861	0.332842
C	-1.256210	-2.984279	-2.025634
C	-0.954305	-4.351882	-0.141448
H	-0.251352	-2.569326	0.943433
H	-2.020130	-2.748302	0.894025
C	-1.704289	-4.317010	-1.467479
H	-1.958593	-2.524127	-2.730960
H	-0.271696	-3.055918	-2.511104
H	-1.363204	-5.066377	0.577999
H	0.103576	-4.598505	-0.309207
H	-2.789674	-4.315593	-1.295948
H	-1.463228	-5.150262	-2.133095
Cl	-1.965655	0.138799	1.484471
O	-3.078681	0.136486	-1.589369
C	-4.062103	-0.847410	-1.217044
C	-3.546284	0.769497	-2.788842
C	-4.808172	-1.212596	-2.508867
H	-3.522182	-1.685332	-0.763809
H	-4.726542	-0.412557	-0.460052
C	-4.106841	-0.383579	-3.590799
H	-4.323045	1.503956	-2.527700
H	-2.696865	1.284648	-3.244843
H	-5.863644	-0.930977	-2.431703
H	-4.770431	-2.286792	-2.716142
H	-4.780297	-0.064001	-4.390691
H	-3.277051	-0.942751	-4.043814
Cl	-0.731857	2.732724	-0.640587
C	-0.106643	0.080267	-3.104107
H	0.916896	0.491079	-3.051437
H	-0.015272	-0.886466	-3.628604
H	-0.637326	0.747439	-3.804828

PR_{vi}_MeMg(μ-Cl)$_2$MeMgZn$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	2.362859	-2.513665	-0.876552
C	2.880151	-1.241689	-1.145463
C	3.812985	-1.099011	-2.177357
C	4.191952	-2.195798	-2.942394
C	3.673222	-3.457673	-2.664783
C	2.763016	-3.616009	-1.624016
H	1.658674	-2.631145	-0.052988
H	4.224297	-0.118207	-2.407736
H	4.899839	-2.065885	-3.757362
H	3.983685	-4.316650	-3.254501
H	2.369842	-4.603329	-1.387558
C	2.423736	-0.083000	-0.312199
N	1.182973	0.101144	-0.048166
Mg	-0.153408	-0.722518	-1.469470
Mg	0.181031	1.780148	0.838222
C	1.635899	1.751335	2.880853
H	1.169210	1.868961	3.867731
H	1.507042	2.735320	2.397921
O	-1.076302	3.221648	1.765771
C	-1.381772	3.232977	3.182597
C	-2.243535	3.628922	1.014200
H	-1.072224	2.273628	3.608179
H	-0.800641	4.042981	3.642390
C	-2.875288	3.472707	3.272285
C	-3.141322	4.305904	2.025402
H	-1.905178	4.263398	0.190771
H	-2.721173	2.725988	0.596025
H	-3.159948	3.969236	4.203896
H	-3.412365	2.517391	3.211296
H	-4.189385	4.307039	1.713809
H	-2.826011	5.345324	2.179740
H	2.720285	1.708092	3.053007
Zn	1.274107	-0.141210	2.302901
C	3.552394	0.767620	0.214202
H	4.224234	1.066744	-0.597931
H	3.193185	1.669646	0.714149
H	4.163474	0.187578	0.921158
C	1.844204	-1.969663	2.661885
H	1.138064	-2.722068	2.284956
H	2.814867	-2.180848	2.192776
H	1.957451	-2.163807	3.735654
O	-0.909015	-2.579366	-0.881030
C	-1.253094	-3.095434	0.421808
C	-0.982549	-3.638824	-1.867073
C	-0.968702	-4.575532	0.318253
H	-0.665064	-2.546393	1.163586
H	-2.319420	-2.898864	0.611564
C	-1.438192	-4.871082	-1.102755
H	-1.671125	-3.328066	-2.661859
H	0.019519	-3.758809	-2.299273
H	-1.493590	-5.158271	1.079830
H	0.108678	-4.764076	0.423359
H	-2.531674	-4.955662	-1.125669
H	-1.019083	-5.790233	-1.520934
Cl	-1.321339	0.070103	1.911761
O	-2.023457	0.252369	-1.421558
C	-3.238436	-0.443398	-1.060500
C	-2.307046	1.255139	-2.427477
C	-4.354805	0.346301	-1.713509
H	-3.179015	-1.467566	-1.460762
H	-3.283141	-0.489100	0.033152
C	-3.668755	0.877861	-2.966467
H	-2.306155	2.240634	-1.940625
H	-1.498351	1.227727	-3.165429
H	-4.665501	1.178792	-1.068823
H	-5.233046	-0.271566	-1.919599
H	-4.186051	1.723616	-3.427367
H	-3.571613	0.080631	-3.716112
Cl	0.439393	3.179728	-1.069315
C	0.235867	-0.848452	-3.548506
H	0.737850	0.046350	-3.952800
H	0.882434	-1.698465	-3.819282
H	-0.687647	-0.965993	-4.143898

RC_{gm}_MeMg(μ-Cl)(μ-Me)MgCl Zn$_{THF3}$

Atom	Coordinate (Å)		
	x	y	z
C	-3.830675	-2.809575	-1.347627
C	-3.751084	-1.733861	-0.454331
C	-4.872636	-1.293414	0.261294
C	-6.081518	-1.946517	0.075857

C	-6.167759	-3.018038	-0.810211
C	-5.048625	-3.448442	-1.520105
H	-2.944786	-3.129847	-1.890106
H	-4.774996	-0.454108	0.947560
H	-6.959814	-1.619862	0.624550
H	-7.118999	-3.524761	-0.949303
H	-5.126703	-4.285085	-2.207899
C	-2.513049	-1.061725	-0.269411
N	-1.515564	-0.489919	-0.115503
Mg	0.233611	0.704875	0.503711
C	-0.047604	1.301096	2.636282
H	0.807795	0.679017	2.944218
H	-0.594002	1.466764	3.580578
Mg	2.853562	-0.287150	-0.341888
O	4.475882	-0.511355	0.973055
C	5.671022	0.283403	0.784385
C	4.833548	-1.831843	1.446497
H	5.626260	0.749525	-0.206936
H	5.680644	1.066469	1.553752
C	6.824322	-0.687941	0.935577
C	6.260871	-1.695868	1.929690
H	4.110260	-2.118460	2.214565
H	4.758623	-2.536756	0.604707
H	7.739328	-0.196456	1.276700
H	7.031050	-1.177461	-0.024697
H	6.790468	-2.652279	1.929899
H	6.284116	-1.288050	2.947907
H	0.344995	2.304059	2.405392
Zn	-2.016753	0.447537	2.385997
C	-3.438616	1.712786	1.803847
H	-4.419131	1.483386	2.248249
H	-3.231972	2.759072	2.076702
H	-3.594460	1.712629	0.713154
C	-2.030664	-1.357229	3.211267
H	-1.337560	-1.436679	4.061832
H	-3.016219	-1.647807	3.605249
H	-1.738848	-2.147341	2.503995
O	-0.812266	2.393145	-0.405277
C	-0.815254	3.680449	0.256362
C	-1.835889	2.381494	-1.427996
C	-1.486710	4.612822	-0.724452
H	-1.383745	3.588917	1.192548
H	0.220964	3.945342	0.490249
C	-2.565164	3.706144	-1.301548
H	-1.339803	2.279397	-2.404895
H	-2.482797	1.513018	-1.269372
H	-0.778424	4.920293	-1.504708
H	-1.881455	5.510739	-0.241800
H	-2.965216	4.049099	-2.259346
H	-3.396284	3.611149	-0.591046
O	1.029299	0.060735	-1.702419
C	1.240315	1.148514	-2.653163
C	0.530610	-1.087918	-2.436512
C	0.606249	0.691829	-3.964199
H	0.773382	2.041379	-2.222682
H	2.317430	1.323032	-2.753195
C	-0.284282	-0.476475	-3.548640
H	1.393486	-1.649551	-2.822299
H	-0.021732	-1.710499	-1.729465
H	1.383407	0.338654	-4.652052
H	0.060817	1.499746	-4.461276
H	-0.478593	-1.178868	-4.363772
H	-1.249399	-0.125304	-3.157784
Cl	4.134829	-0.864702	-2.243037
Cl	1.350901	-1.707756	0.874563
C	2.335765	1.729005	0.429544
H	3.249447	1.989098	-0.139983
H	1.705711	2.599842	0.197099
H	2.632033	1.836853	1.483456

TS_{gm}_MeMg(μ-Cl)(μ-Me)MgCl Zn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
C	-3.816924	-0.518987	-2.494948
C	-3.695455	-1.129673	-1.240865
C	-4.784239	-1.795650	-0.679821
C	-5.986824	-1.855276	-1.370707
C	-6.102714	-1.263418	-2.625866
C	-5.017178	-0.596215	-3.187490
H	-2.960322	0.006612	-2.912609
H	-4.676350	-2.252202	0.300912
H	-6.836622	-2.369342	-0.929721
H	-7.043221	-1.321106	-3.167993
H	-5.106674	-0.132972	-4.166574
C	-2.421788	-0.954917	-0.554873
N	-1.460939	-0.242833	-0.546227
Mg	0.242164	0.143496	0.653451
C	-0.300137	-1.243610	2.484570
H	0.534442	-1.776432	2.000389
H	-0.653538	-1.986262	3.217112
Mg	2.955513	0.025689	-0.385988
O	4.531688	-1.078253	0.435434
C	5.678874	-0.397728	0.997766
C	4.950913	-2.312206	-0.194876
H	5.648718	0.650967	0.680830
H	5.599557	-0.449271	2.091544
C	6.884637	-1.148187	0.469936
C	6.342423	-2.566487	0.342221
H	4.212633	-3.080424	0.050527
H	4.961206	-2.161943	-1.284896
H	7.749214	-1.064575	1.133721
H	7.166909	-0.759425	-0.516908
H	6.932785	-3.201563	-0.323530
H	6.291643	-3.049854	1.325742
H	0.121229	-0.447830	3.115562
Zn	-2.196934	-1.174333	1.698100
C	-3.777684	-0.216299	2.402763
H	-4.550047	-0.908664	2.766921
H	-3.548917	0.460991	3.238086
H	-4.261234	0.390456	1.622335
C	-2.149090	-2.942284	0.548737
H	-2.429978	-3.525788	1.444354
H	-2.725252	-3.371632	-0.273876
H	-1.083287	-3.105197	0.350638
O	-0.826969	1.908735	1.369738
C	-0.932506	2.236706	2.776320
C	-1.850361	2.622068	0.630189
C	-1.792162	3.480269	2.829348
H	-1.407512	1.390210	3.292004
H	0.078712	2.377252	3.173063
C	-2.757626	3.234968	1.677135
H	-1.354069	3.395831	0.024483
H	-2.348860	1.912407	-0.038888
H	-1.185535	4.375441	2.642875
H	-2.287916	3.595813	3.797113
H	-3.247979	4.142702	1.315416
H	-3.530272	2.516160	1.976488
O	1.129046	1.296462	-1.116743
C	1.334021	2.732565	-0.933325
C	0.637649	1.070857	-2.467678
C	0.773482	3.397712	-2.184535
H	0.809133	3.014814	-0.013220

H	2.406360	2.917406	-0.807733
C	-0.134913	2.327135	-2.781748
H	1.507237	0.943989	-3.128085
H	0.047408	0.151809	-2.446218
H	1.587027	3.626351	-2.883366
H	0.254804	4.333114	-1.954273
H	-0.306823	2.458209	-3.853570
H	-1.109329	2.300537	-2.273743
Cl	4.305889	1.109173	-1.986876
Cl	1.485474	-1.824362	-0.766051
C	2.261636	0.724671	1.618280
H	3.158351	1.363997	1.502856
H	1.602771	1.412707	2.168510
H	2.558573	-0.047106	2.343895

PR_{gm}_MeMg(μ-Cl)(μ-Me)MgCl Zn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
C	3.094538	-2.891858	-0.117393
C	2.422131	-2.270183	-1.171965
C	1.484281	-2.998908	-1.905578
C	1.209267	-4.322560	-1.576216
C	1.868661	-4.930612	-0.510402
C	2.812643	-4.212855	0.218742
H	3.837982	-2.330039	0.450168
H	0.958364	-2.514262	-2.726241
H	0.474445	-4.880664	-2.151849
H	1.650445	-5.964056	-0.252161
H	3.332037	-4.682942	1.051078
C	2.716608	-0.835044	-1.502928
N	1.949481	0.110553	-1.156003
Mg	0.194217	0.650137	-0.229649
C	0.539945	2.843530	-1.970289
H	-0.367658	2.222540	-2.042036
H	0.729999	3.144514	-3.011933
Mg	-2.589107	0.018800	0.218610
O	-4.283570	0.726754	-0.782154
C	-5.233165	1.582434	-0.101187
C	-4.976398	-0.121954	-1.730006
H	-5.013149	1.564120	0.972565
H	-5.100463	2.604756	-0.479132
C	-6.592993	1.014365	-0.448366
C	-6.358471	0.482375	-1.856868
H	-4.394447	-0.136187	-2.655670
H	-5.018299	-1.141152	-1.317675
H	-7.385231	1.765175	-0.387397
H	-6.841370	0.190909	0.233469
H	-7.102142	-0.252505	-2.176054
H	-6.352819	1.304977	-2.582587
H	0.240439	3.759581	-1.443633
Zn	2.309352	2.097392	-1.407679
C	4.122504	2.774332	-1.036452
H	4.690119	2.983765	-1.954703
H	4.127184	3.707291	-0.455070
H	4.723696	2.043745	-0.473848
C	4.017454	-0.651273	-2.245517
H	4.857139	-1.028733	-1.645090
H	4.015613	-1.236633	-3.174115
H	4.192172	0.403698	-2.477310
O	1.577014	1.604072	1.211674
C	1.408168	2.862636	1.915636
C	2.749330	0.917118	1.719553
C	2.407243	2.826040	3.054815
H	1.615407	3.676619	1.207061
H	0.366689	2.935808	2.246460
C	3.526348	1.974091	2.471352
H	2.414674	0.104259	2.384938
H	3.279073	0.485587	0.865392
H	1.969331	2.333162	3.932783
H	2.726763	3.828058	3.352887
H	4.188124	1.543470	3.227555
H	4.131436	2.559882	1.767485
O	-0.544319	-0.759480	1.314925
C	-0.509286	-0.348682	2.718342
C	-0.286133	-2.193459	1.244400
C	-0.124421	-1.590150	3.508440
H	0.229632	0.456335	2.798138
H	-1.496796	0.037553	2.990039
C	0.552119	-2.472522	2.465755
H	-1.254627	-2.711383	1.285120
H	0.199507	-2.393054	0.285913
H	-1.024617	-2.085778	3.891017
H	0.518629	-1.347583	4.359488
H	0.559899	-3.533657	2.730998
H	1.590519	-2.159963	2.284822
Cl	-3.811459	-1.139349	1.862202
Cl	-1.421051	-0.821107	-1.709915
C	-1.589626	1.981093	0.429635
H	-2.004871	2.143538	1.441642
H	-0.750918	2.688278	0.391409
H	-2.304956	2.437357	-0.274511

RC_{vi}_MgCl(μ-Cl)(μ-Me)MeMg Zn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
C	2.876533	-3.090476	0.320648
C	2.332118	-2.162671	-0.578079
C	2.423900	-2.345183	-1.963689
C	3.062413	-3.478919	-2.445442
C	3.603974	-4.407554	-1.558722
C	3.514939	-4.214720	-0.180944
H	2.793388	-2.915509	1.391513
H	1.976454	-1.606149	-2.627150
H	3.140145	-3.638607	-3.516942
H	4.103315	-5.292052	-1.945290
H	3.943731	-4.942299	0.501732
C	1.638238	-1.038546	-0.053808
N	1.042974	-0.155777	0.412693
Mg	-1.337671	-0.080066	-0.751666
Mg	-0.312295	1.092646	1.827734
C	1.671020	2.665231	1.969962
H	0.720542	3.221577	1.980752
H	2.054235	2.738670	0.943615
O	-1.331774	2.309369	3.231481
C	-0.716513	2.727533	4.474415
C	-2.433533	3.189751	2.913497
H	-0.671554	1.864777	5.147284
H	0.307983	3.053674	4.248955
C	-1.574445	3.869437	4.988494
C	-2.144409	4.448076	3.699141
H	-2.452715	3.317249	1.826872
H	-3.369177	2.712822	3.240382
H	-0.993089	4.587259	5.573274
H	-2.384853	3.489503	5.622777
H	-3.034697	5.064387	3.850103
H	-1.388356	5.050698	3.178306
H	2.337432	3.282929	2.591008
Zn	2.067850	0.838168	2.762930
C	3.776904	-0.141875	2.881855
H	4.162591	-0.397197	1.883767
H	4.582398	0.410396	3.384079
H	3.662981	-1.090817	3.426806

C	0.489949	-0.307323	3.544696
H	0.601958	-1.333876	3.161468
H	0.969566	-0.306354	4.536977
H	-0.578303	-0.185729	3.784448
O	-1.171799	-2.234053	-0.896630
C	-1.093254	-3.154571	0.215094
C	-1.158764	-2.972969	-2.142676
C	-0.680286	-4.476207	-0.395626
H	-0.383076	-2.751395	0.946873
H	-2.084023	-3.217064	0.688710
C	-1.382589	-4.416535	-1.745677
H	-1.933471	-2.557755	-2.797402
H	-0.185114	-2.819660	-2.625001
H	-0.977265	-5.328895	0.220627
H	0.409875	-4.511364	-0.532208
H	-2.454694	-4.623694	-1.626255
H	-0.979345	-5.114697	-2.484103
Cl	-0.143937	0.077811	-2.859313
O	-3.257554	-0.041318	-1.606318
C	-4.224467	-1.107861	-1.481577
C	-3.572804	0.749795	-2.771190
C	-5.042961	-1.089618	-2.770782
H	-3.665179	-2.042340	-1.338758
H	-4.834810	-0.931774	-0.587909
C	-4.192185	-0.248772	-3.719987
H	-4.280084	1.540315	-2.483070
H	-2.638397	1.197401	-3.121865
H	-6.009496	-0.601819	-2.600373
H	-5.239564	-2.097937	-3.145426
H	-4.775498	0.224592	-4.514299
H	-3.401581	-0.852445	-4.184650
C	-2.051239	-0.339678	1.403302
H	-2.901013	-0.751099	0.835491
H	-1.750934	-1.165030	2.064255
H	-2.562982	0.393570	2.052027
Cl	-1.053713	2.393563	-0.239386

TS_{vi}_MgCl(μ-Cl)(μ-Me)MeMgZn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
C	2.737280	-3.038333	0.707808
C	2.334851	-2.046668	-0.189328
C	2.282343	-2.310017	-1.562219
C	2.653731	-3.564992	-2.031352
C	3.054648	-4.555304	-1.138897
C	3.085202	-4.294430	0.230211
H	2.761376	-2.817779	1.773100
H	1.934439	-1.533599	-2.243700
H	2.625049	-3.768886	-3.098777
H	3.342620	-5.535794	-1.509630
H	3.389516	-5.070767	0.926989
C	1.853524	-0.747053	0.254407
N	0.982928	0.054034	0.082343
Mg	-0.998217	0.073384	-0.907981
Mg	-0.144118	1.677235	1.334625
C	1.896918	2.214305	2.269378
H	1.226820	3.017478	2.611035
H	2.354308	2.550057	1.325969
O	-1.163223	3.010899	2.614473
C	-1.089820	2.858069	4.050985
C	-2.448284	3.572346	2.246041
H	-0.619341	1.893570	4.274186
H	-0.453324	3.658197	4.453354
C	-2.520294	2.982371	4.527540
C	-3.072861	4.015686	3.553021
H	-2.272716	4.374579	1.524256
H	-3.039659	2.782988	1.762315
H	-2.585670	3.285173	5.575834
H	-3.044387	2.024800	4.409024
H	-4.164723	4.031759	3.502829
H	-2.726726	5.020102	3.826369
H	2.705615	2.257668	3.012781
Zn	1.905242	0.142713	2.446594
C	3.716831	-0.112018	1.419399
H	3.938227	0.470442	0.518318
H	4.149251	0.459020	2.260703
H	4.241317	-1.067410	1.372611
C	1.035663	-1.149385	3.656482
H	0.415986	-1.873529	3.107799
H	1.772203	-1.736500	4.221755
H	0.373300	-0.675384	4.392906
O	-1.105522	-2.104198	-0.899970
C	-1.027827	-3.013453	0.218766
C	-1.253960	-2.856214	-2.128293
C	-0.794341	-4.378883	-0.391040
H	-0.228161	-2.671248	0.887443
H	-1.985628	-2.980899	0.761974
C	-1.584492	-4.266597	-1.688871
H	-2.033044	-2.375208	-2.730165
H	-0.307250	-2.799944	-2.681096
H	-1.133334	-5.186430	0.263398
H	0.272985	-4.527381	-0.602562
H	-2.661017	-4.366435	-1.491619
H	-1.304788	-5.009570	-2.440711
Cl	-0.116373	0.091819	-3.159266
O	-3.020275	0.087204	-1.499459
C	-4.023152	-0.873440	-1.116750
C	-3.494100	0.784028	-2.666716
C	-4.892764	-1.102609	-2.358815
H	-3.493873	-1.771631	-0.780064
H	-4.597441	-0.471482	-0.272656
C	-4.192236	-0.298343	-3.457365
H	-4.185580	1.579363	-2.351544
H	-2.622854	1.222813	-3.160448
H	-5.905210	-0.720620	-2.190310
H	-4.978407	-2.165070	-2.607255
H	-4.885566	0.100568	-4.202714
H	-3.442547	-0.906548	-3.979902
C	-1.761207	0.175285	1.408128
H	-2.772966	0.591557	1.282491
H	-1.836951	-0.897540	1.187824
H	-1.583269	0.160682	2.499666
Cl	-0.756412	2.735647	-0.745700

PR_{vi}_MgCl(μ-Cl)(μ-Me)MeMg Zn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
C	3.265470	-2.638404	-0.499250
C	2.406540	-1.534921	-0.428870
C	2.008420	-0.916659	-1.616206
C	2.434385	-1.401430	-2.846119
C	3.264170	-2.518718	-2.907714
C	3.680679	-3.135064	-1.730746
H	3.591845	-3.134035	0.413574
H	1.364562	-0.041535	-1.570150
H	2.116867	-0.901264	-3.758741
H	3.594156	-2.902536	-3.870142
H	4.333122	-4.004118	-1.770731
C	1.877815	-1.057164	0.881463
N	0.694352	-0.586880	1.013190
Mg	-1.085524	-0.565039	-0.119604
Mg	0.252038	1.613571	1.552283

C	0.528486	1.049697	3.920593
H	-0.256363	1.521747	4.525410
H	1.190506	1.869785	3.587899
O	-0.377160	3.589675	2.007322
C	-1.171237	4.040422	3.122752
C	-0.575162	4.472661	0.873853
H	-1.581895	3.162368	3.632267
H	-0.517470	4.578505	3.823003
C	-2.216359	4.946632	2.511215
C	-1.420613	5.617373	1.397984
H	0.408837	4.765836	0.497206
H	-1.095048	3.902227	0.088168
H	-2.637759	5.649192	3.235136
H	-3.034641	4.346345	2.091944
H	-2.045403	6.058264	0.616890
H	-0.781729	6.407579	1.810917
H	1.172959	0.513089	4.631928
Zn	-0.198358	-0.540138	2.879579
C	2.804703	-1.233941	2.061308
H	3.862075	-1.169022	1.787062
H	2.590867	-0.478581	2.824243
H	2.638078	-2.222198	2.516948
C	-1.298627	-2.130543	3.223136
H	-2.010121	-2.323952	2.406301
H	-0.681356	-3.033974	3.322083
H	-1.890773	-2.043179	4.142106
O	-0.759998	-2.586572	-0.701508
C	-0.204789	-3.672235	0.069102
C	-1.044261	-3.026302	-2.049578
C	0.167892	-4.721439	-0.955944
H	0.640230	-3.287948	0.650403
H	-0.972709	-4.033072	0.771376
C	-0.927254	-4.535229	-1.999211
H	-2.037524	-2.651668	-2.323716
H	-0.296420	-2.578764	-2.719411
H	0.206446	-5.727578	-0.530050
H	1.150932	-4.485733	-1.388335
H	-1.868183	-4.984358	-1.652452
H	-0.683303	-4.964560	-2.974545
Cl	-1.133627	0.633839	-2.171774
O	-3.133657	-1.221827	-0.348046
C	-3.750532	-2.411777	0.157984
C	-4.206438	-0.420511	-0.864482
C	-4.915313	-2.706503	-0.794098
H	-2.983790	-3.191879	0.189180
H	-4.101088	-2.218244	1.184123
C	-5.044467	-1.422686	-1.633451
H	-4.760046	0.020821	-0.019562
H	-3.760903	0.374273	-1.468430
H	-5.828540	-2.919932	-0.230780
H	-4.708048	-3.577272	-1.424201
H	-6.079642	-1.093619	-1.757505
H	-4.614046	-1.566152	-2.631495
C	-1.948228	1.062510	1.413064
H	-2.397843	1.787095	0.712666
H	-2.666711	0.229075	1.464719
H	-2.065835	1.518908	2.407894
Cl	2.236947	2.419043	0.555769

RC_{vi}_MgCl(μ-Cl)Me_2Mg Zn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
Mg	-2.241131	-0.513276	1.088820
Mg	1.776332	-0.813609	0.010112
C	-0.051115	1.212677	-2.087758
H	-0.613856	0.883022	-1.201143
H	-0.400874	0.593277	-2.927121
H	-0.394723	2.237008	-2.300042
Zn	1.914154	1.056019	-1.822843
C	3.571252	1.229313	-2.889304
H	3.717327	0.367368	-3.556245
H	3.589791	2.119404	-3.533811
H	4.468809	1.287497	-2.255963
O	-3.642847	0.333682	-0.234571
C	-3.536563	1.499510	-1.088106
C	-4.920659	-0.315740	-0.440601
C	-4.925901	1.699871	-1.657701
H	-3.177751	2.338297	-0.482506
H	-2.789086	1.287730	-1.866151
C	-5.447504	0.270250	-1.732935
H	-4.745767	-1.396458	-0.465068
H	-5.569348	-0.079298	0.412951
H	-4.904381	2.209921	-2.624400
H	-5.541273	2.292970	-0.970119
H	-5.015804	-0.250388	-2.597598
H	-6.536442	0.204742	-1.803580
O	3.327582	-1.819078	0.999895
C	3.099723	-3.150202	1.524002
C	4.617464	-1.767560	0.341983
C	4.444076	-3.842416	1.441668
H	2.695049	-3.051071	2.535069
H	2.352470	-3.651186	0.889935
C	5.036526	-3.213498	0.186617
H	4.499551	-1.234489	-0.608986
H	5.305985	-1.202933	0.984082
H	4.345268	-4.929544	1.383002
H	5.056866	-3.599043	2.318379
H	4.575298	-3.646160	-0.711026
H	6.120802	-3.326583	0.106146
N	-1.417750	1.481198	1.289508
C	-0.724401	2.410050	1.262786
C	0.136414	3.537932	1.185218
C	0.922342	3.898150	2.286273
C	0.218019	4.235584	-0.026620
C	1.799299	4.964972	2.163483
H	0.846648	3.336817	3.213261
C	1.102470	5.297945	-0.132889
H	-0.398251	3.925179	-0.867048
C	1.890753	5.658268	0.958449
H	2.417919	5.253900	3.007870
H	1.179659	5.845056	-1.067709
H	2.585024	6.489396	0.868493
C	1.715726	-1.869416	-1.849218
H	1.095397	-1.496400	-2.677169
H	2.726442	-2.011699	-2.266386
H	1.339865	-2.885832	-1.628181
C	2.558124	1.226196	0.299699
H	2.439637	2.294595	0.058880
H	2.130857	1.156208	1.318452
H	3.642363	1.072609	0.412240
Cl	0.067568	-1.336305	1.701310
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C	-1.887562	-2.079582	-1.505561
C	-2.280100	-3.537703	0.325600
C	-1.629871	-3.508266	-1.942621
H	-2.634269	-1.550164	-2.109636
H	-0.957920	-1.489362	-1.490530
C	-1.299828	-4.193774	-0.621211
H	-1.946659	-3.508309	1.367651
H	-3.276324	-3.998261	0.279039
H	-0.816738	-3.564091	-2.672631
H	-2.530273	-3.947625	-2.389171

H	-0.271453	-3.956061	-0.316726
H	-1.412563	-5.280742	-0.652860
Cl	-3.591683	-1.013430	2.912273

TS_{vi}_MgCl(μ-Cl)Me_2Mg Zn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
Mg	1.552610	-2.285473	0.579127
Mg	0.312897	1.136670	1.639112
C	-2.212409	-1.537711	3.066886
H	-2.221838	-1.754963	1.990058
H	-3.235980	-1.270282	3.382839
H	-2.016501	-2.491400	3.574738
Zn	-1.690769	0.549252	3.050946
C	-3.054816	1.658703	3.997324
H	-4.070981	1.557755	3.587853
H	-3.125442	1.369046	5.057937
H	-2.824891	2.735077	3.995623
O	0.789344	-4.234115	0.863336
C	-0.002051	-4.737264	1.963727
C	0.961032	-5.262418	-0.136768
C	-0.120918	-6.227941	1.715852
H	0.501872	-4.478883	2.901280
H	-0.980691	-4.235097	1.943694
C	-0.090445	-6.299595	0.194087
H	0.849405	-4.795336	-1.122819
H	1.980180	-5.661494	-0.056929
H	-1.028309	-6.648419	2.157245
H	0.742427	-6.756596	2.138073
H	-1.064300	-6.007870	-0.221376
H	0.164806	-7.289095	-0.194027
O	0.464578	3.108567	1.023121
C	0.901053	3.482404	-0.308179
C	-0.525637	4.055287	1.502451
C	0.364457	4.882909	-0.516414
H	1.990724	3.399741	-0.343426
H	0.468753	2.770289	-1.026712
C	-0.936726	4.840411	0.275913
H	-1.339822	3.491997	1.973996
H	-0.048494	4.691959	2.258678
H	0.225500	5.117078	-1.575028
H	1.049624	5.624179	-0.087369
H	-1.709168	4.297583	-0.284312
H	-1.328933	5.828618	0.529607
N	0.588297	-1.761249	2.336446
C	0.050251	-1.579723	3.376365
C	0.217315	-1.688620	4.819993
C	-0.770592	-1.398059	5.760751
C	1.484283	-2.109991	5.247044
C	-0.494595	-1.527981	7.114970
H	-1.746478	-1.065281	5.415625
C	1.751817	-2.242011	6.602426
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C	0.763083	-1.950392	7.537879
H	-1.266407	-1.298060	7.844510
H	2.734989	-2.570828	6.928391
H	0.973177	-2.051184	8.599677
C	-1.672324	0.631949	0.829291
H	-1.262788	-0.189823	0.218902
H	-2.734530	0.384791	0.949592
H	-1.672510	1.530501	0.186037
C	0.256415	1.423677	3.803670
H	-0.103304	1.080318	4.779633
H	1.335488	1.171322	3.829452
H	0.196322	2.522631	3.850425
Cl	2.089215	0.260097	0.302679
O	0.214383	-2.142979	-0.993637
C	-1.144123	-2.616521	-1.002337
C	0.488596	-1.616501	-2.302711
C	-1.880190	-1.753887	-2.034302
H	-1.145851	-3.680636	-1.280703
H	-1.529050	-2.519603	0.019231
C	-0.782691	-0.872687	-2.649602
H	1.383427	-0.992399	-2.228350
H	0.683698	-2.457072	-2.986826
H	-2.662207	-1.148983	-1.565134
H	-2.354739	-2.386643	-2.790475
H	-0.768852	0.114316	-2.170106
H	-0.903009	-0.728346	-3.726465
Cl	3.593537	-3.012045	-0.318402

PR_{vi}_MgCl(μ-Cl)Me_2Mg Zn_{THF3}

Atom	Coordinate (Å)		
	x	y	z
Mg	1.328785	-1.197611	-0.374338
Mg	-0.220515	1.701721	0.014971
C	-2.074774	-0.372033	2.271199
H	-2.587212	0.176604	1.473573
H	-2.157503	0.176722	3.218718
H	-2.618805	-1.316714	2.405724
Zn	-2.312502	2.555486	1.150046
C	-3.930498	2.858486	2.219983
H	-4.705278	2.116995	1.980548
H	-3.721467	2.766533	3.294573
H	-4.383415	3.846817	2.068900
O	0.414348	-3.178912	-0.271392
C	-0.763907	-3.630685	0.424597
C	0.873241	-4.205271	-1.181574
C	-0.843874	-5.118997	0.150659
H	-0.654595	-3.384601	1.485460
H	-1.639071	-3.094095	0.025642
C	-0.257996	-5.211279	-1.252016
H	1.110375	-3.728586	-2.139841
H	1.792852	-4.642162	-0.773376
H	-1.865460	-5.501116	0.227046
H	-0.216751	-5.670100	0.862075
H	-1.003443	-4.908308	-1.999300
H	0.095521	-6.211970	-1.514741
O	-0.003957	3.613268	-1.049369
C	0.207654	3.681422	-2.471974
C	-0.490307	4.883519	-0.570010
C	0.328088	5.158477	-2.773103
H	1.095722	3.085116	-2.705043
H	-0.667267	3.245175	-2.983348
C	-0.696895	5.738682	-1.806847
H	-1.414050	4.720276	-0.000746
H	0.263797	5.302034	0.109003
H	0.122031	5.390776	-3.821310
H	1.336639	5.514673	-2.530077
H	-1.710702	5.595145	-2.202487
H	-0.558677	6.803402	-1.601422
N	-0.132700	-0.292127	0.770484
C	-0.639644	-0.650646	1.883105
C	0.156891	-1.379837	2.928720
C	-0.421605	-2.256312	3.854938
C	1.532313	-1.135060	3.015464
C	0.360658	-2.907617	4.802014
H	-1.491605	-2.452959	3.827423
C	2.314755	-1.774857	3.969091
H	1.979250	-0.406945	2.338158
C	1.730884	-2.670906	4.860078
H	-0.102822	-3.601328	5.499437

H	3.380214	-1.565520	4.022527
H	2.340573	-3.175584	5.605458
C	-2.437277	1.890179	-0.814943
H	-1.738158	1.494245	-1.579211
H	-3.231651	1.131386	-0.771761
H	-2.868129	2.771204	-1.316370
C	-0.437162	2.822874	2.029826
H	-0.435510	2.188595	2.927435
H	0.623240	2.853883	1.710646
H	-0.607728	3.850745	2.379593
Cl	2.042688	1.267529	-0.821021
O	0.409862	-1.193755	-2.250881
C	-1.011883	-1.406302	-2.396516
C	0.950391	-0.688171	-3.484559
C	-1.390385	-0.799373	-3.744834
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H	1.832123	-0.089894	-3.235806
H	1.246468	-1.536057	-4.120121
H	-2.336539	-0.252166	-3.694435
H	-1.496438	-1.584253	-4.502377
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H	-0.081580	0.280517	-5.148754
Cl	3.505784	-2.112548	-0.548269

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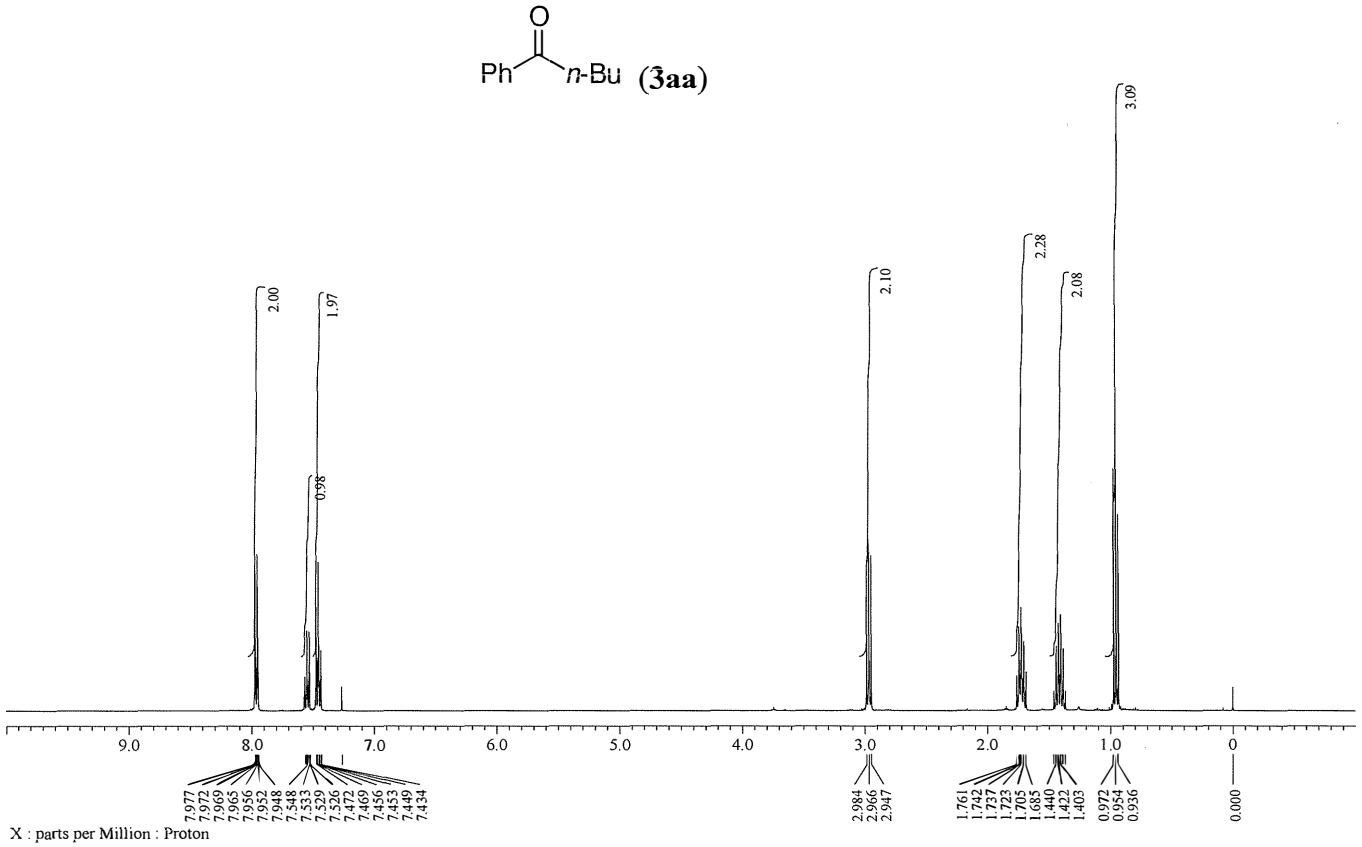

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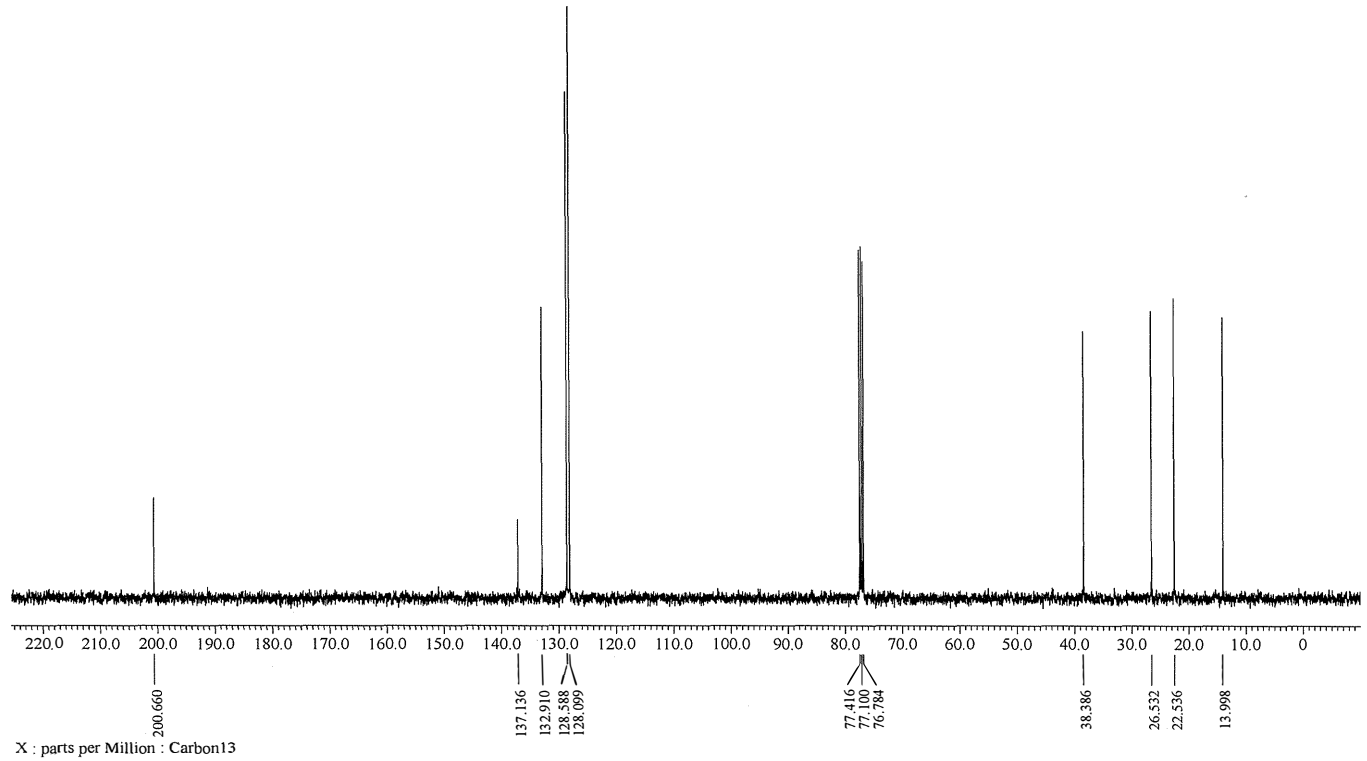

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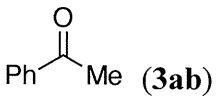

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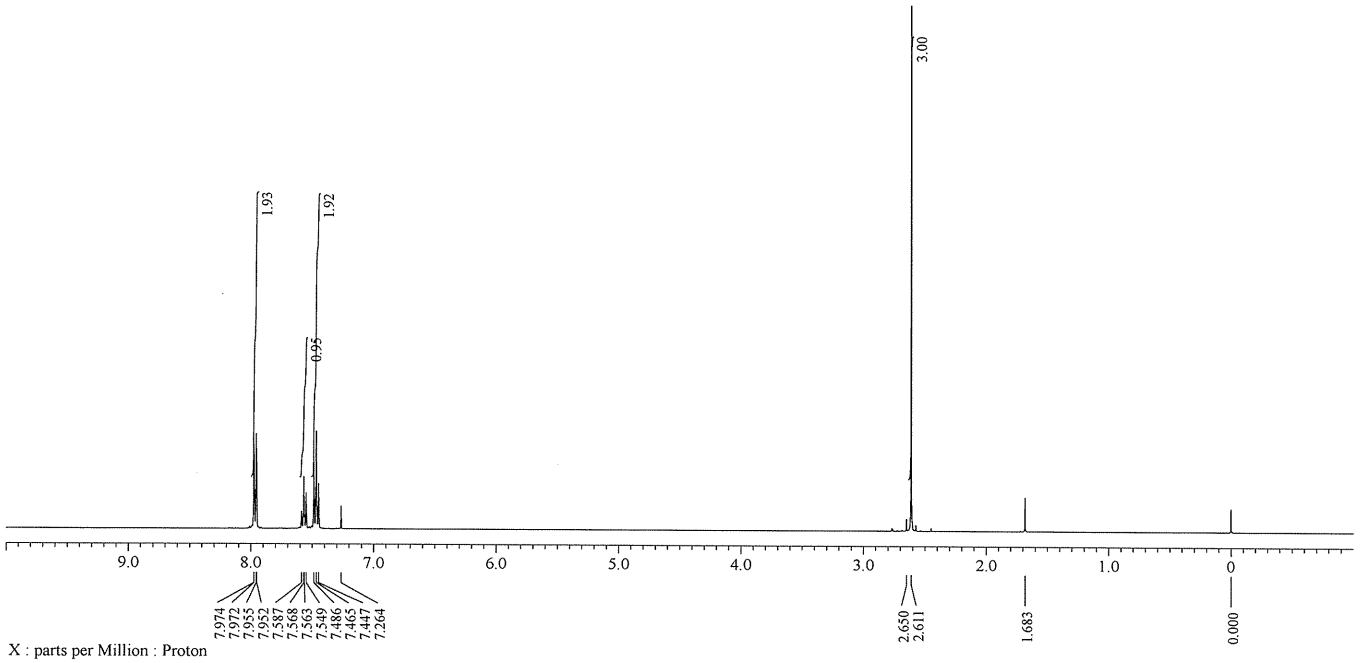

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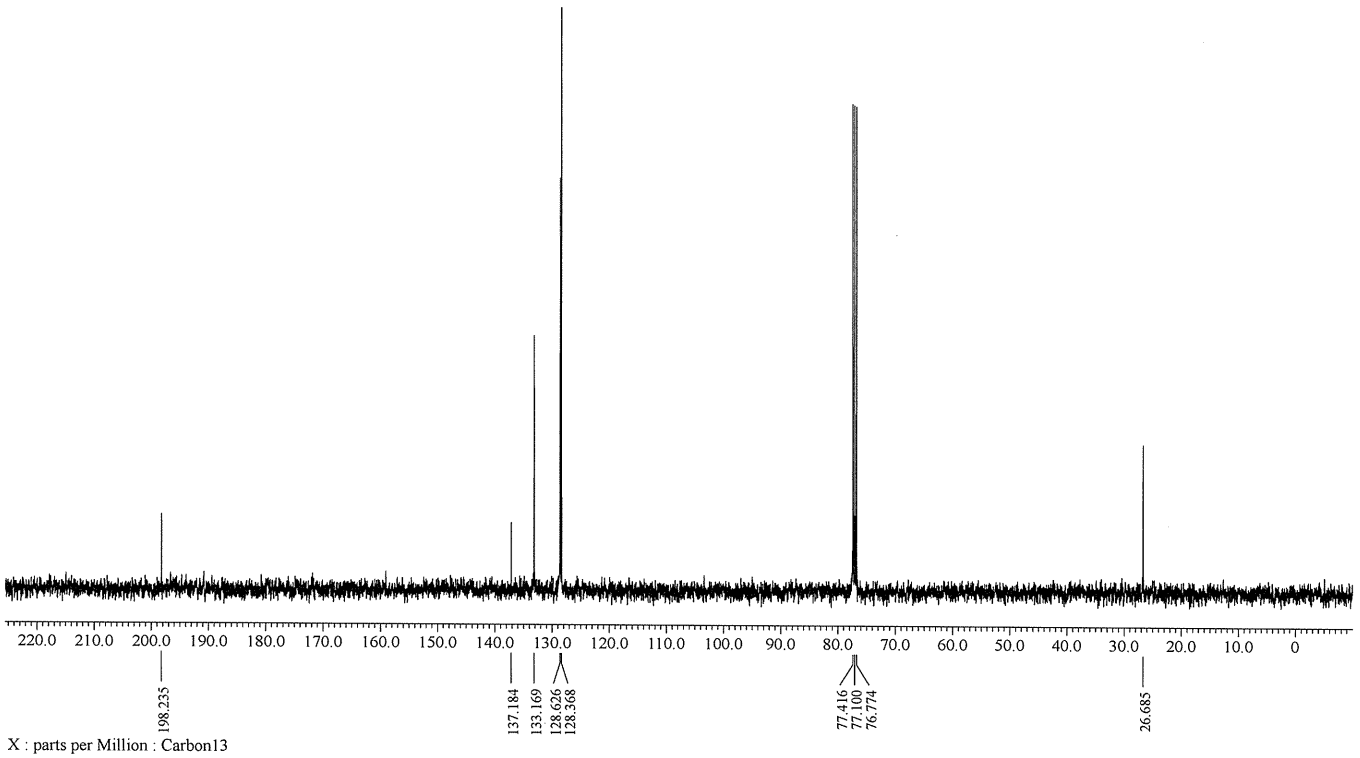

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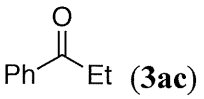

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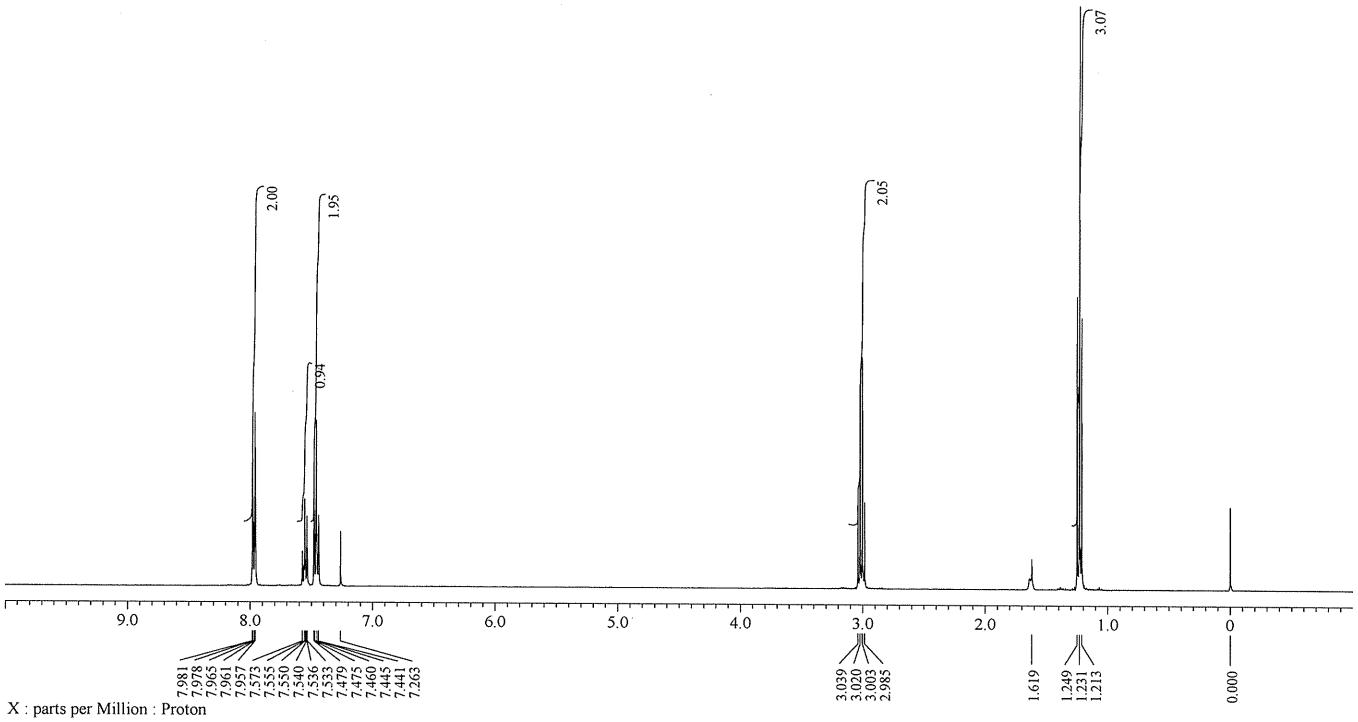

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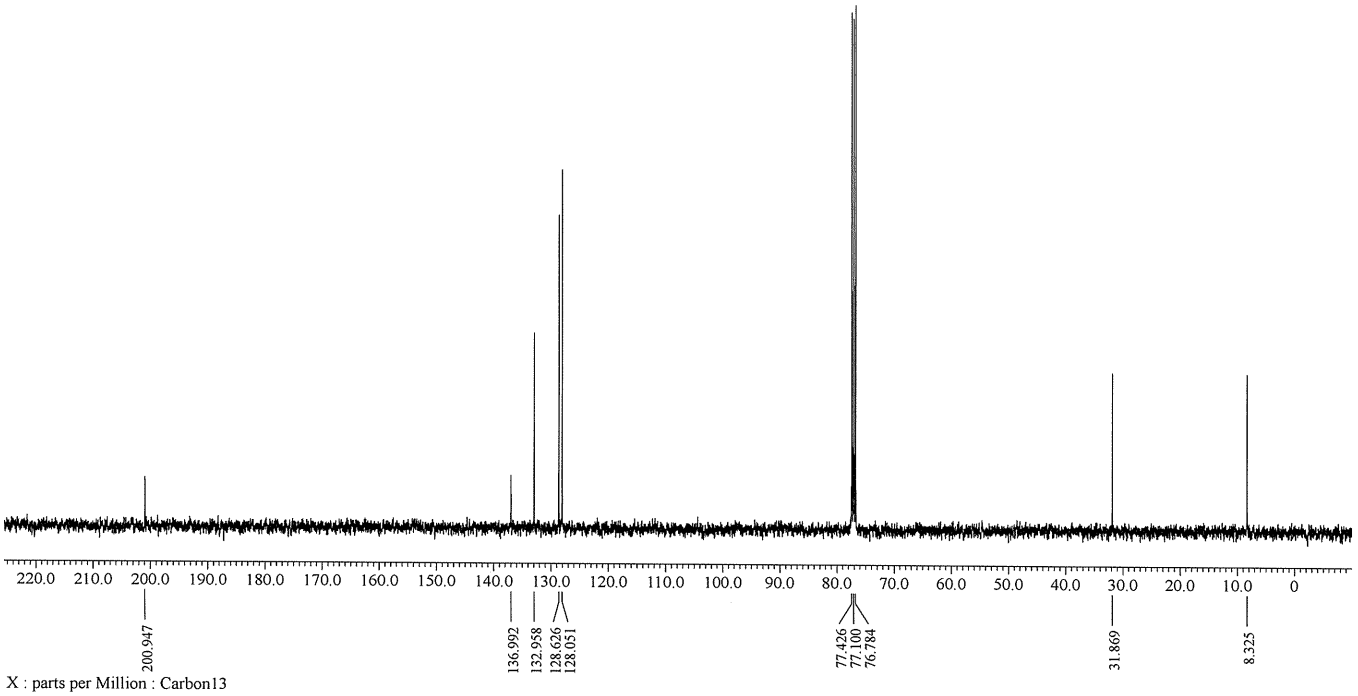

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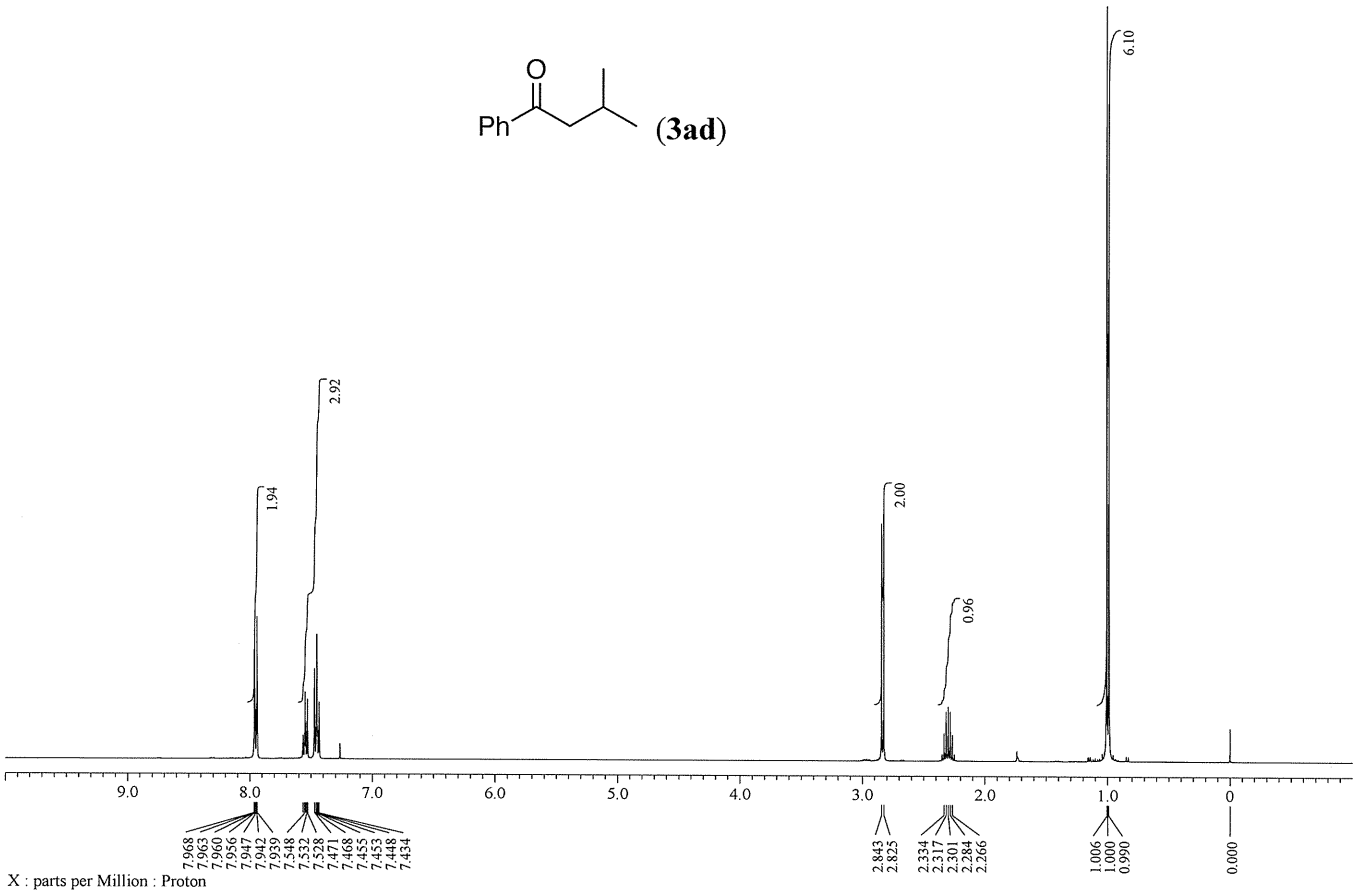

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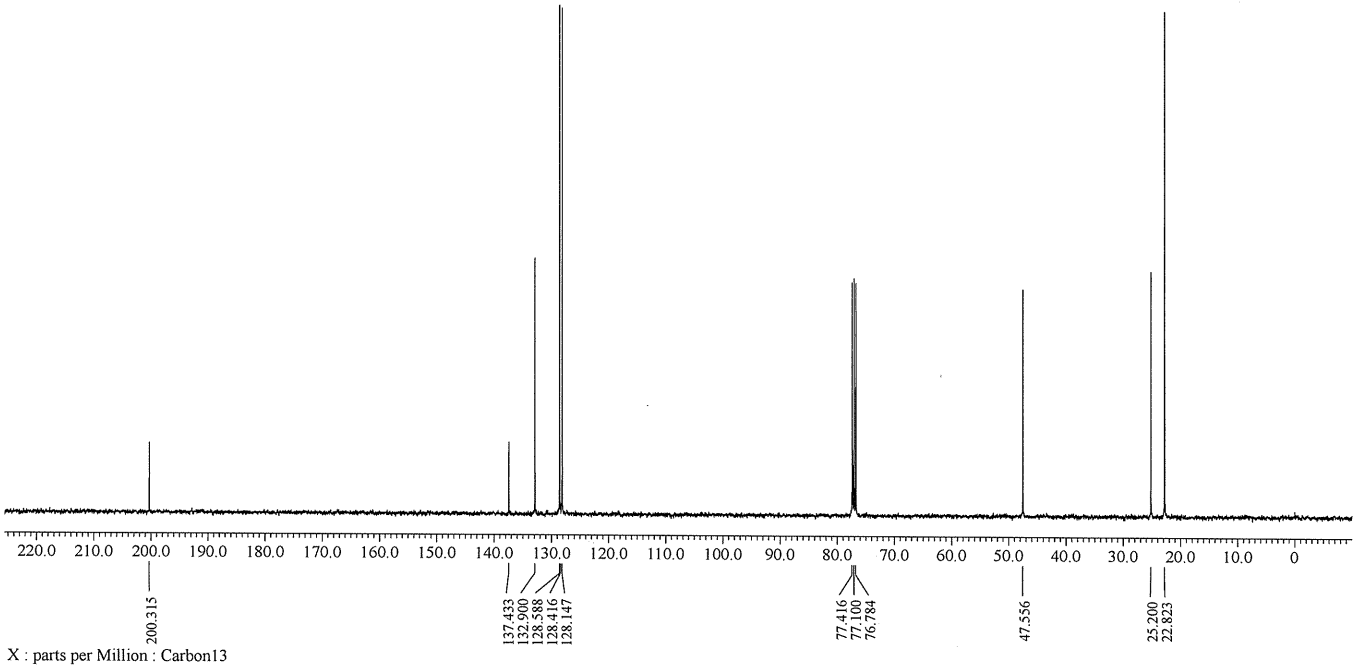

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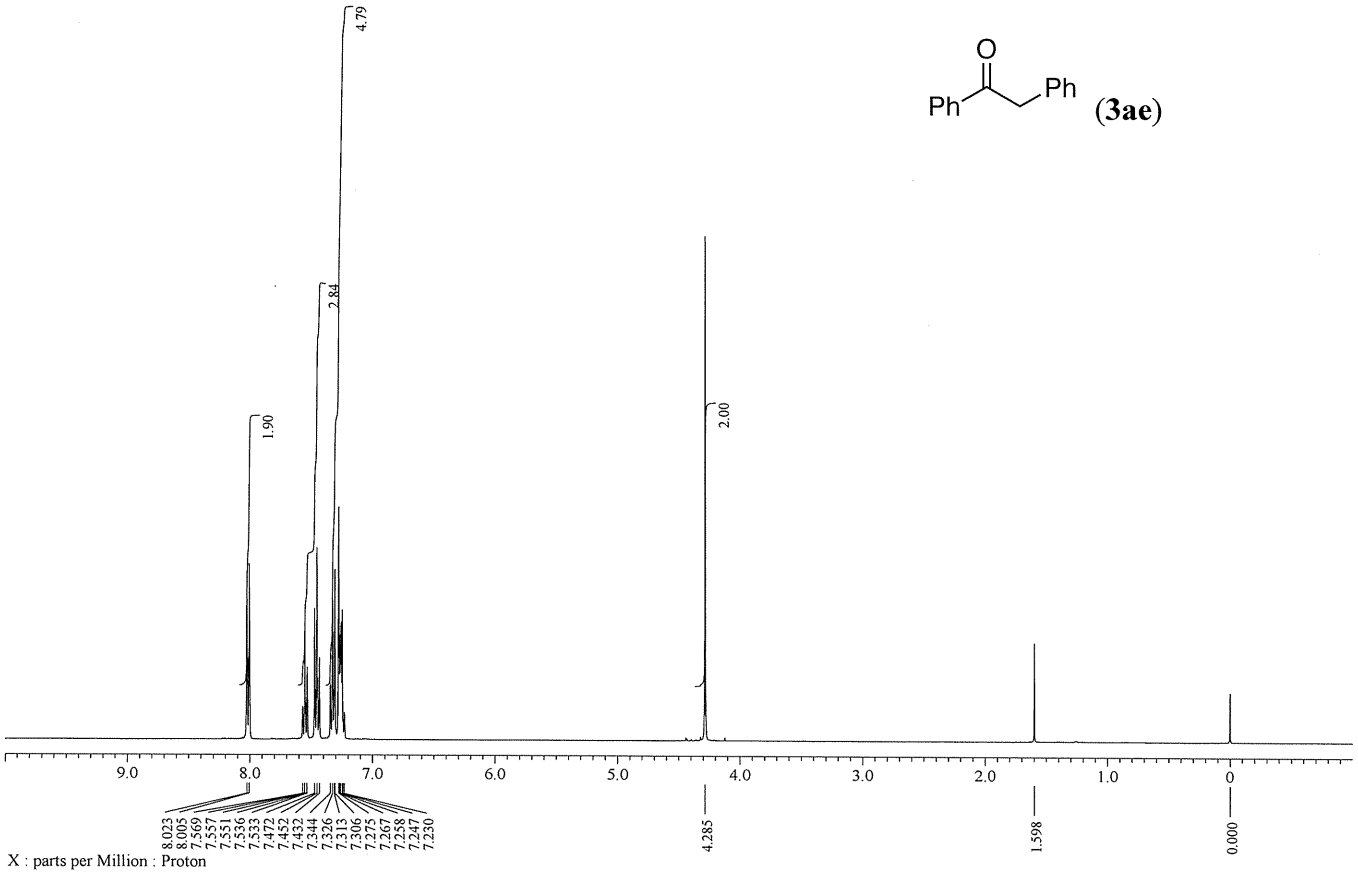
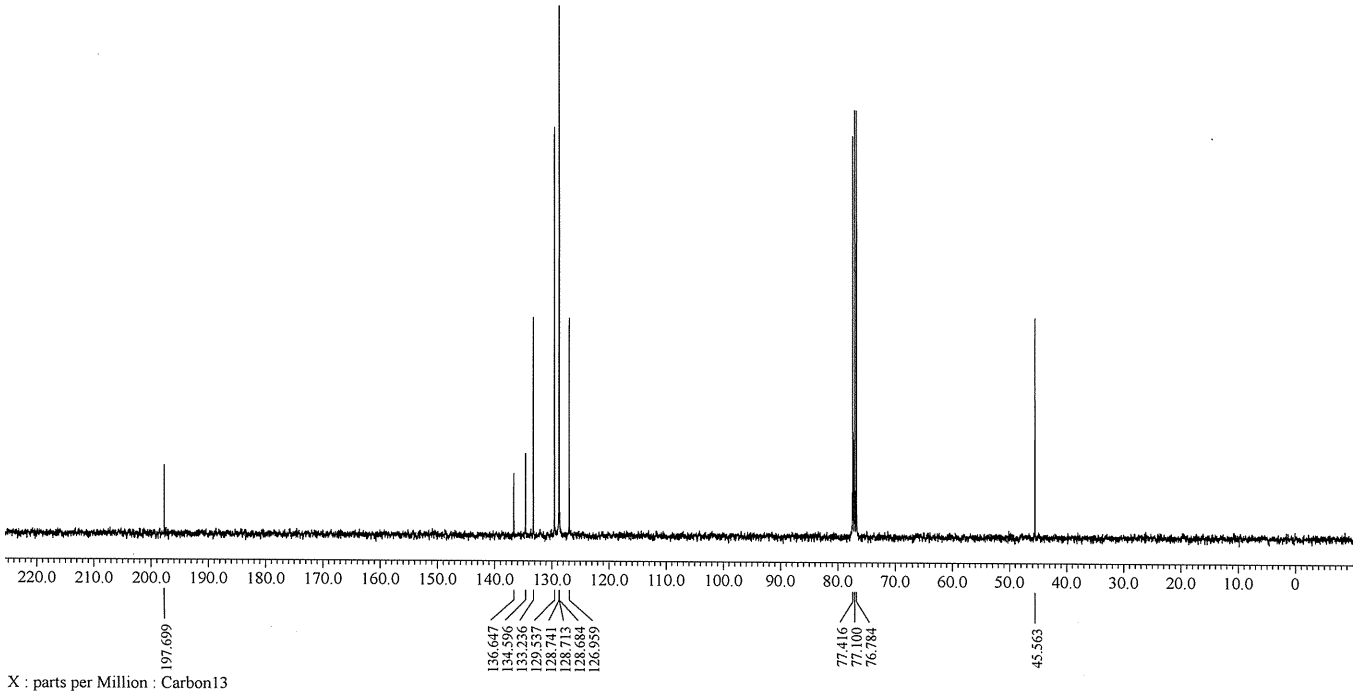
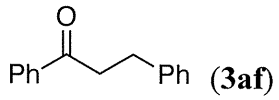


(3ae)

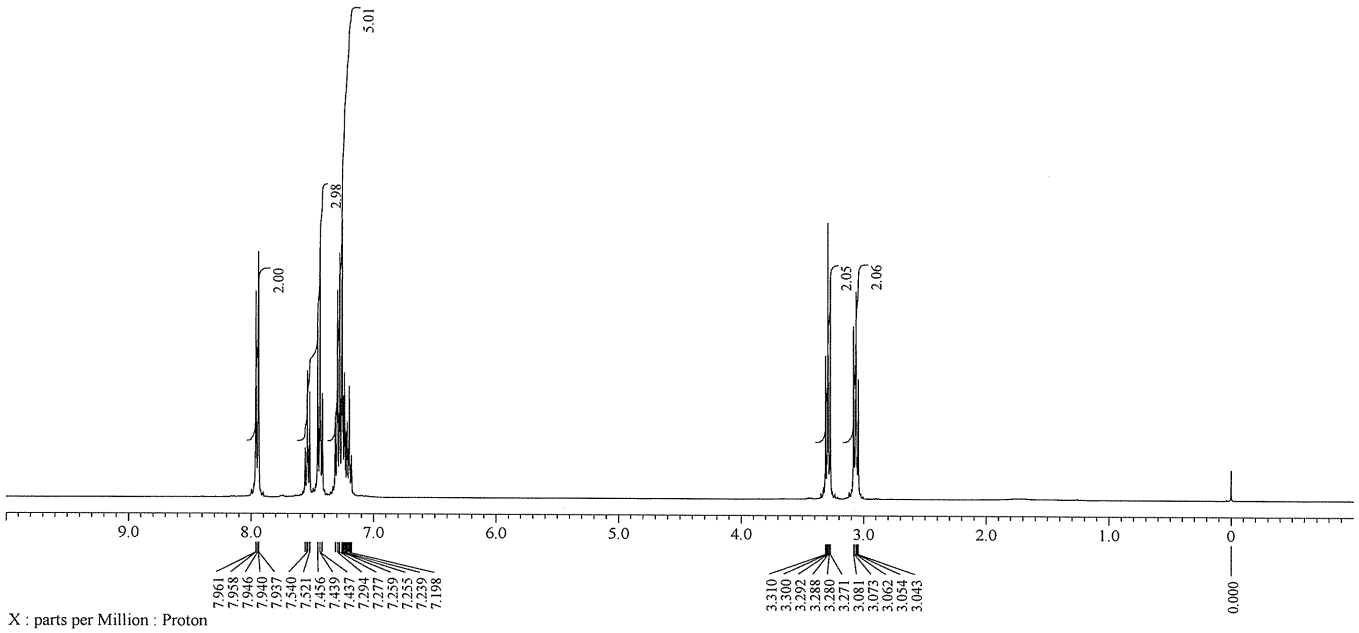
^{1}H NMR, 400 MHz, $CDCl_3$



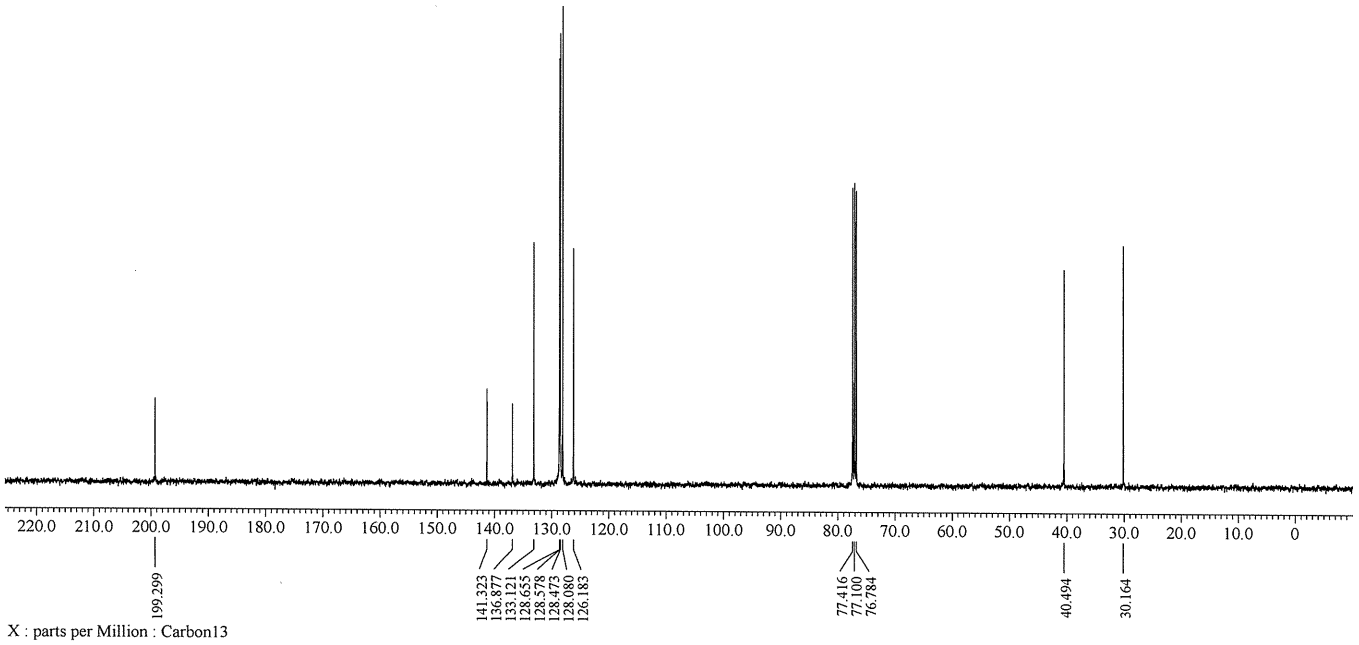
^{13}C NMR, 100 MHz, $CDCl_3$



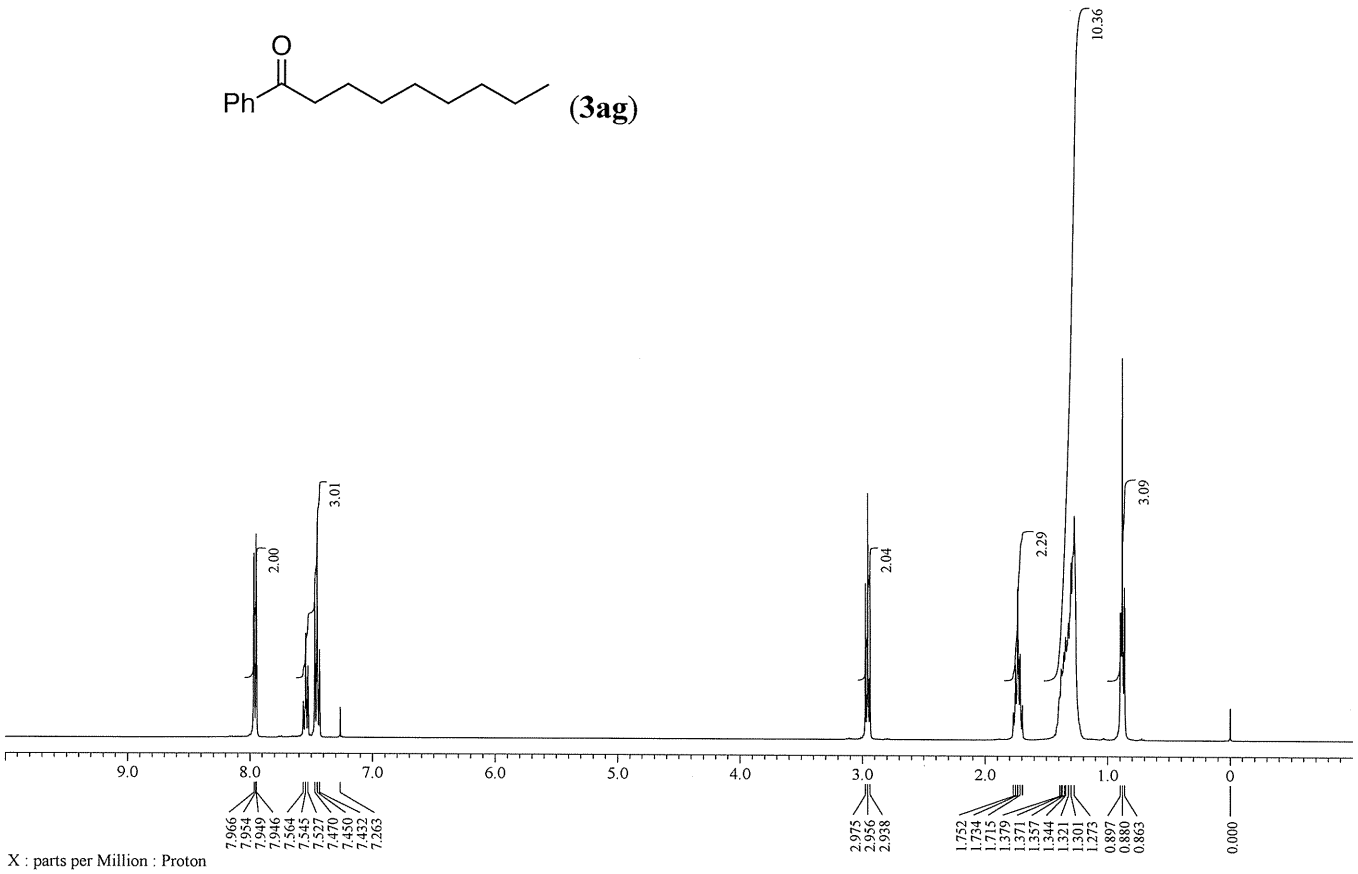
(3af)



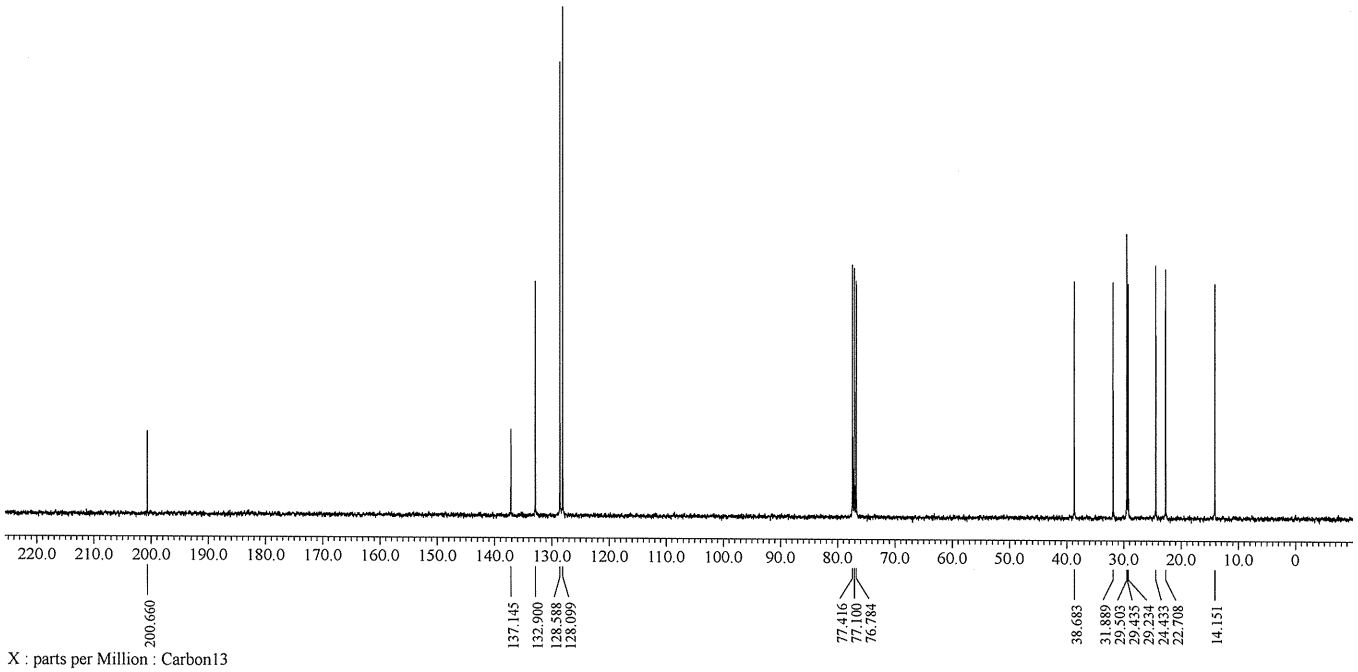
^{1}H NMR, 400 MHz, $CDCl_3$



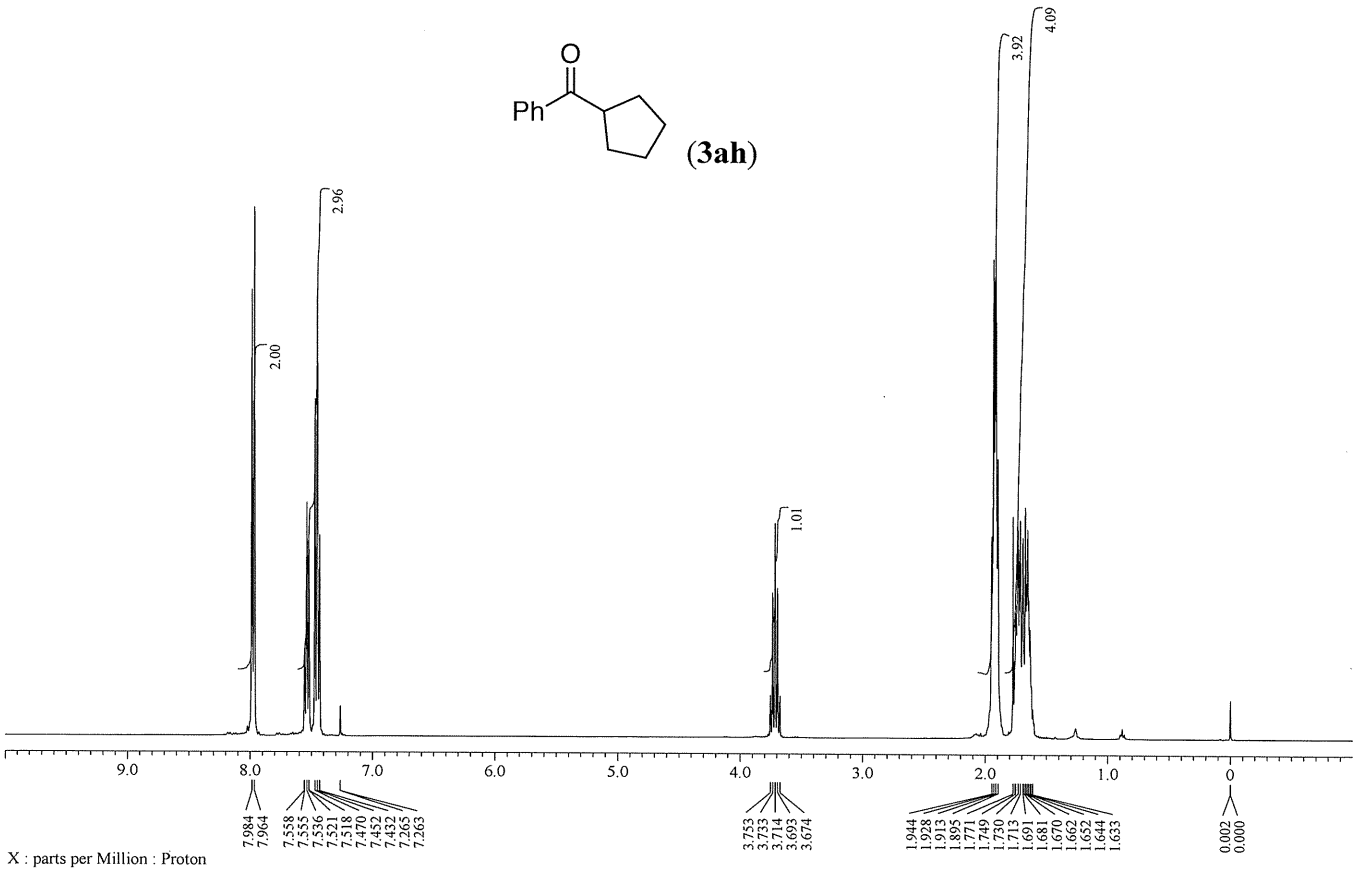
^{13}C NMR, 100 MHz, $CDCl_3$



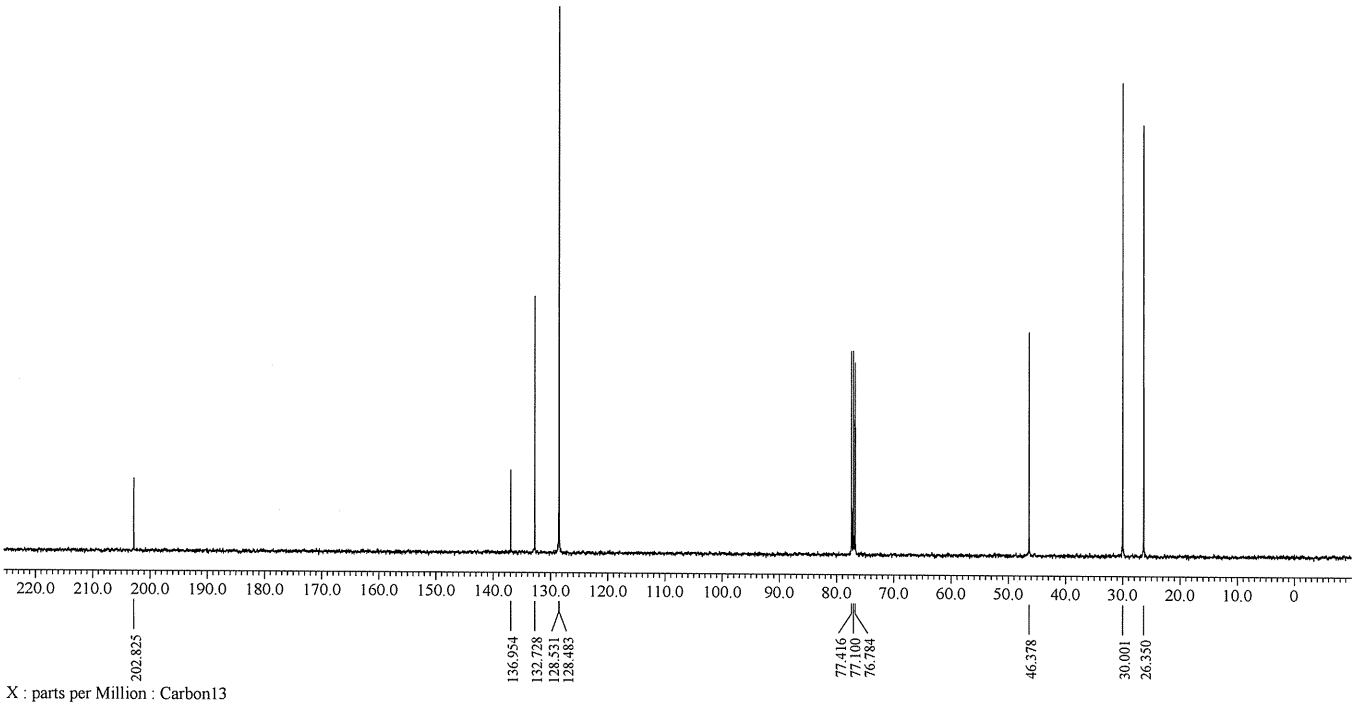
^{1}H NMR, 400 MHz, $CDCl_3$



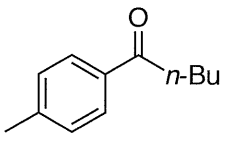
^{13}C NMR, 100 MHz, $CDCl_3$



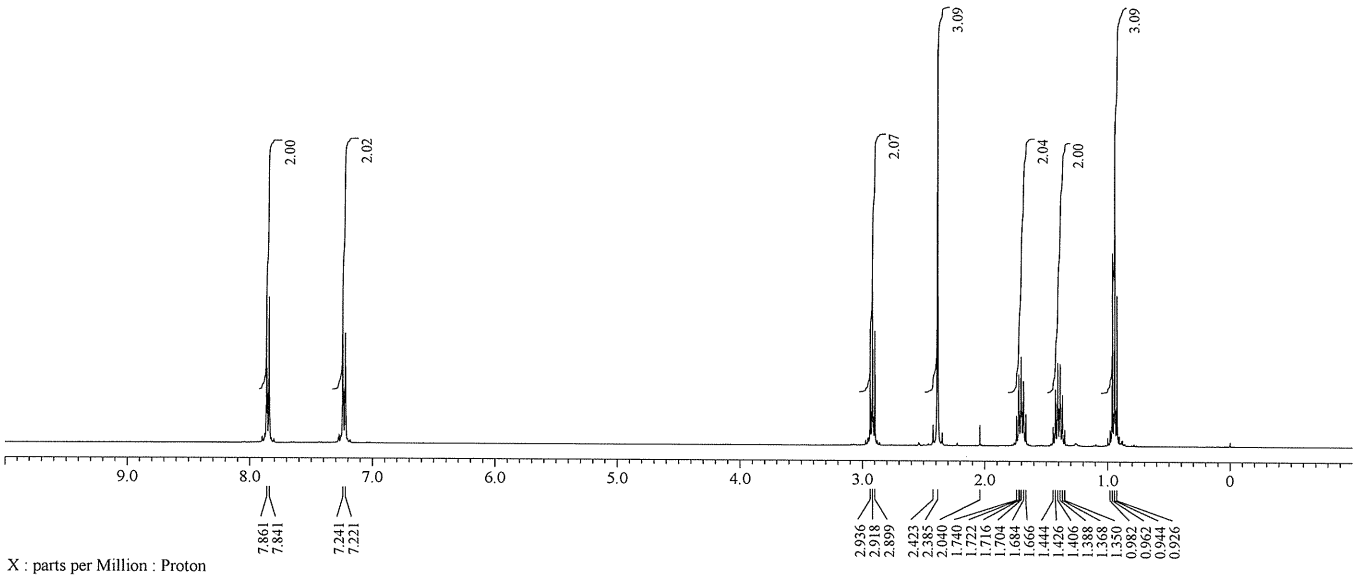
^{1}H NMR, 400 MHz, $CDCl_3$



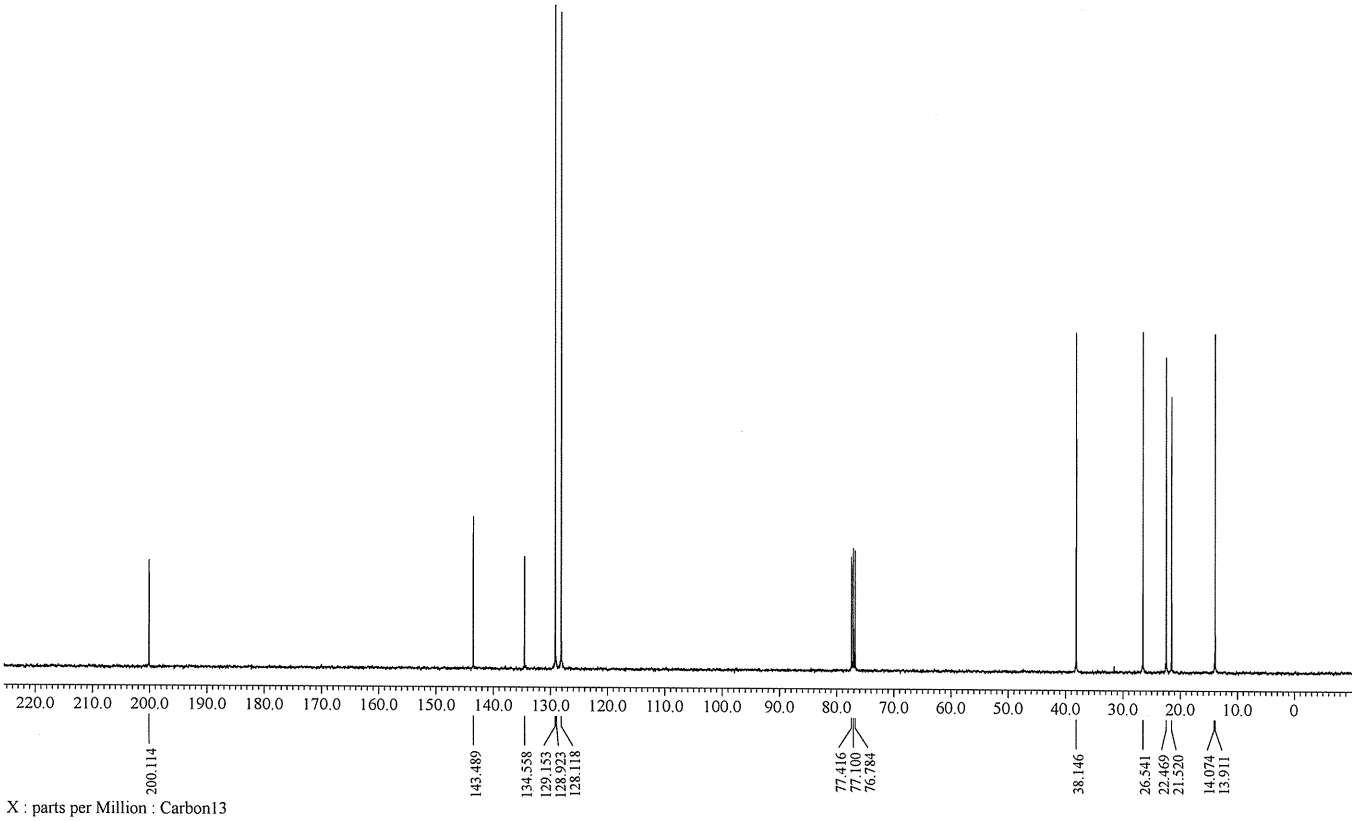
^{13}C NMR, 100 MHz, $CDCl_3$



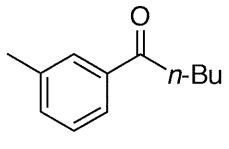
(**3ba**)



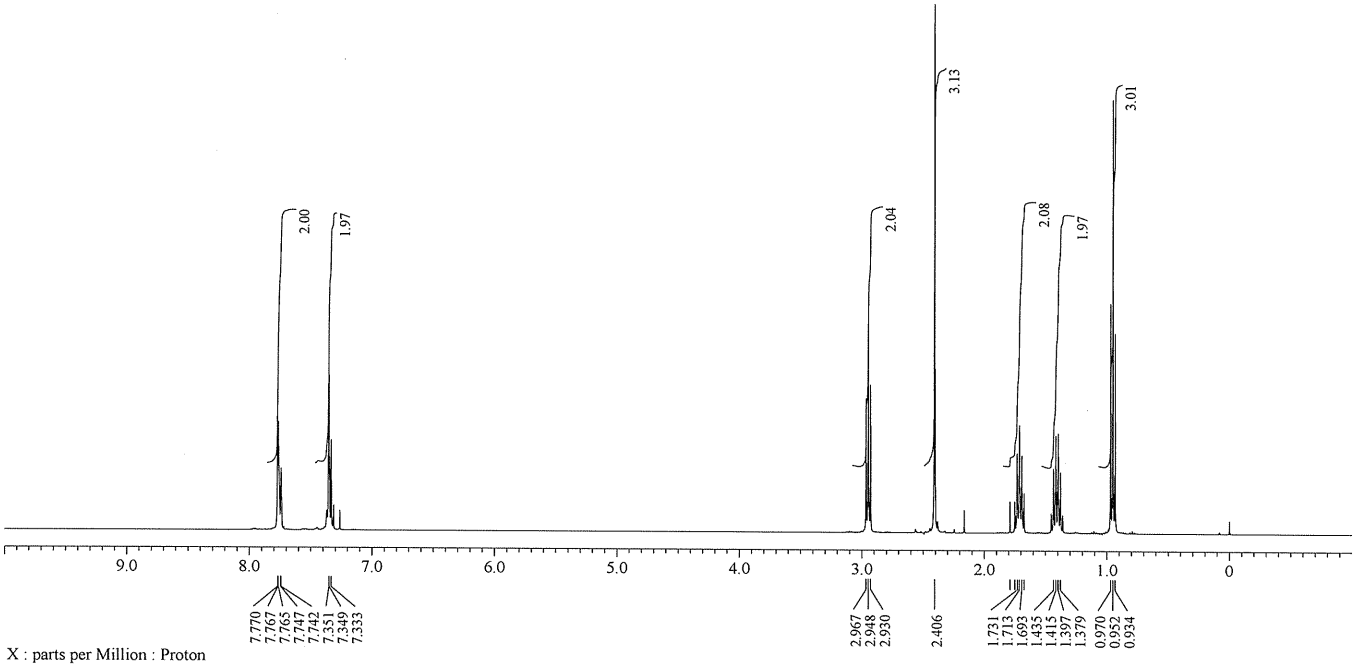
^{1}H NMR, 400 MHz, $CDCl_3$



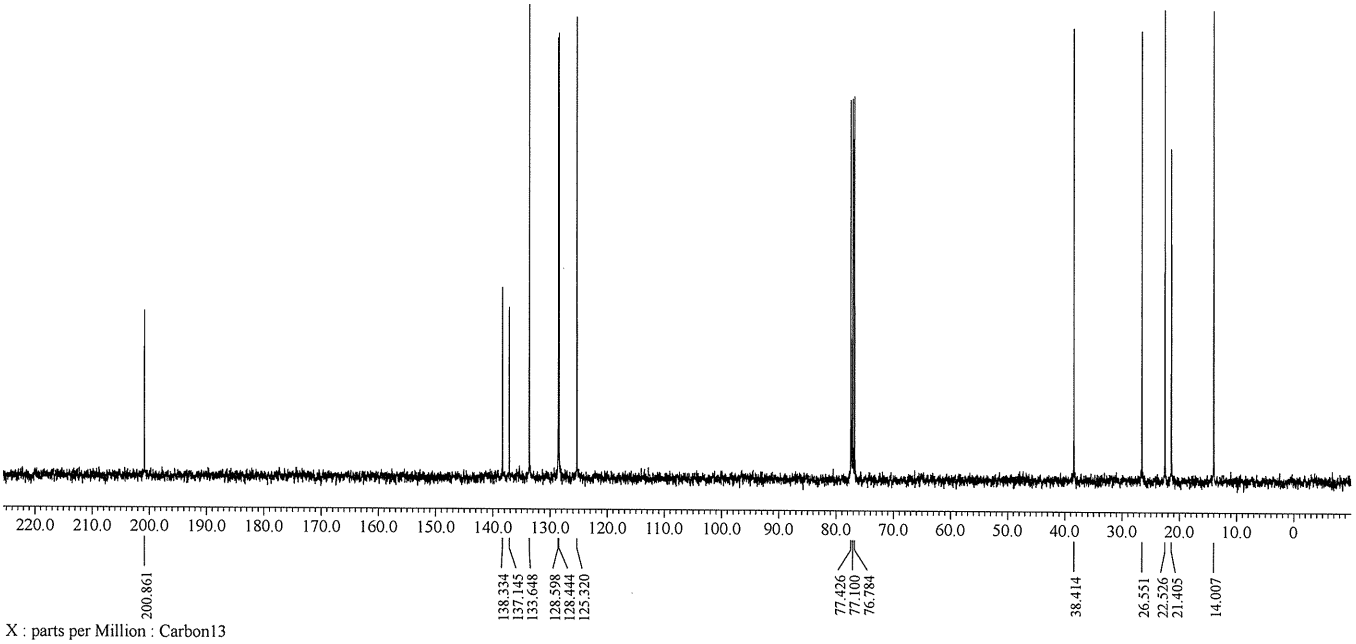
^{13}C NMR, 100 MHz, $CDCl_3$



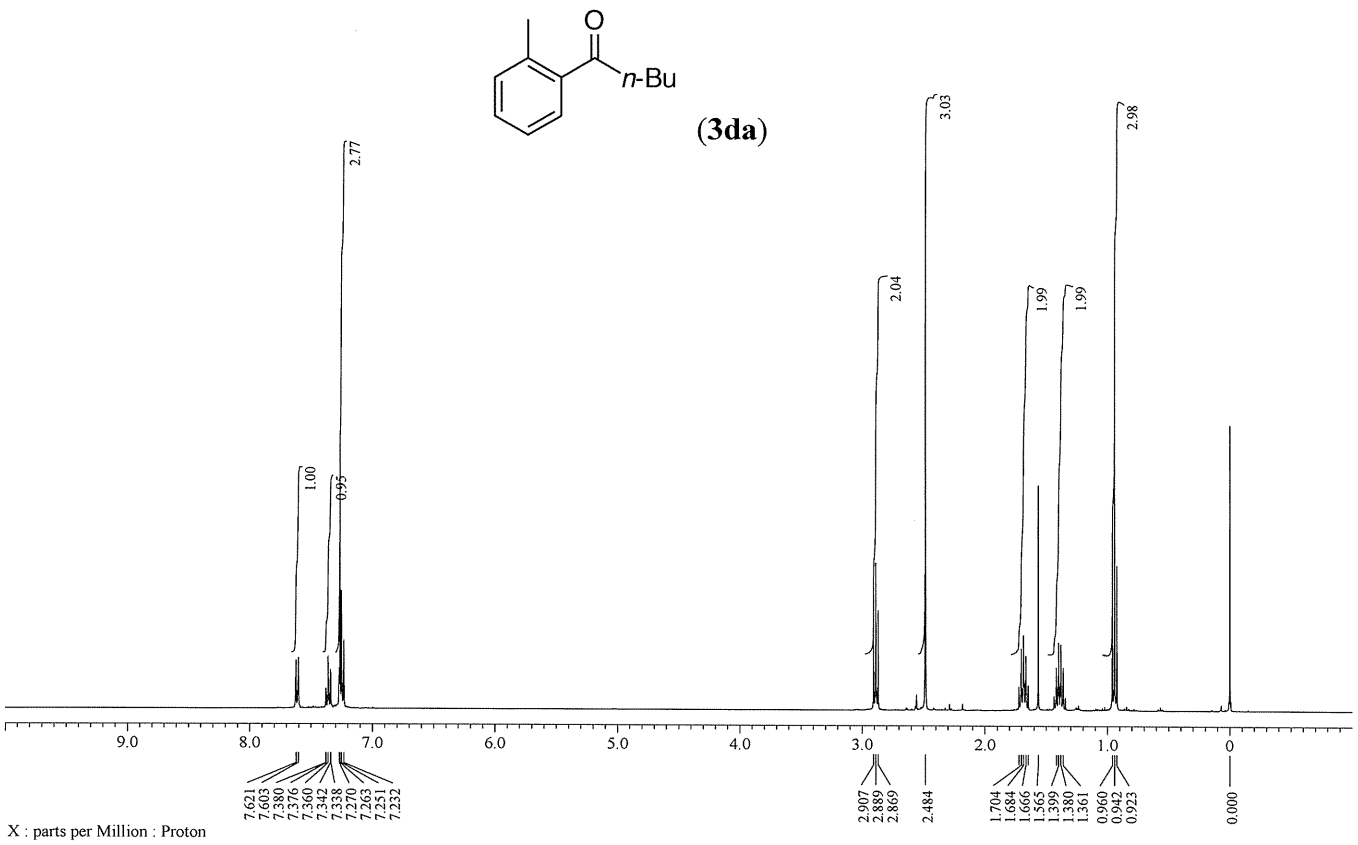
(**3ca**)



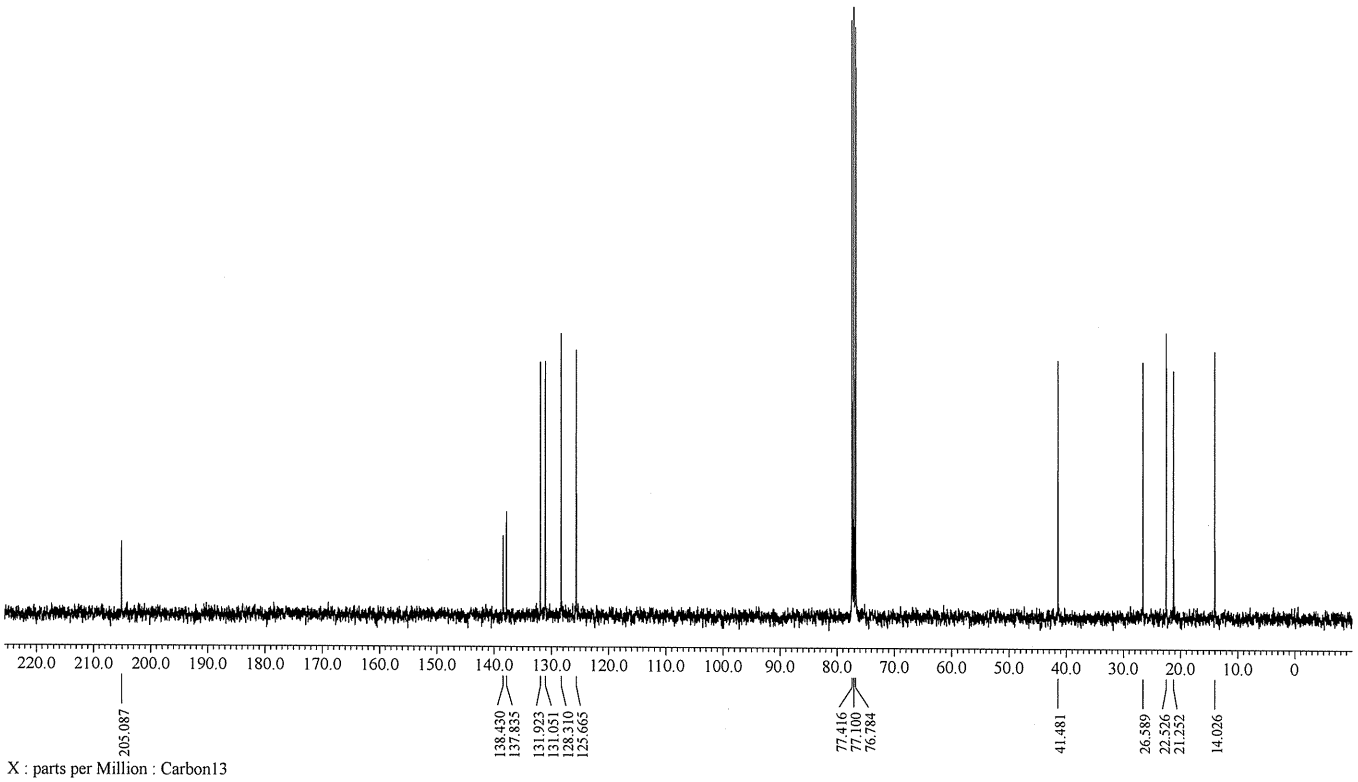
^{1}H NMR, 400 MHz, $CDCl_3$



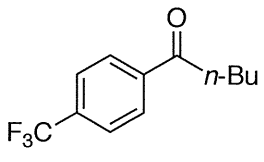
^{13}C NMR, 100 MHz, $CDCl_3$



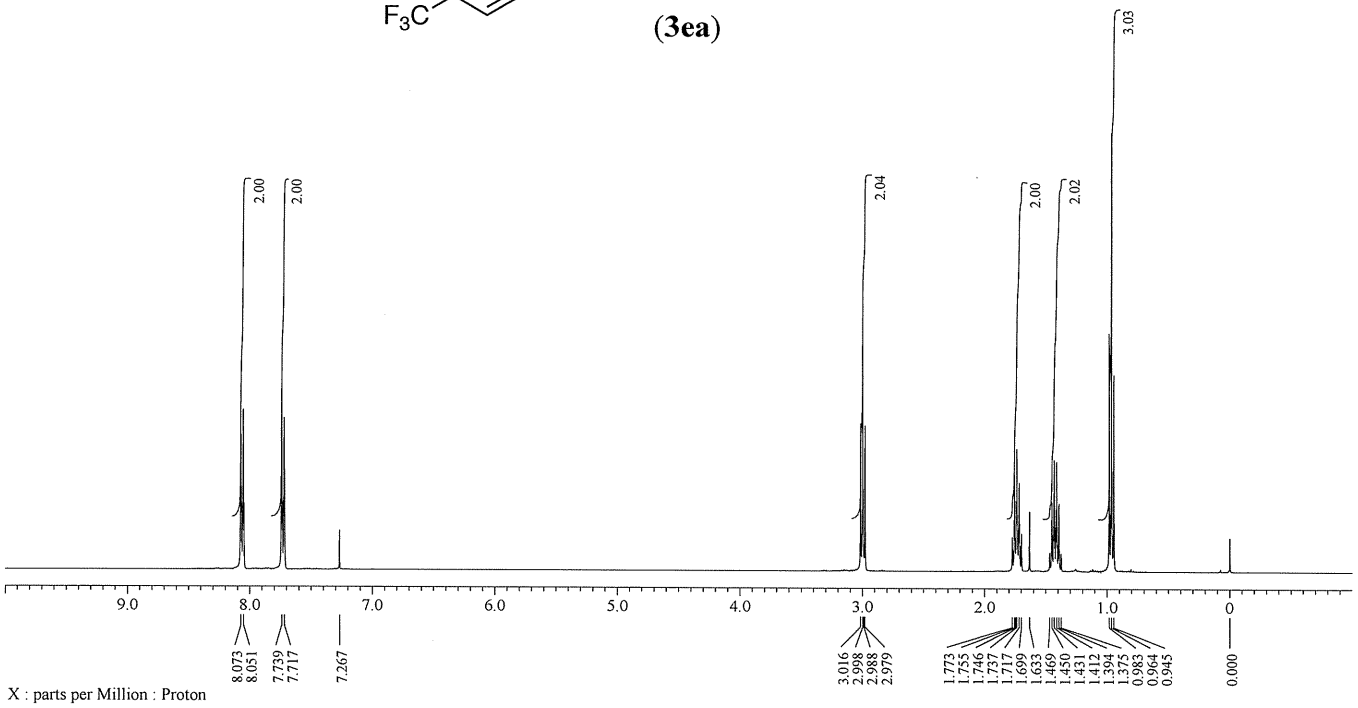
^{1}H NMR, 400 MHz, $CDCl_3$



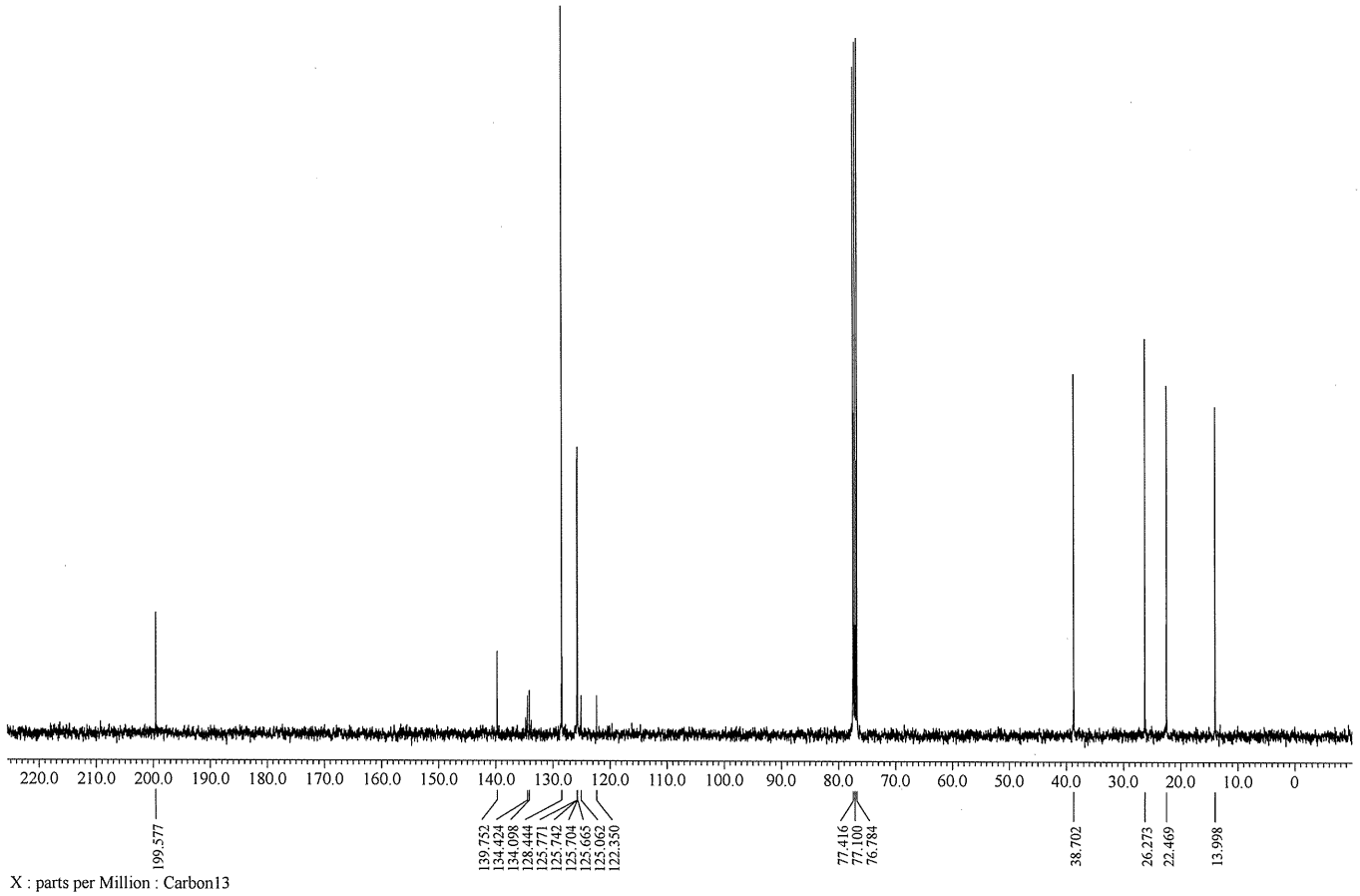
^{13}C NMR, 100 MHz, $CDCl_3$



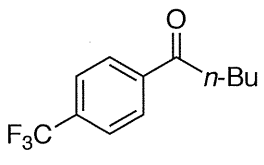
(3ea)



^{1}H NMR, 400 MHz, $CDCl_3$

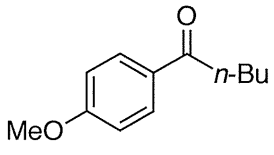


^{13}C NMR, 100 MHz, $CDCl_3$



(3ea)

^{19}F NMR, 376 MHz, $CDCl_3$



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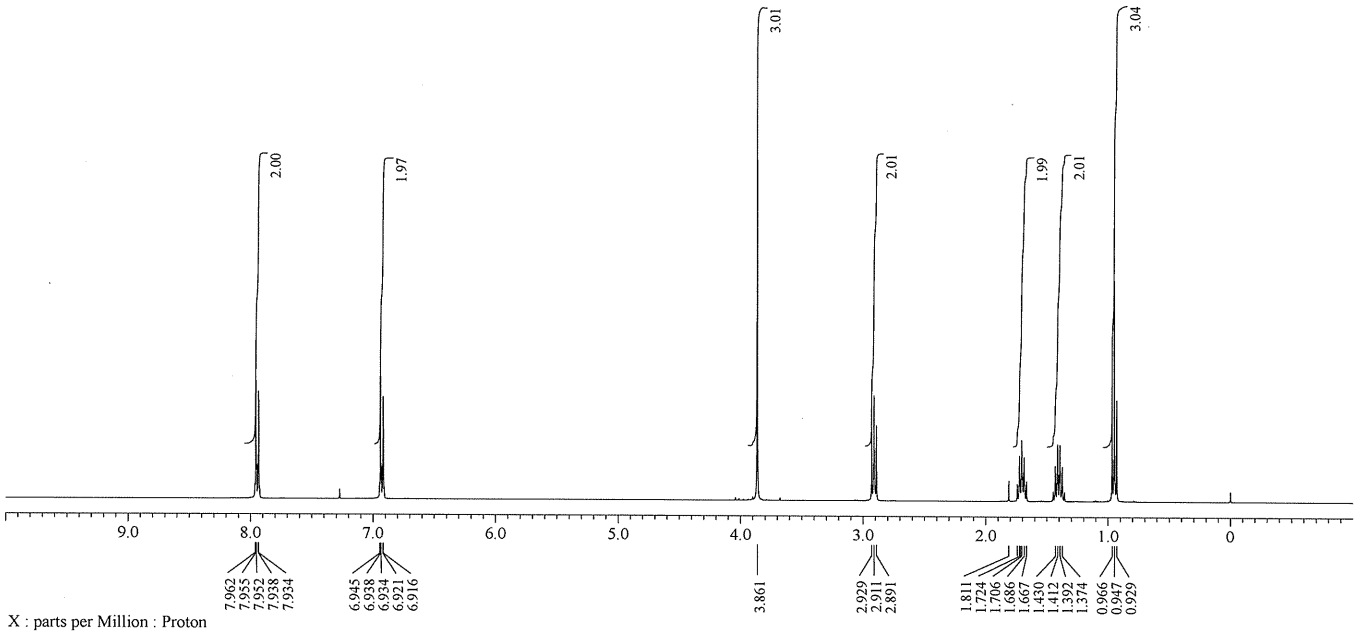
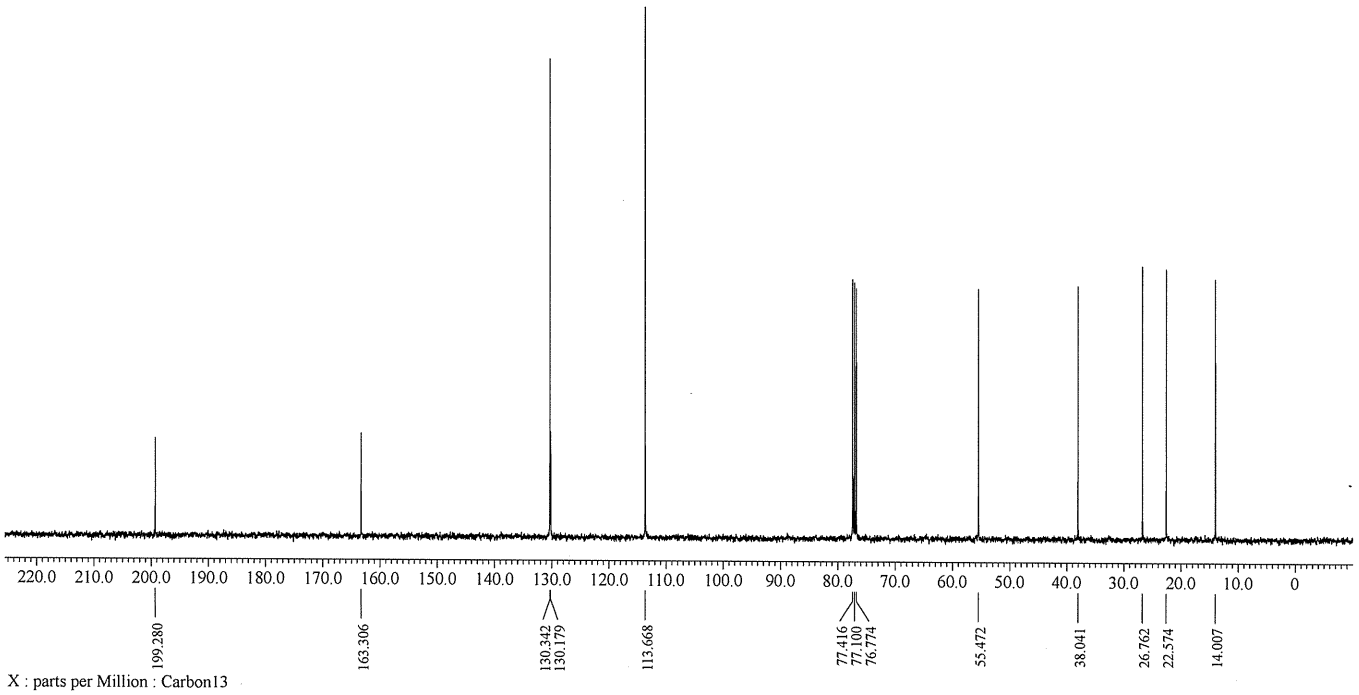
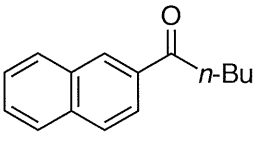


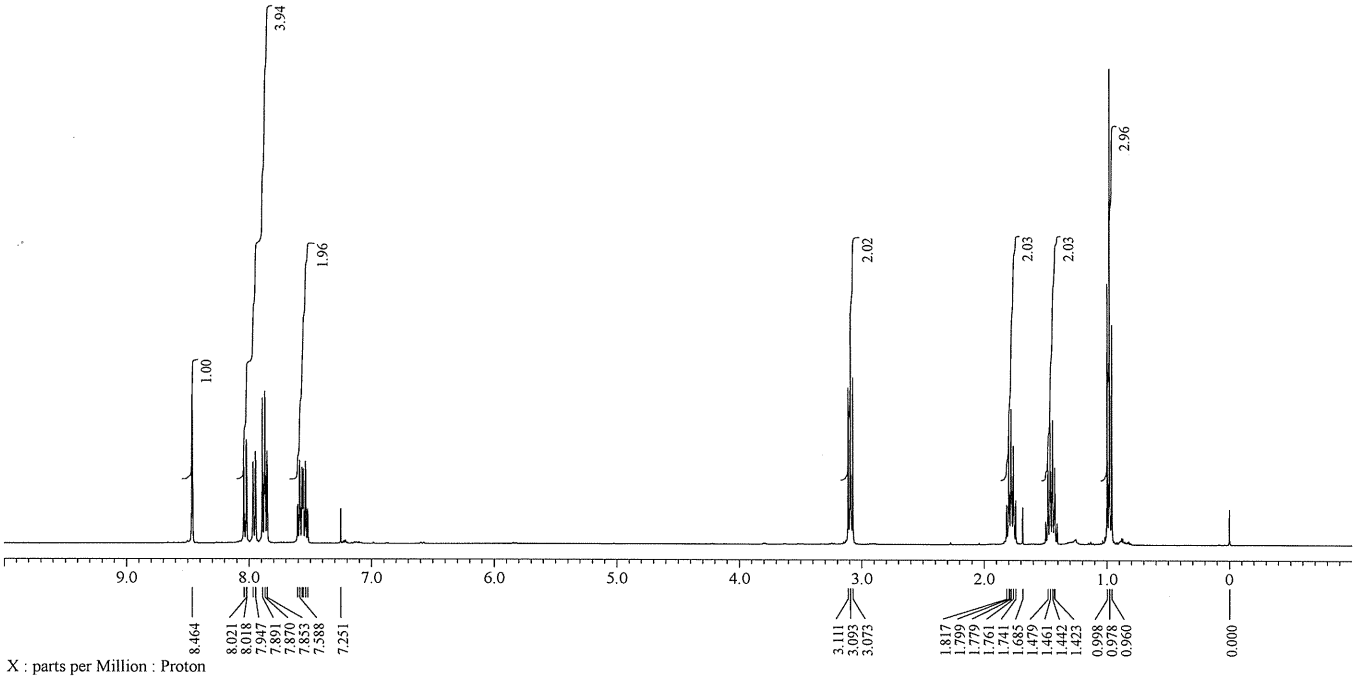
^{1}H NMR, 400 MHz, $CDCl_3$



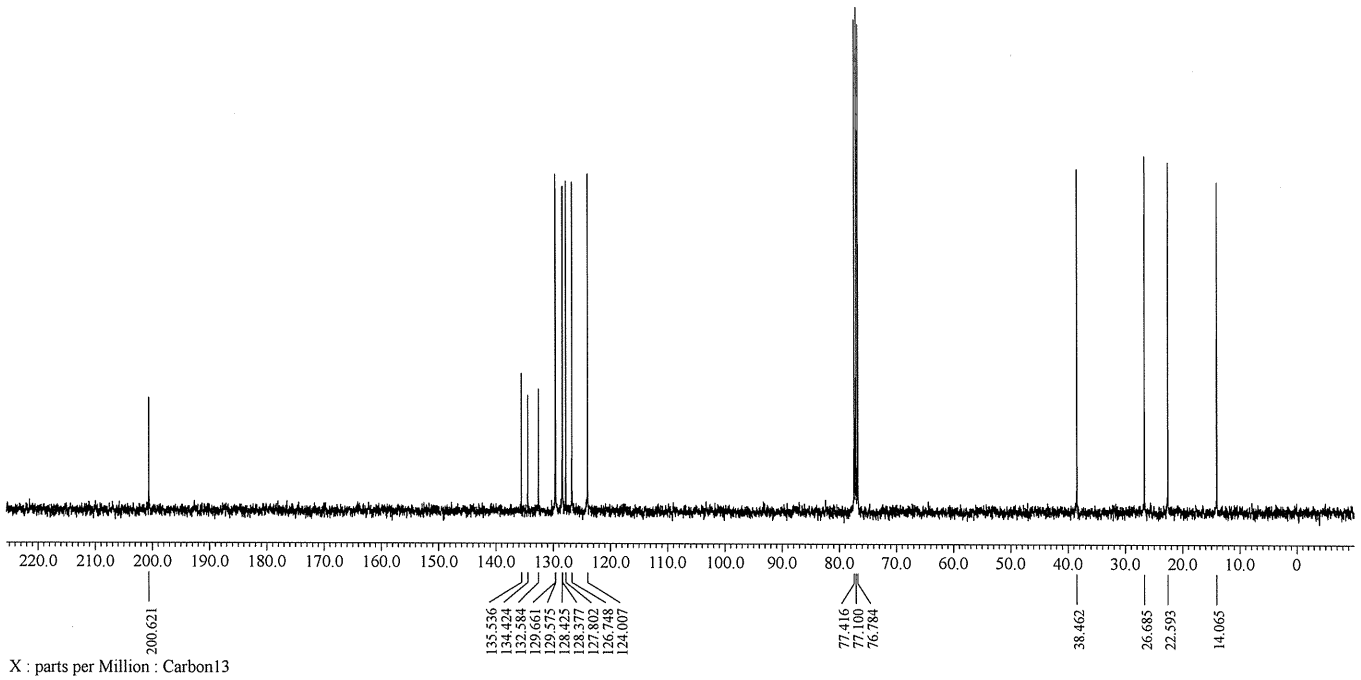
^{13}C NMR, 100 MHz, $CDCl_3$



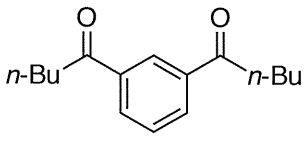
(3ga)



^{1}H NMR, 400 MHz, $CDCl_3$

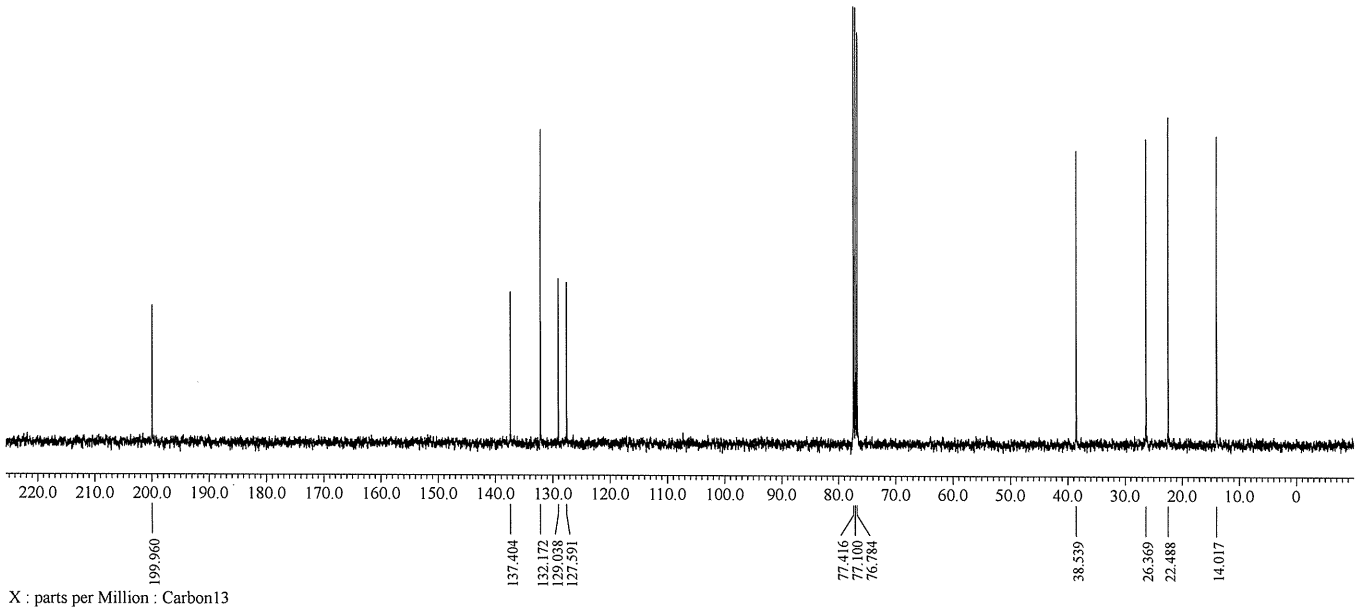


^{13}C NMR, 100 MHz, $CDCl_3$

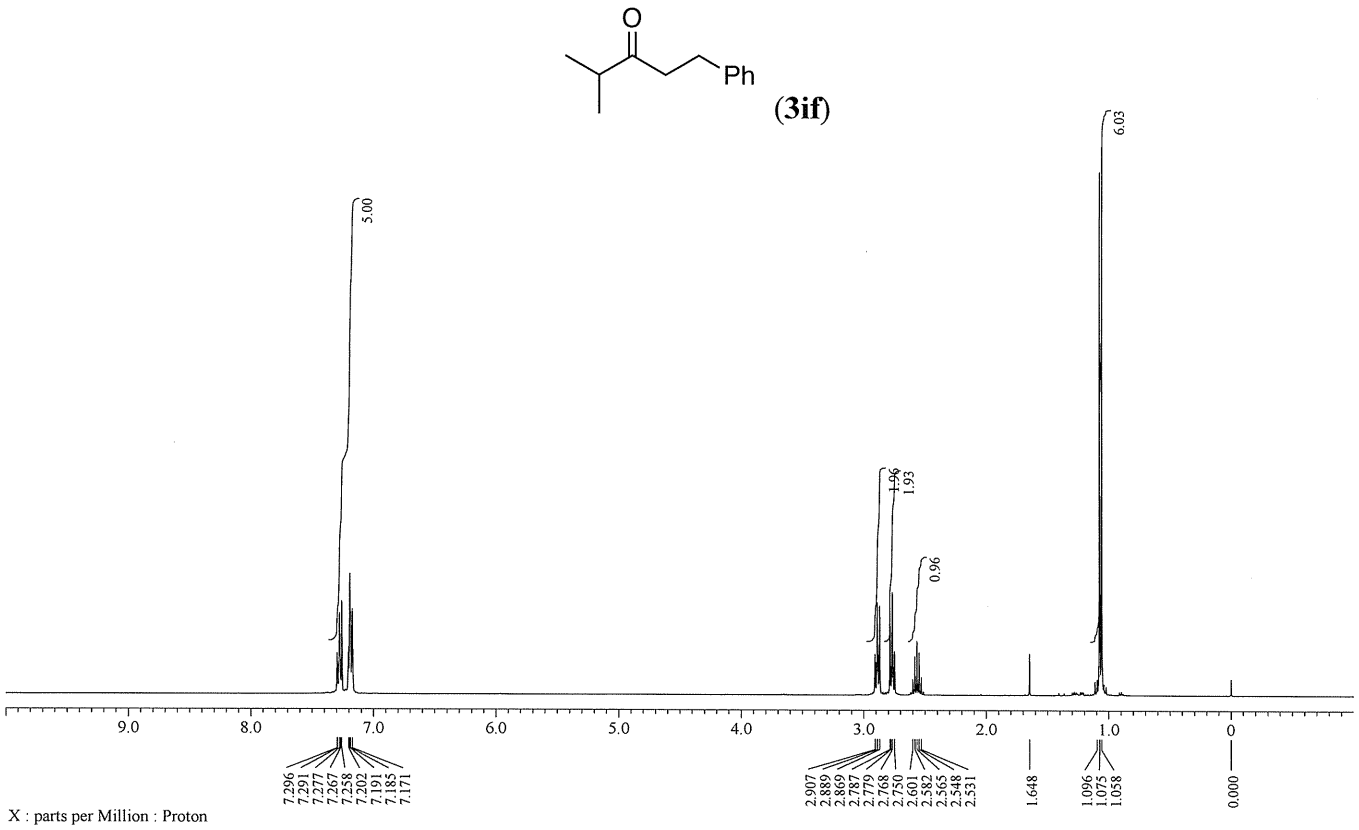


(3ha')

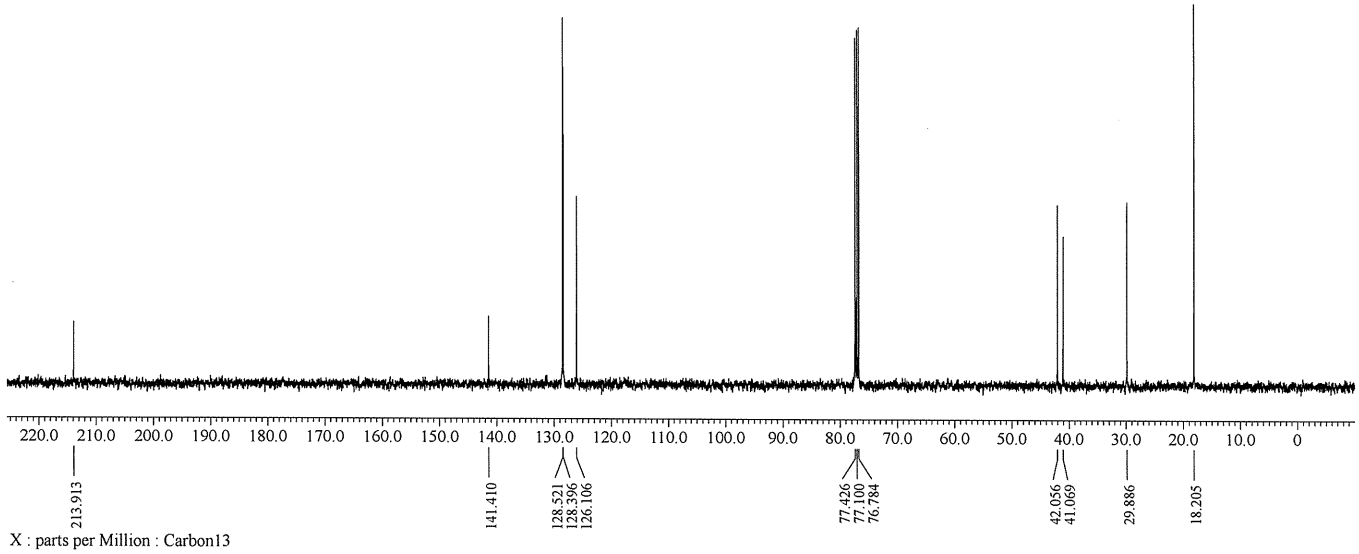
^{1}H NMR, 400 MHz, $CDCl_3$



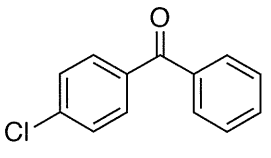
^{13}C NMR, 100 MHz, $CDCl_3$



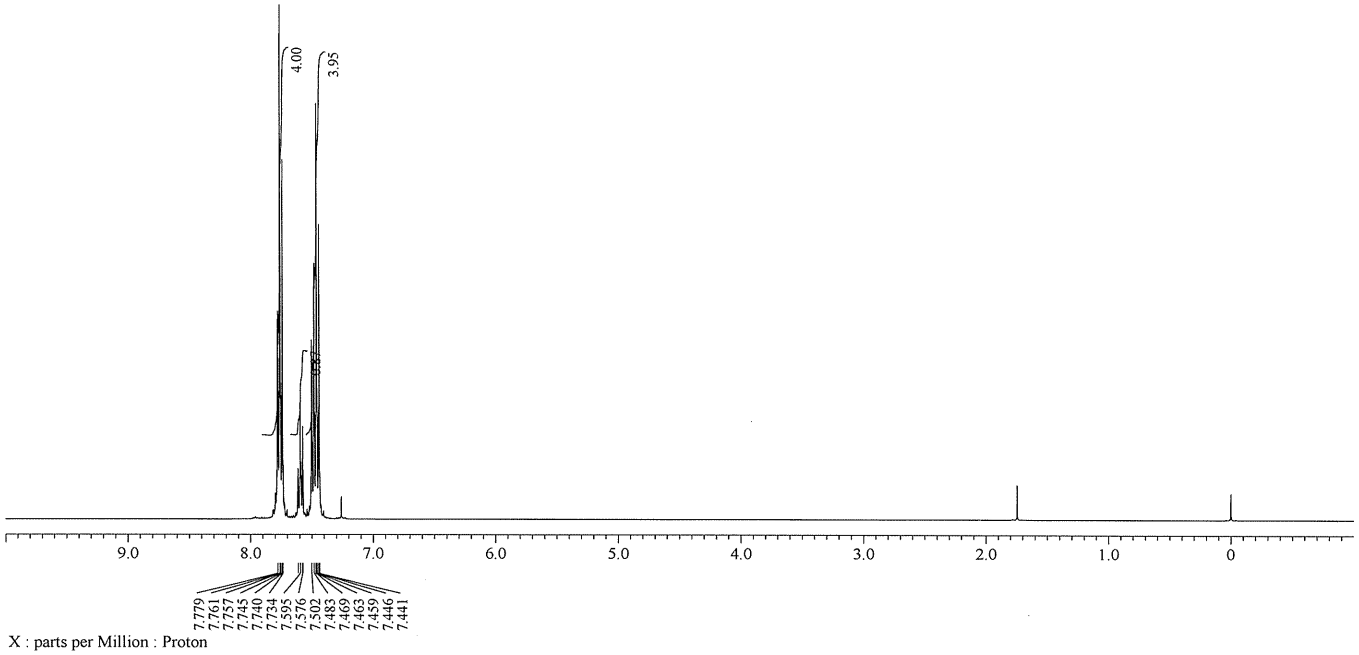
^{1}H NMR, 400 MHz, $CDCl_3$



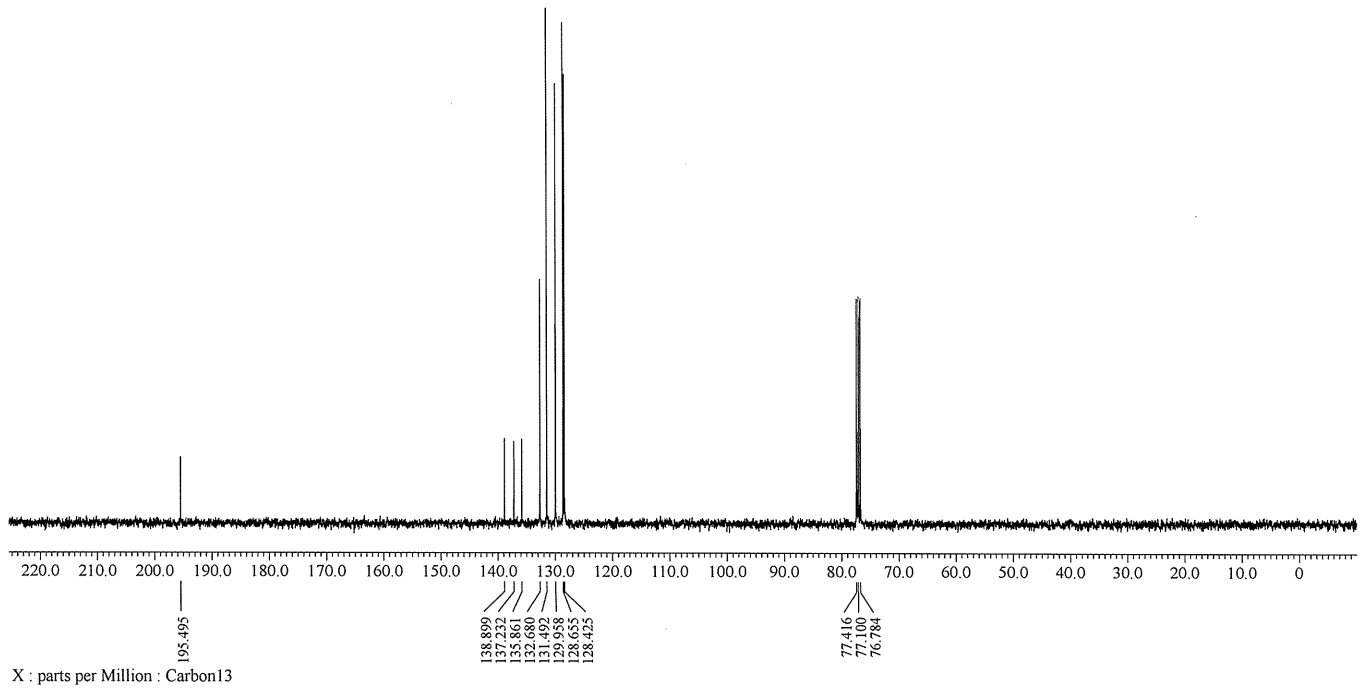
^{13}C NMR, 100 MHz, $CDCl_3$



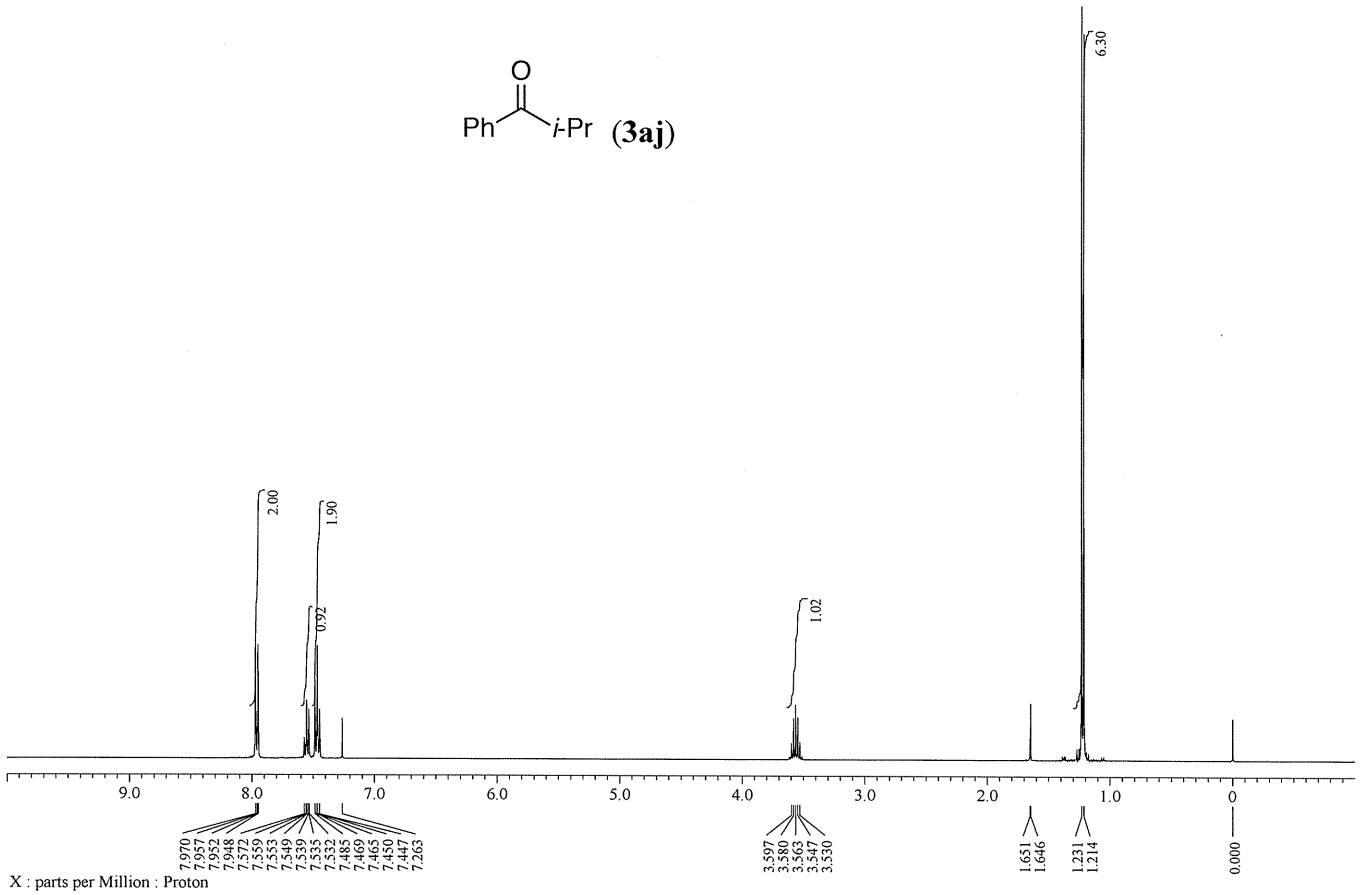
(3ji)



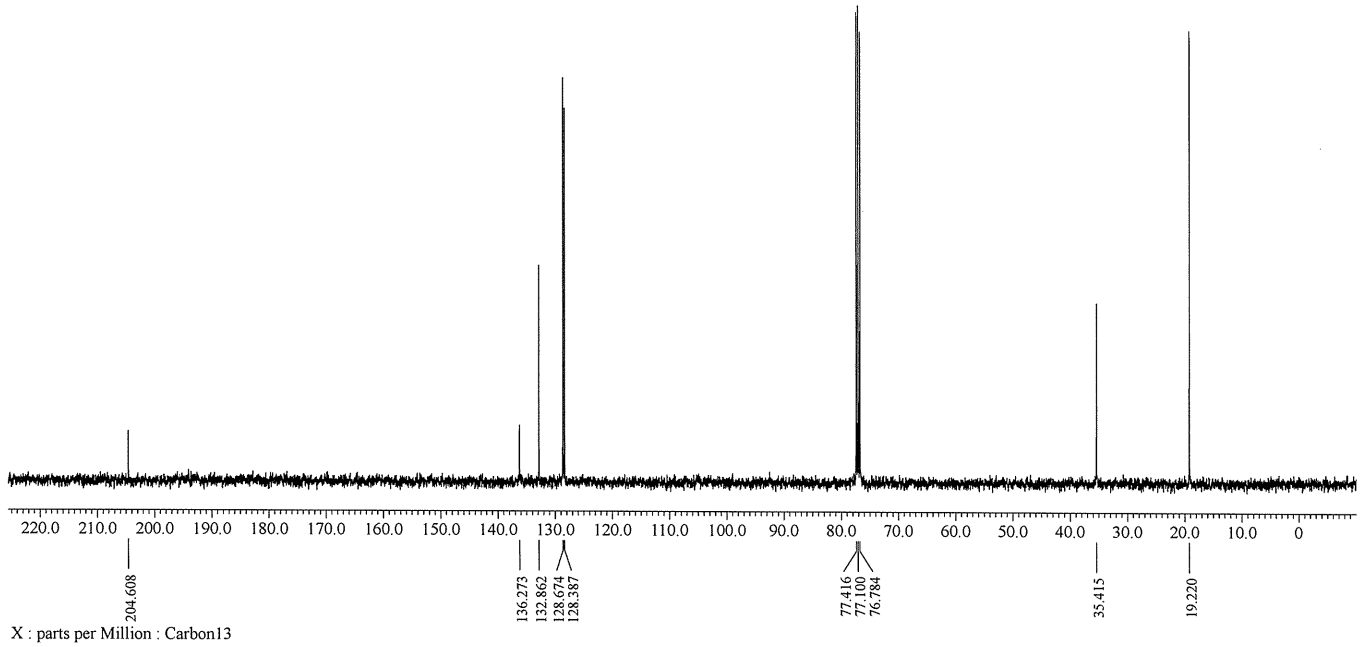
^{1}H NMR, 400 MHz, $CDCl_3$



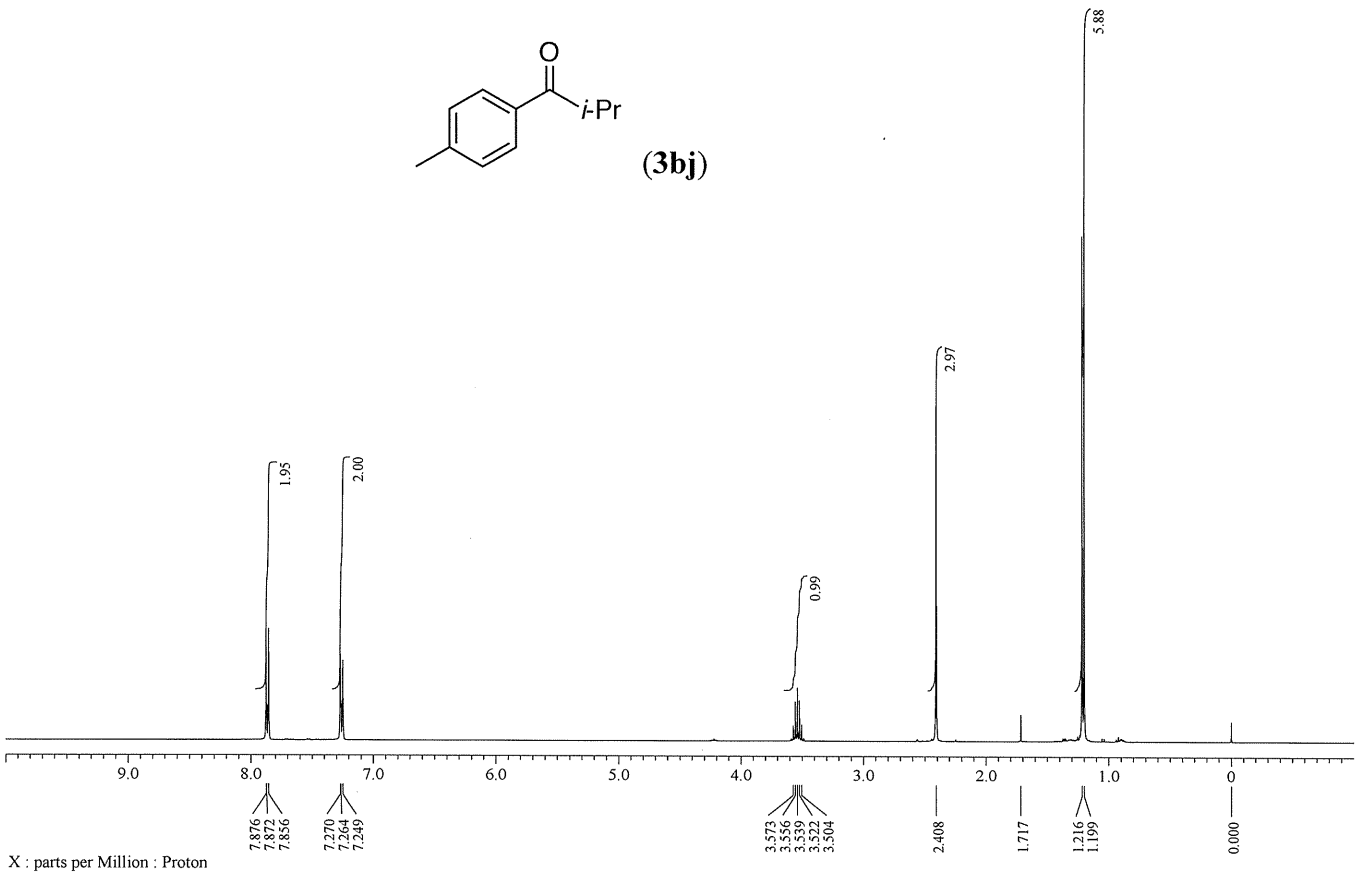
^{13}C NMR, 100 MHz, $CDCl_3$



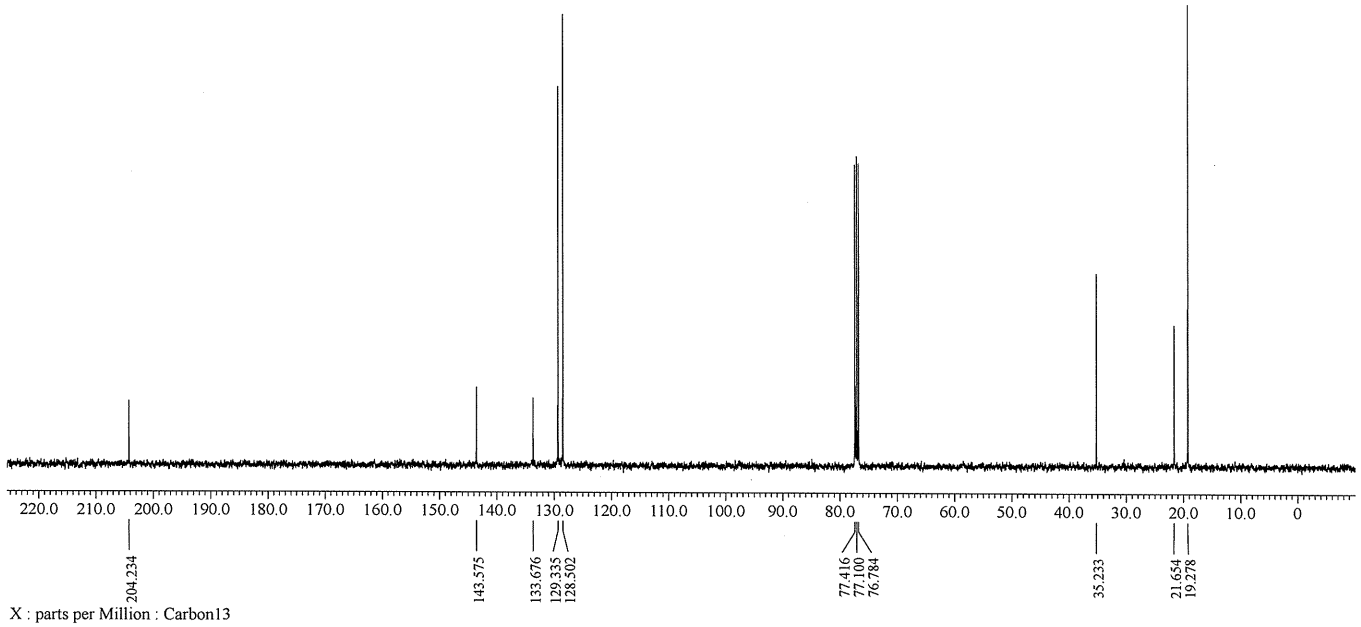
^{1}H NMR, 400 MHz, $CDCl_3$



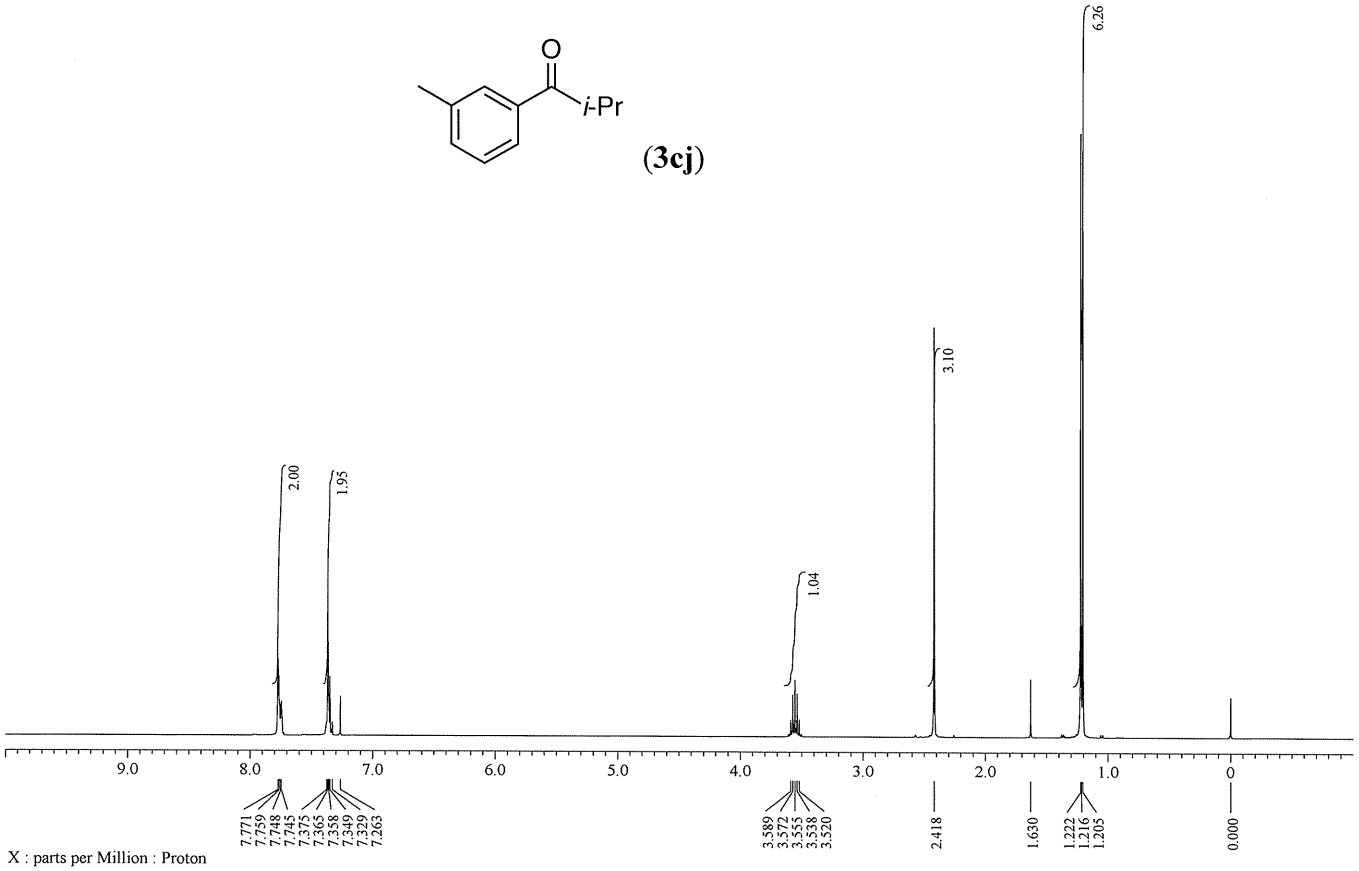
^{13}C NMR, 100 MHz, $CDCl_3$



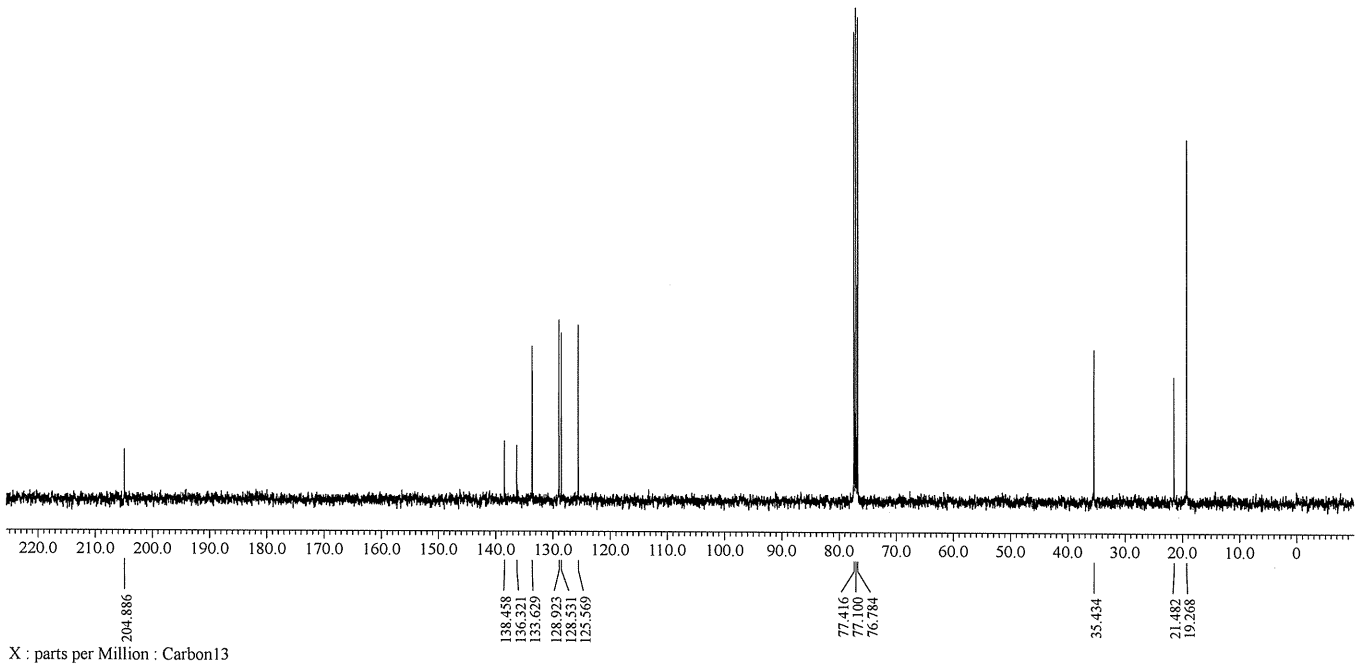
^{1}H NMR, 400 MHz, $CDCl_3$



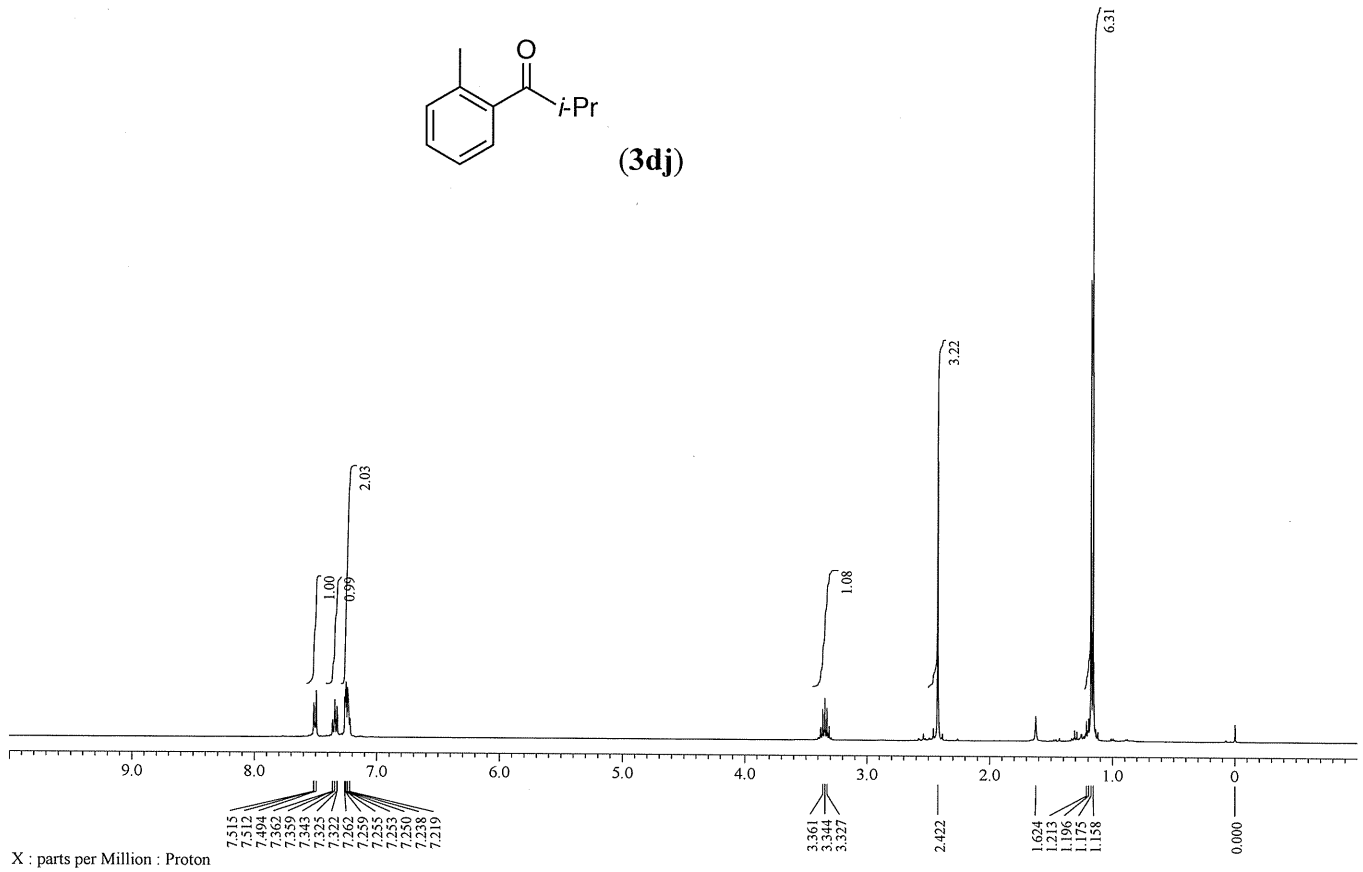
^{13}C NMR, 100 MHz, $CDCl_3$



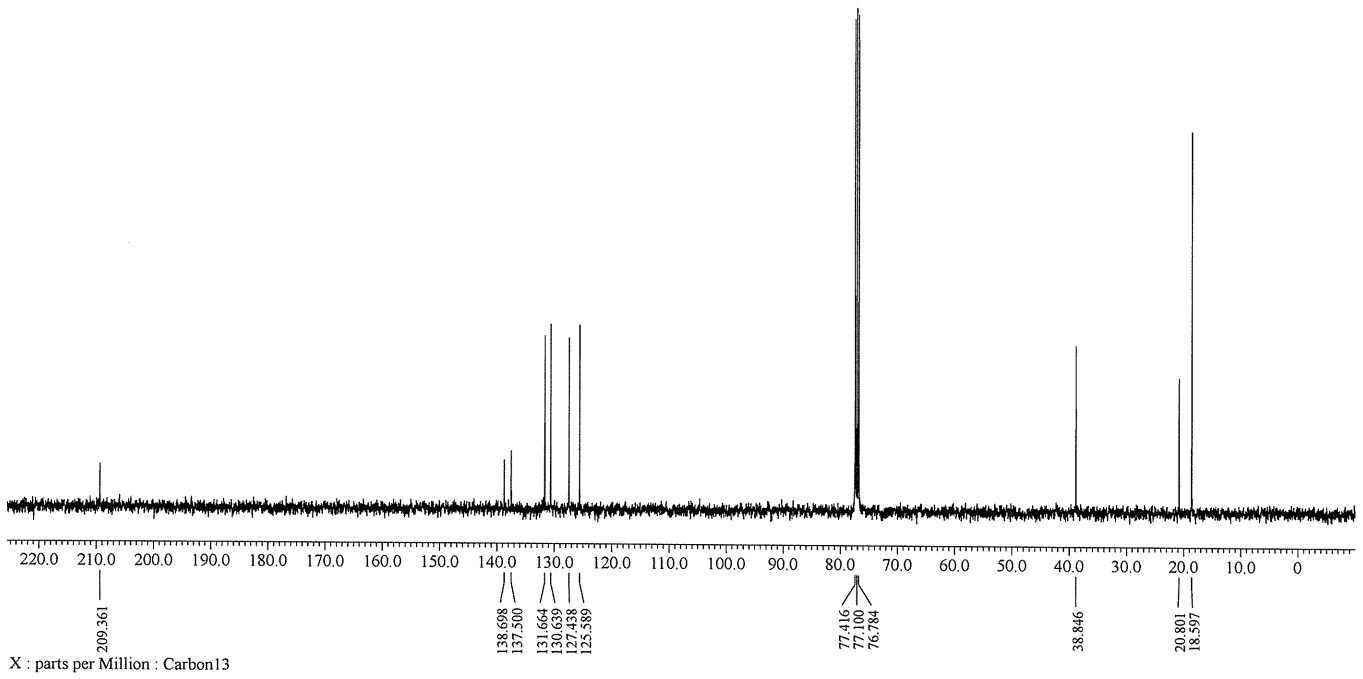
^{1}H NMR, 400 MHz, $CDCl_3$



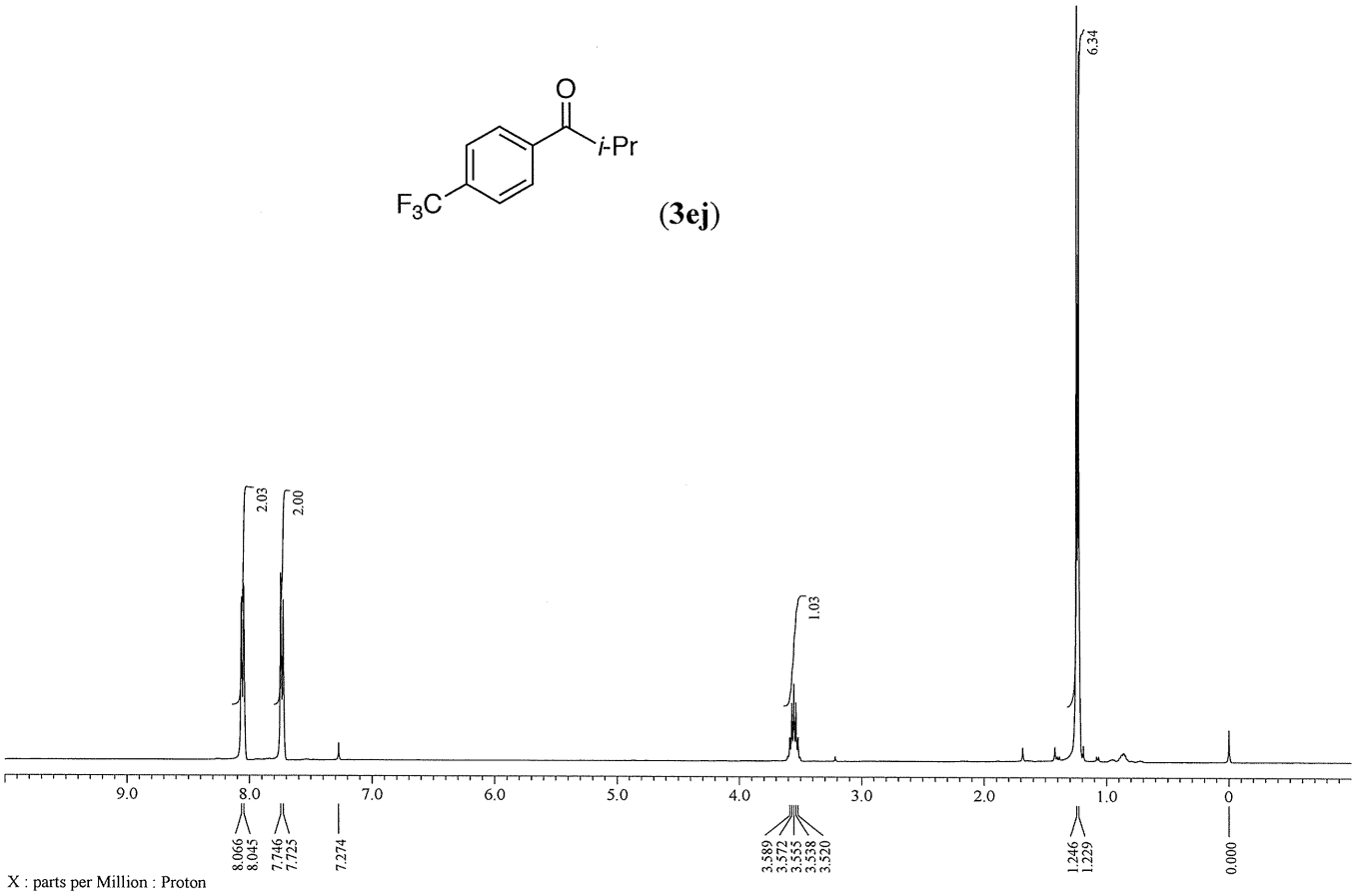
^{13}C NMR, 100 MHz, $CDCl_3$



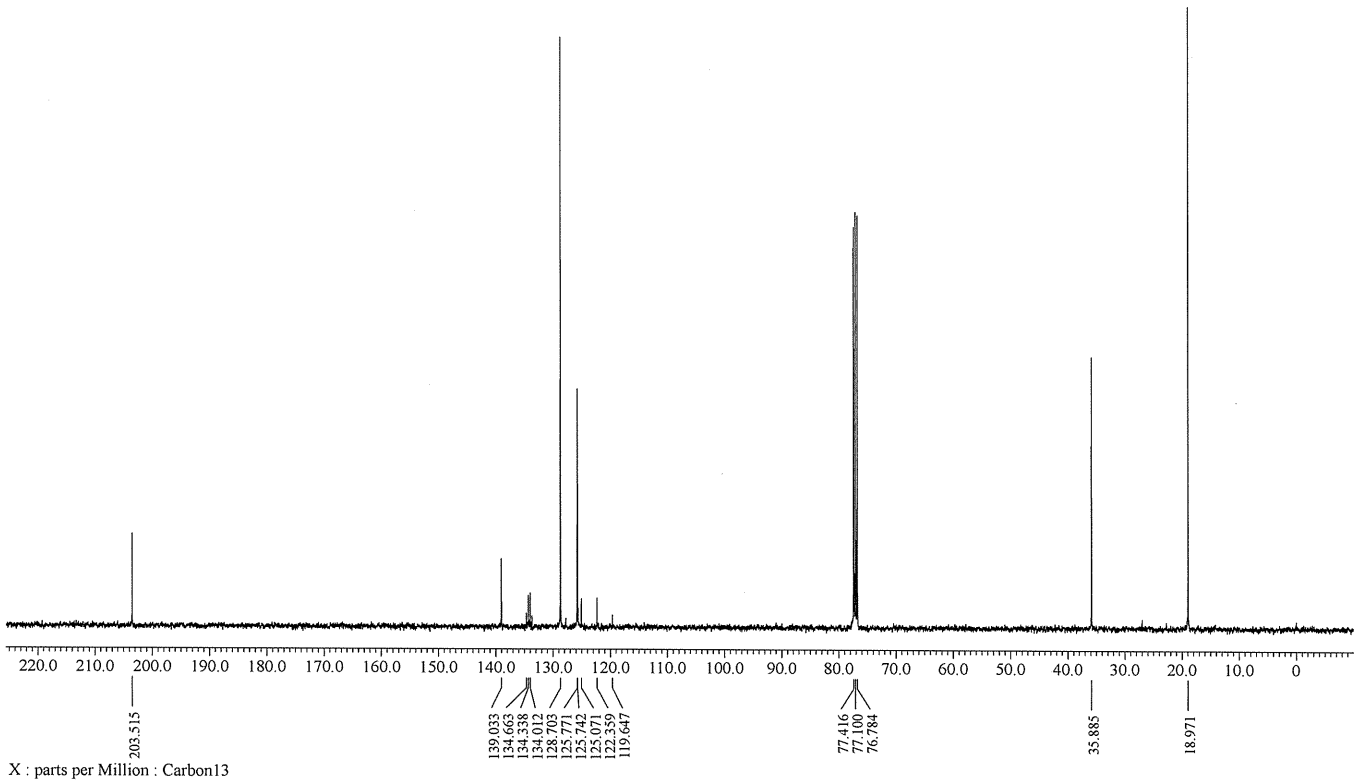
^{1}H NMR, 400 MHz, $CDCl_3$



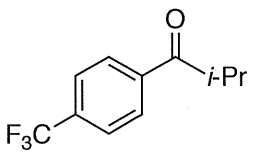
^{13}C NMR, 100 MHz, $CDCl_3$



^{1}H NMR, 400 MHz, $CDCl_3$



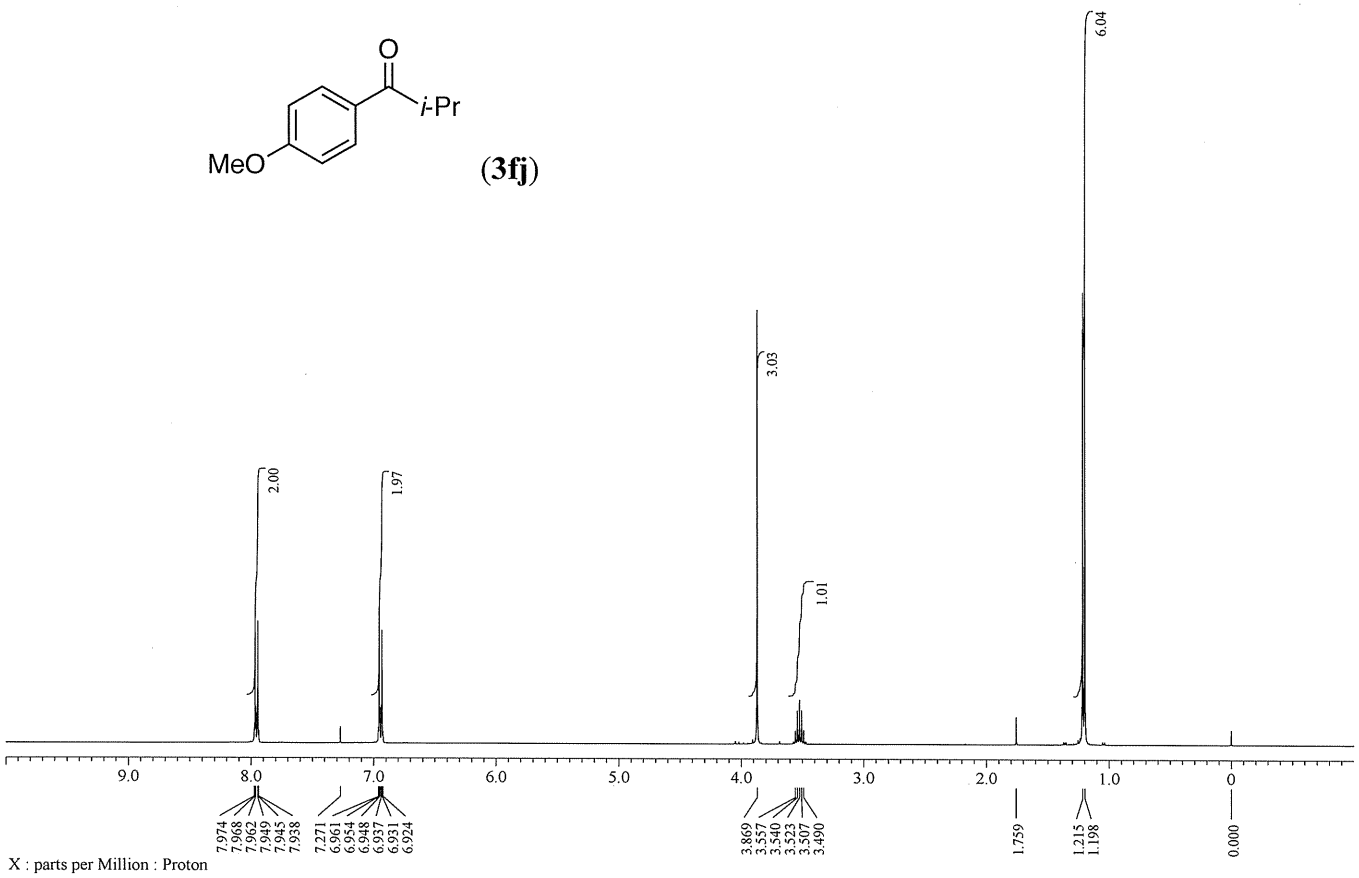
^{13}C NMR, 100 MHz, $CDCl_3$



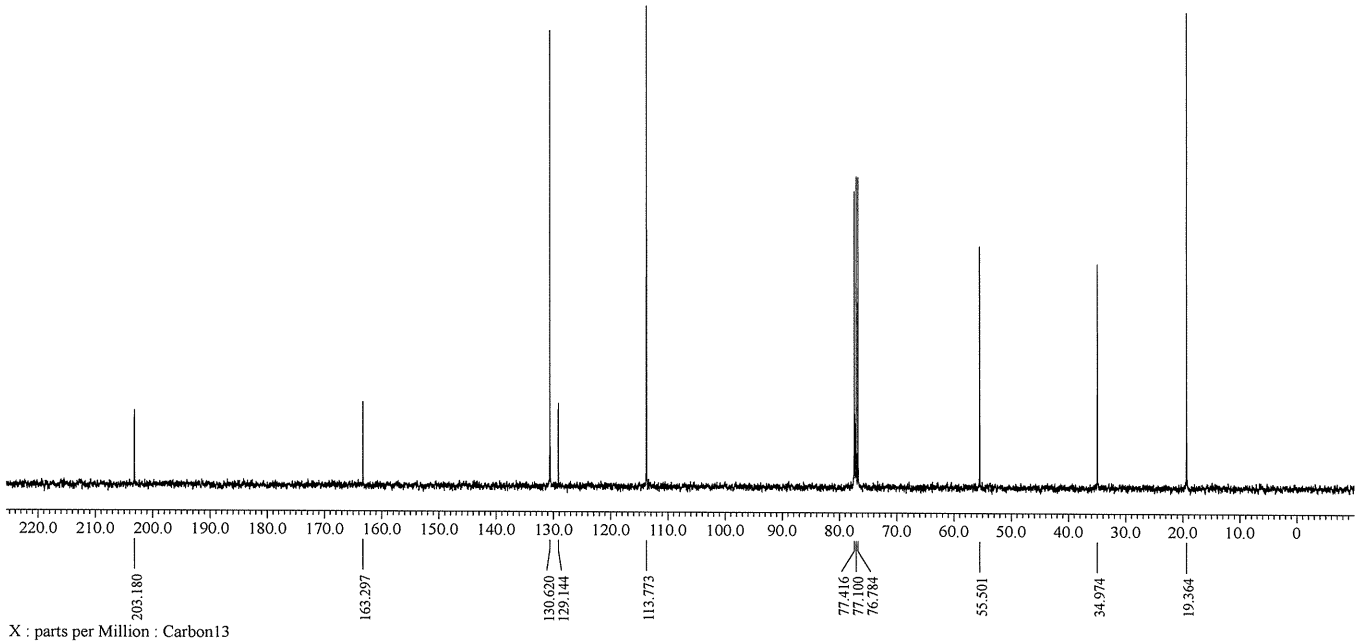
(3ej)

X : parts per Million : Fluorine19

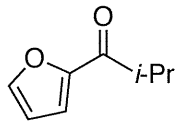
^{19}F NMR, 376 MHz, $CDCl_3$



^{1}H NMR, 400 MHz, $CDCl_3$

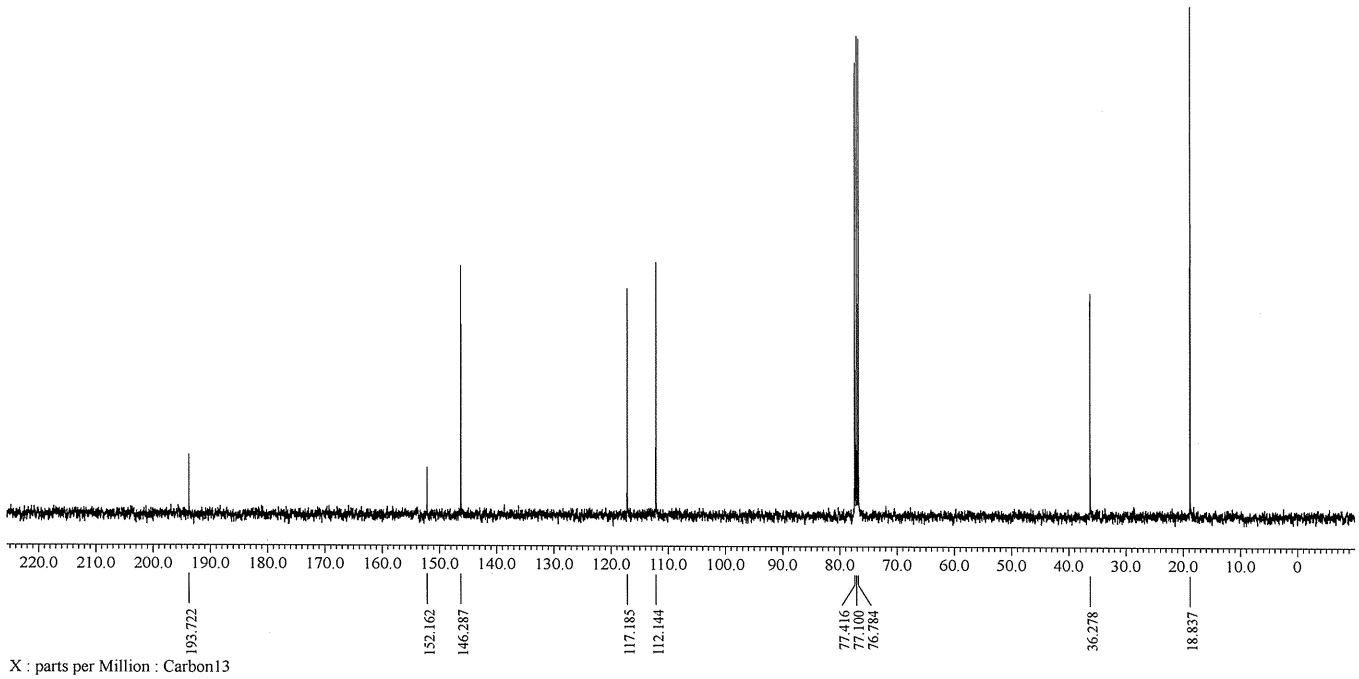


^{13}C NMR, 100 MHz, $CDCl_3$

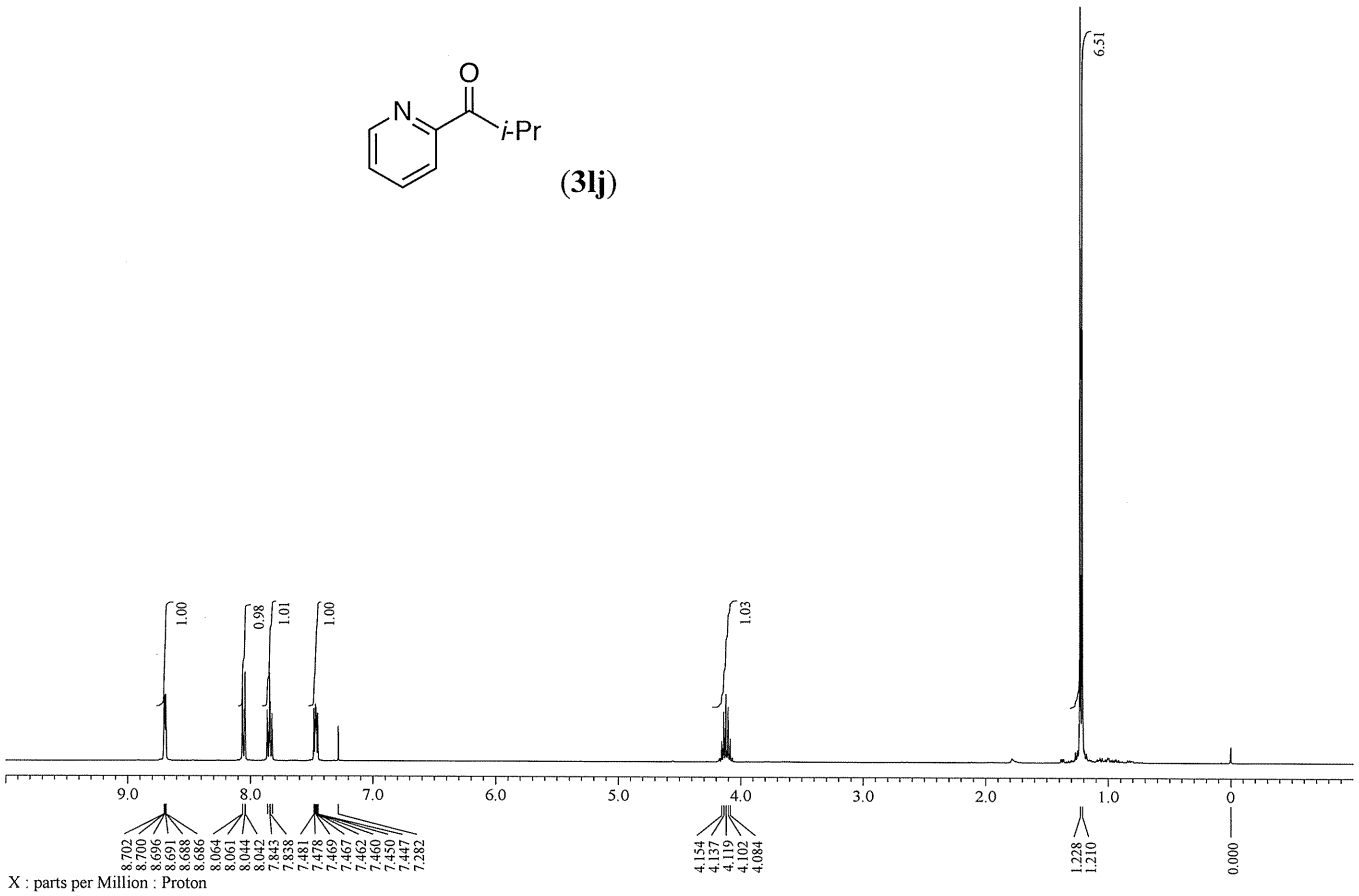


(3kj)

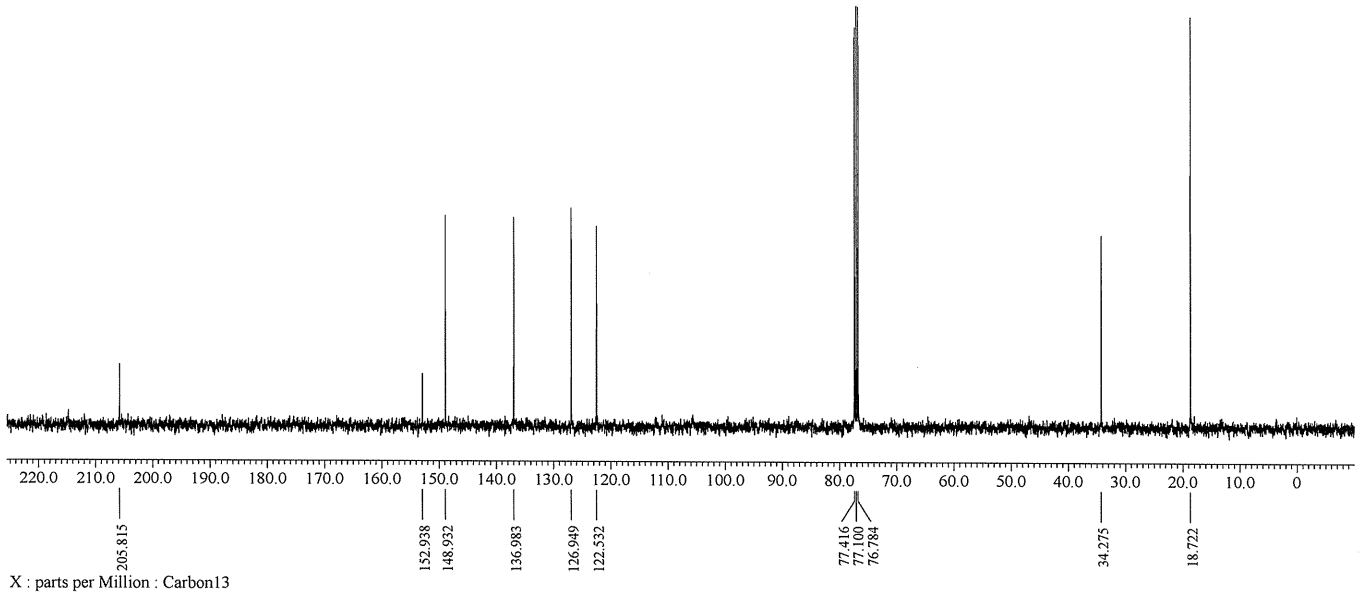
^{1}H NMR, 400 MHz, $CDCl_3$



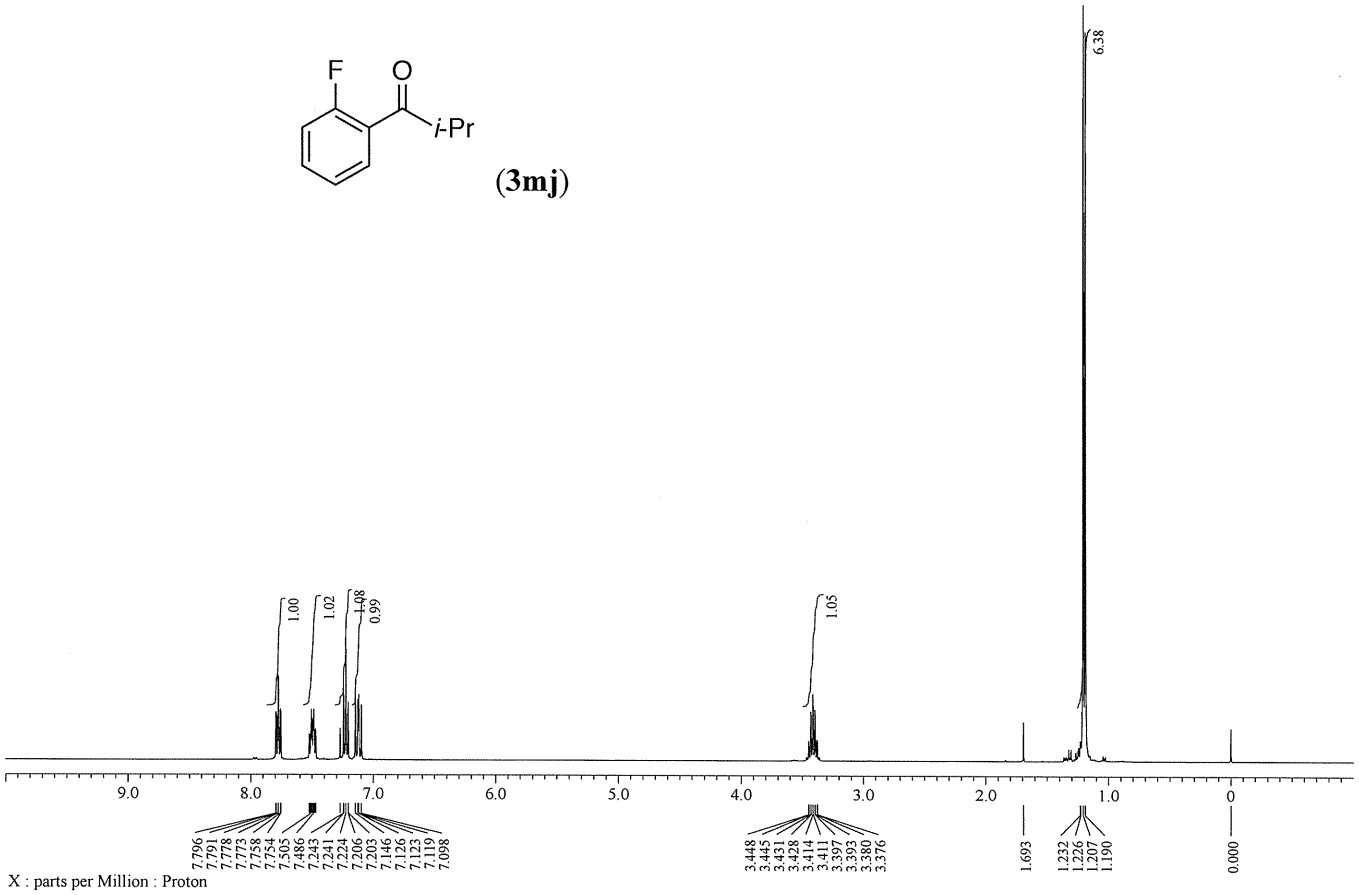
^{13}C NMR, 100 MHz, $CDCl_3$



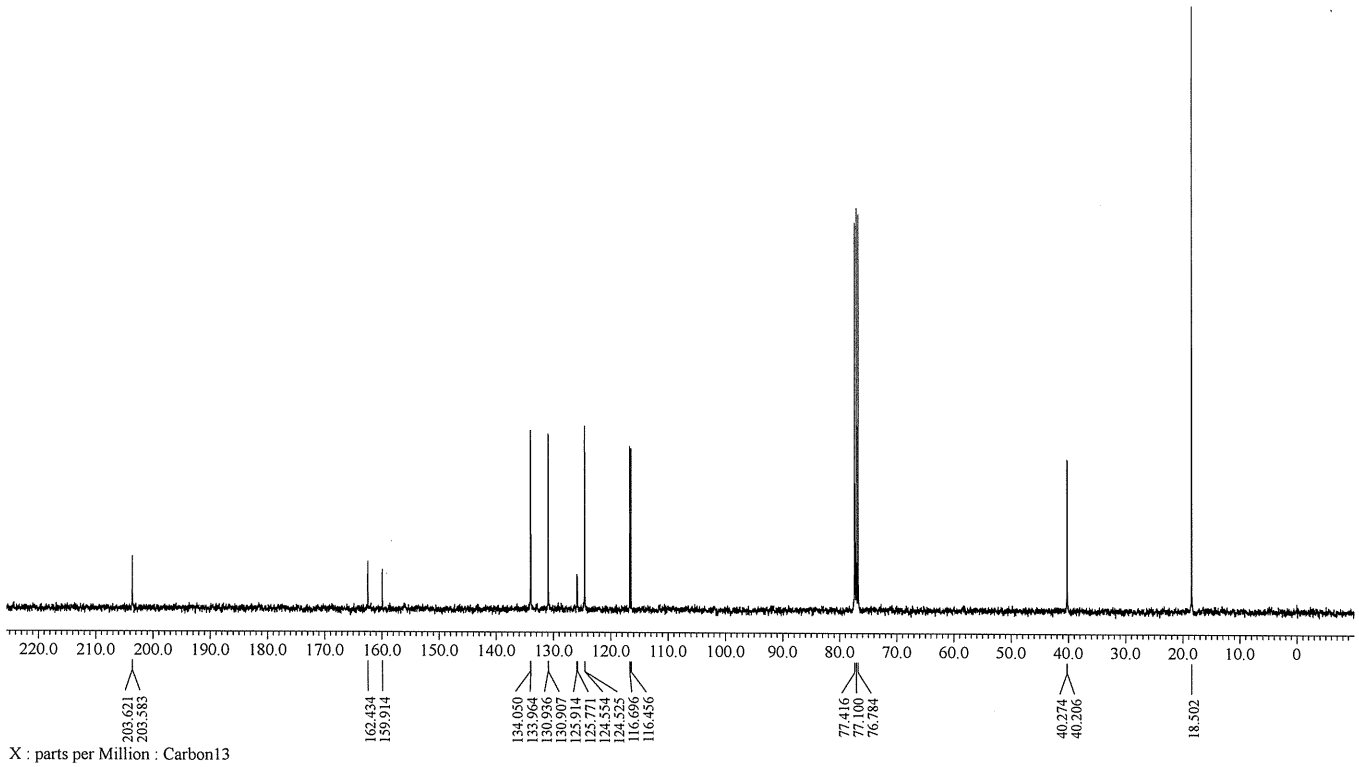
^{1}H NMR, 400 MHz, $CDCl_3$



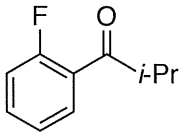
^{13}C NMR, 100 MHz, $CDCl_3$



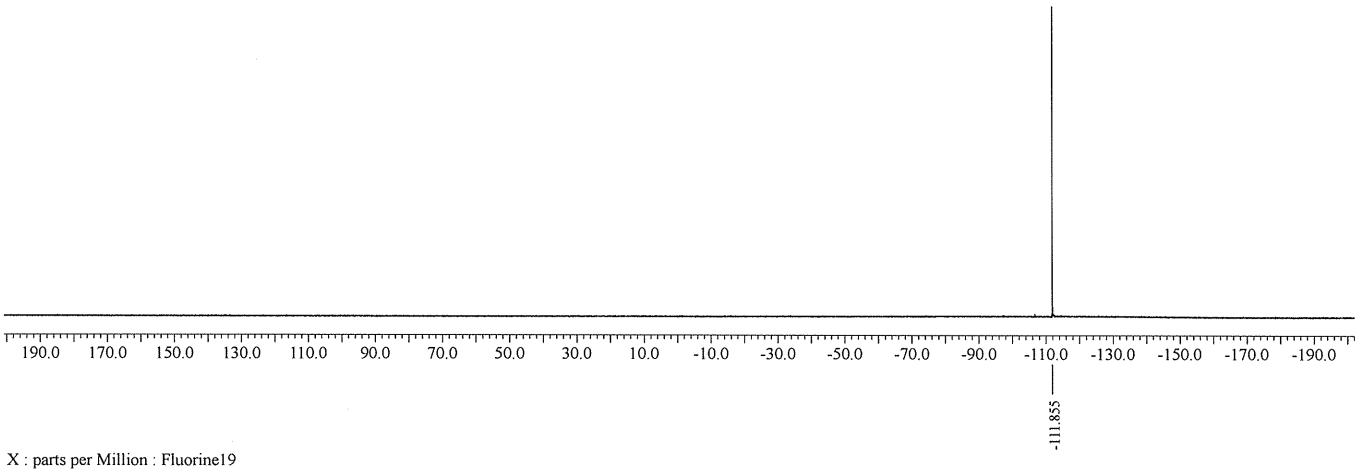
^{1}H NMR, 400 MHz, $CDCl_3$



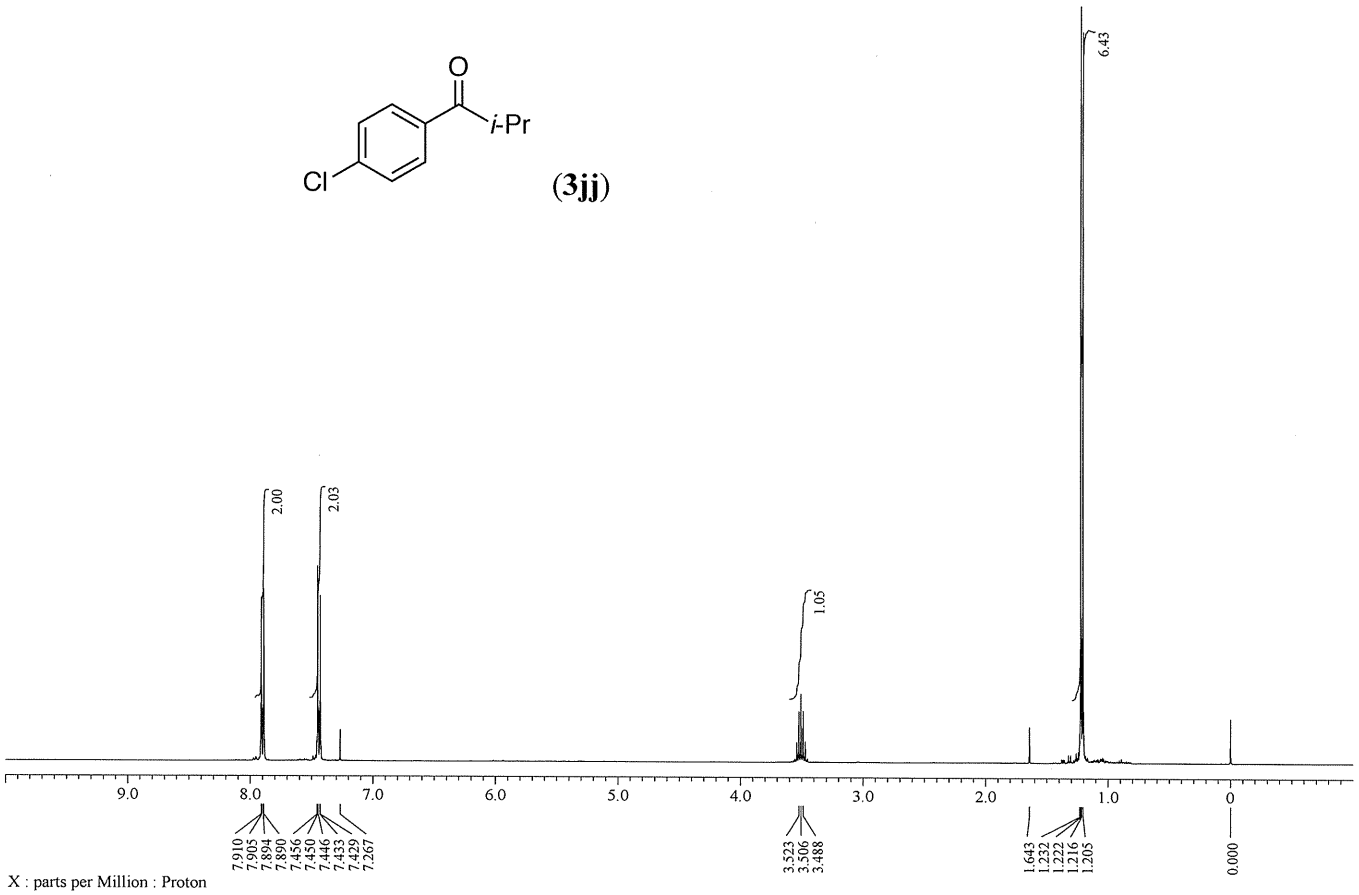
^{13}C NMR, 100 MHz, $CDCl_3$



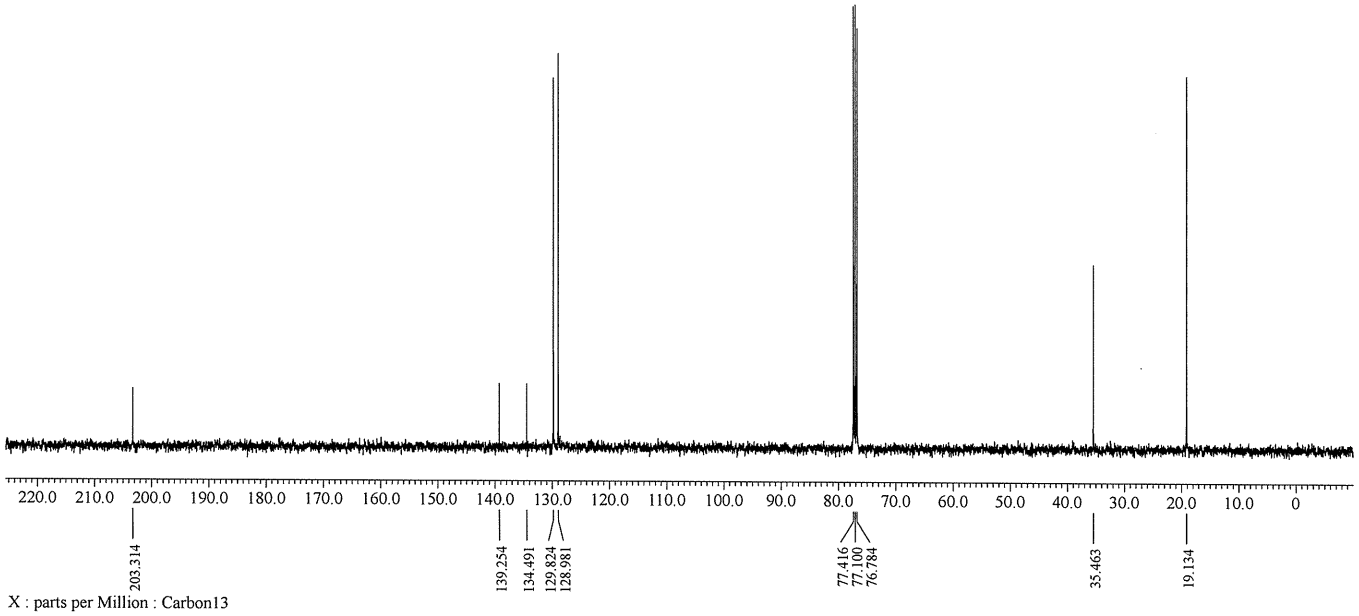
(3mj)



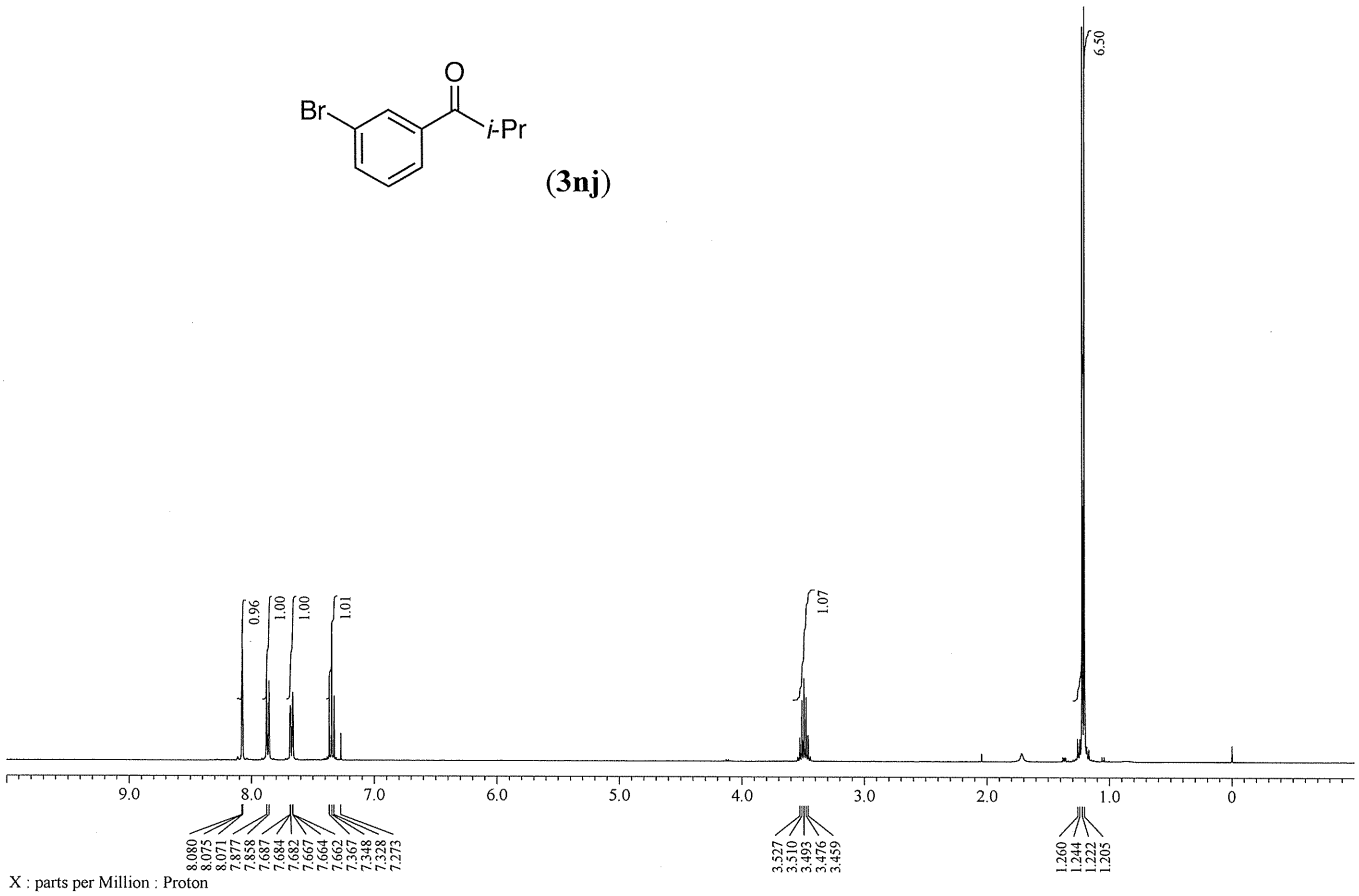
^{19}F NMR, 376 MHz, $CDCl_3$



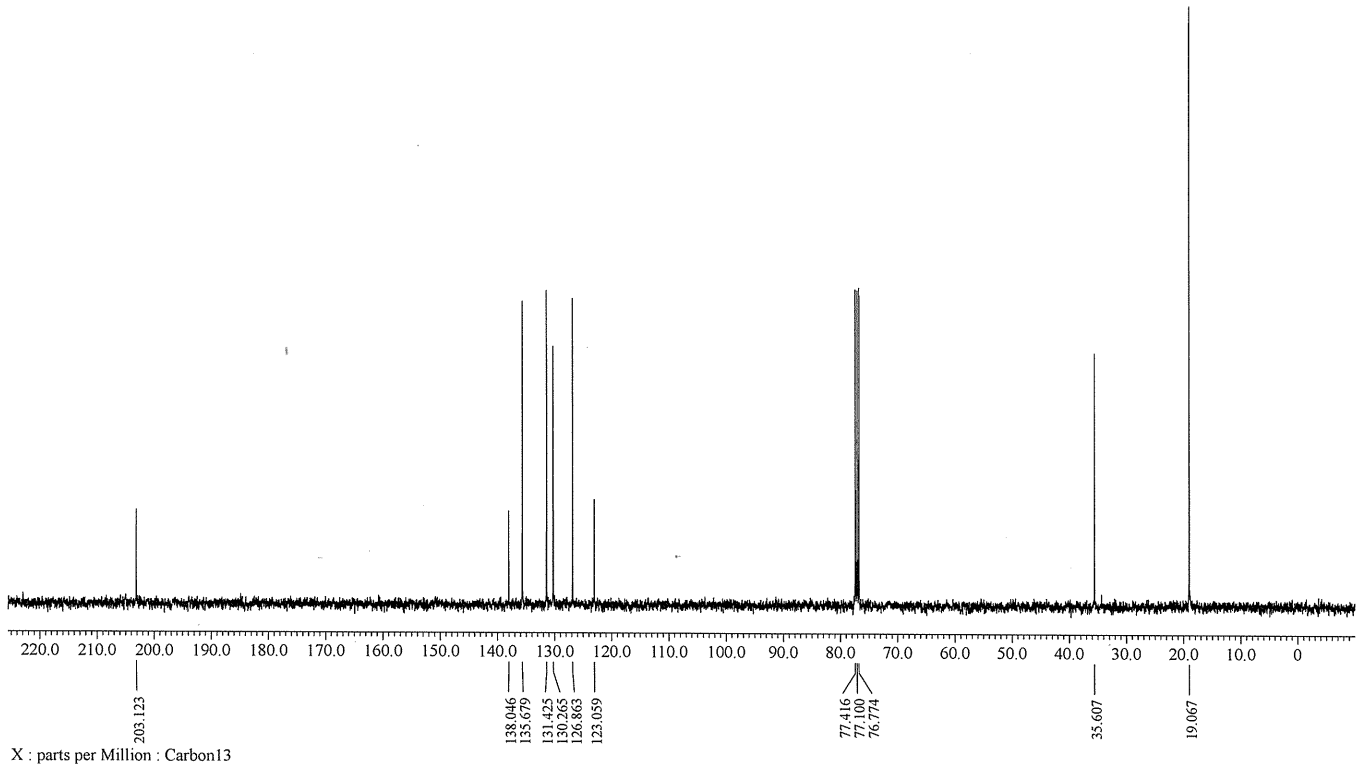
^{1}H NMR, 400 MHz, $CDCl_3$



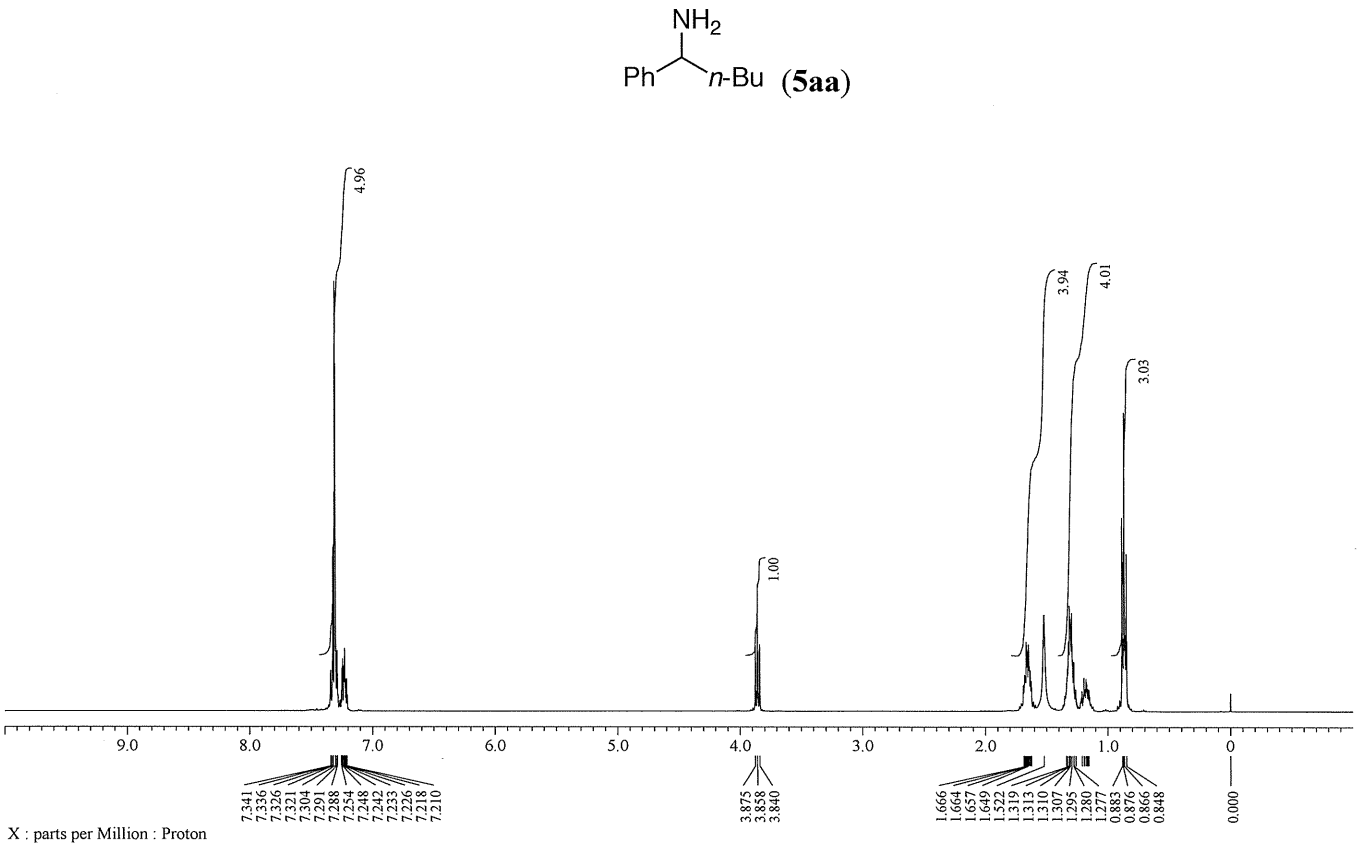
^{13}C NMR, 100 MHz, $CDCl_3$



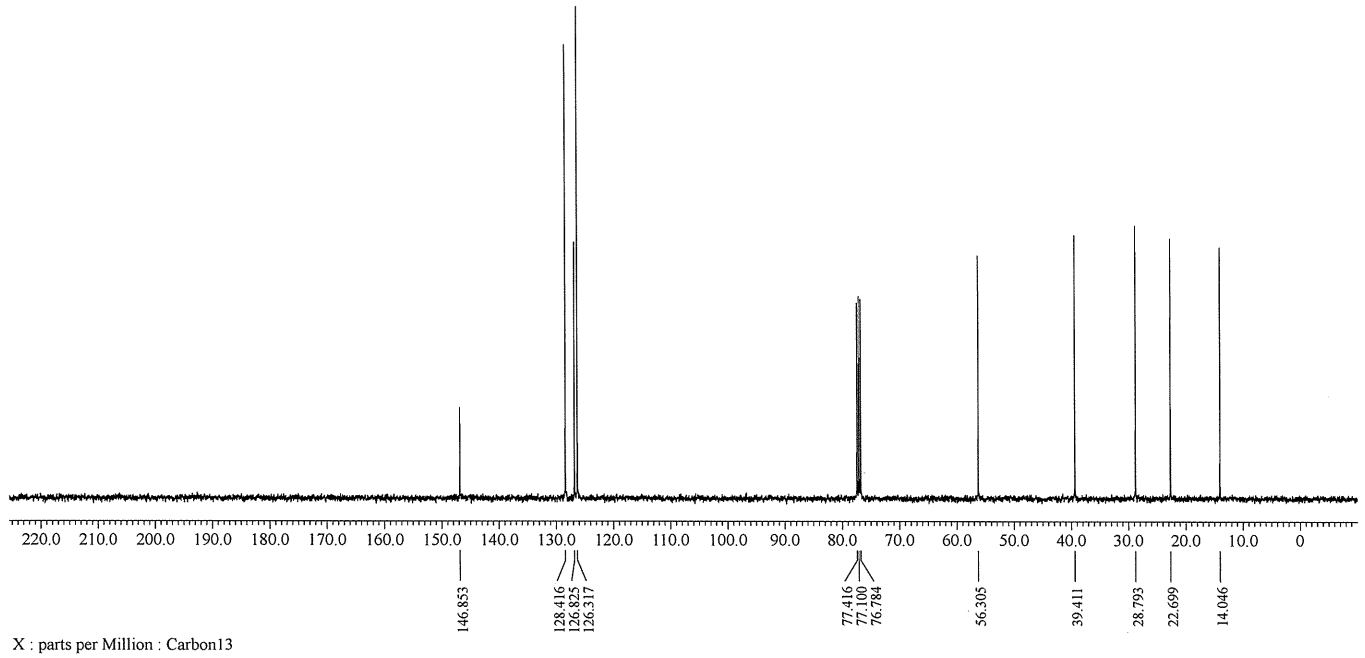
^{1}H NMR, 400 MHz, $CDCl_3$



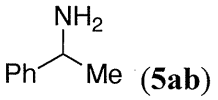
^{13}C NMR, 100 MHz, $CDCl_3$



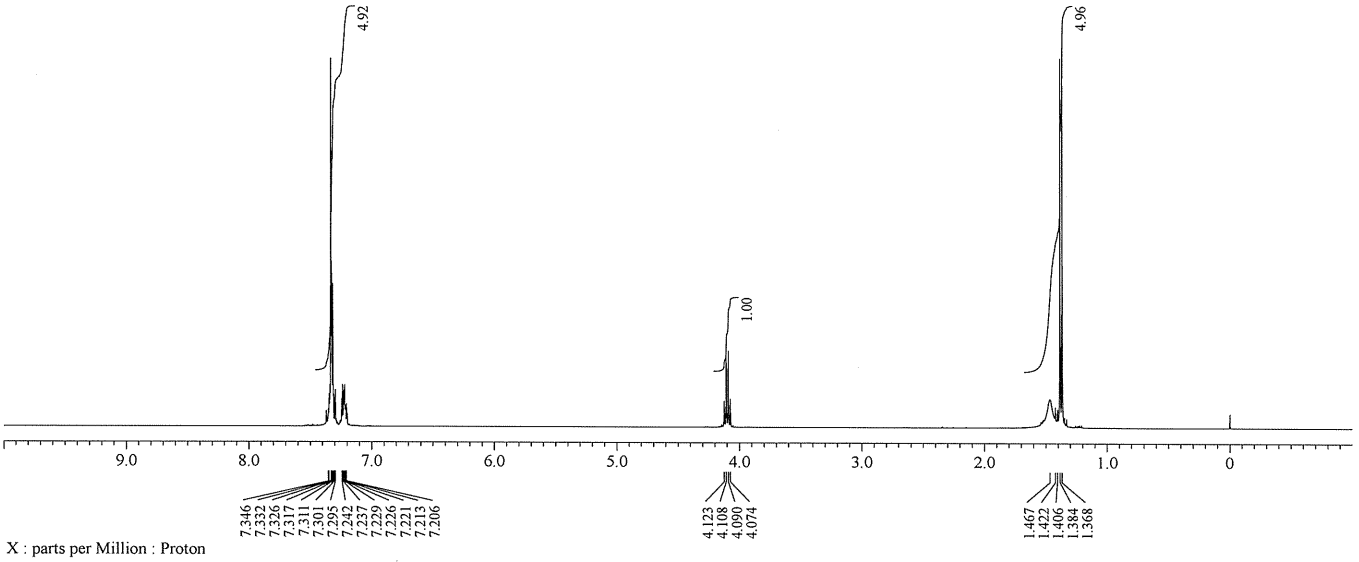
^{1}H NMR, 400 MHz, $CDCl_3$



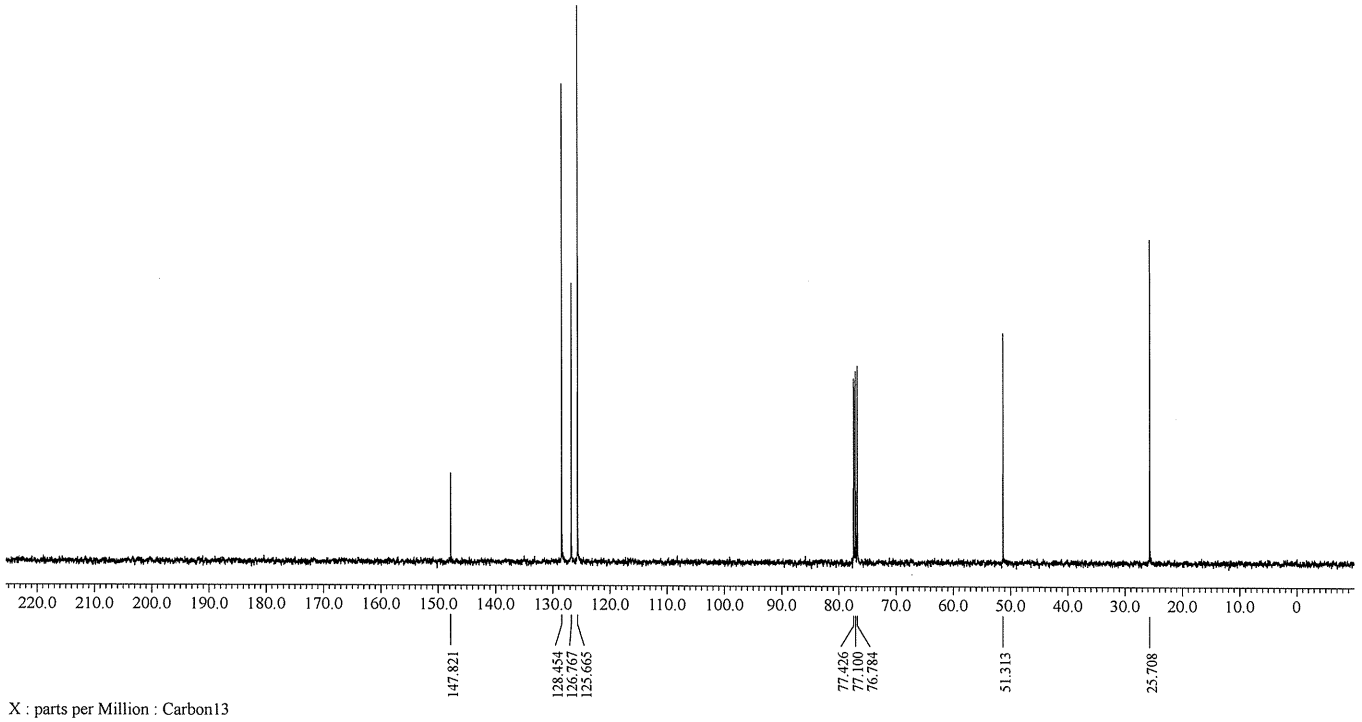
^{13}C NMR, 100 MHz, $CDCl_3$



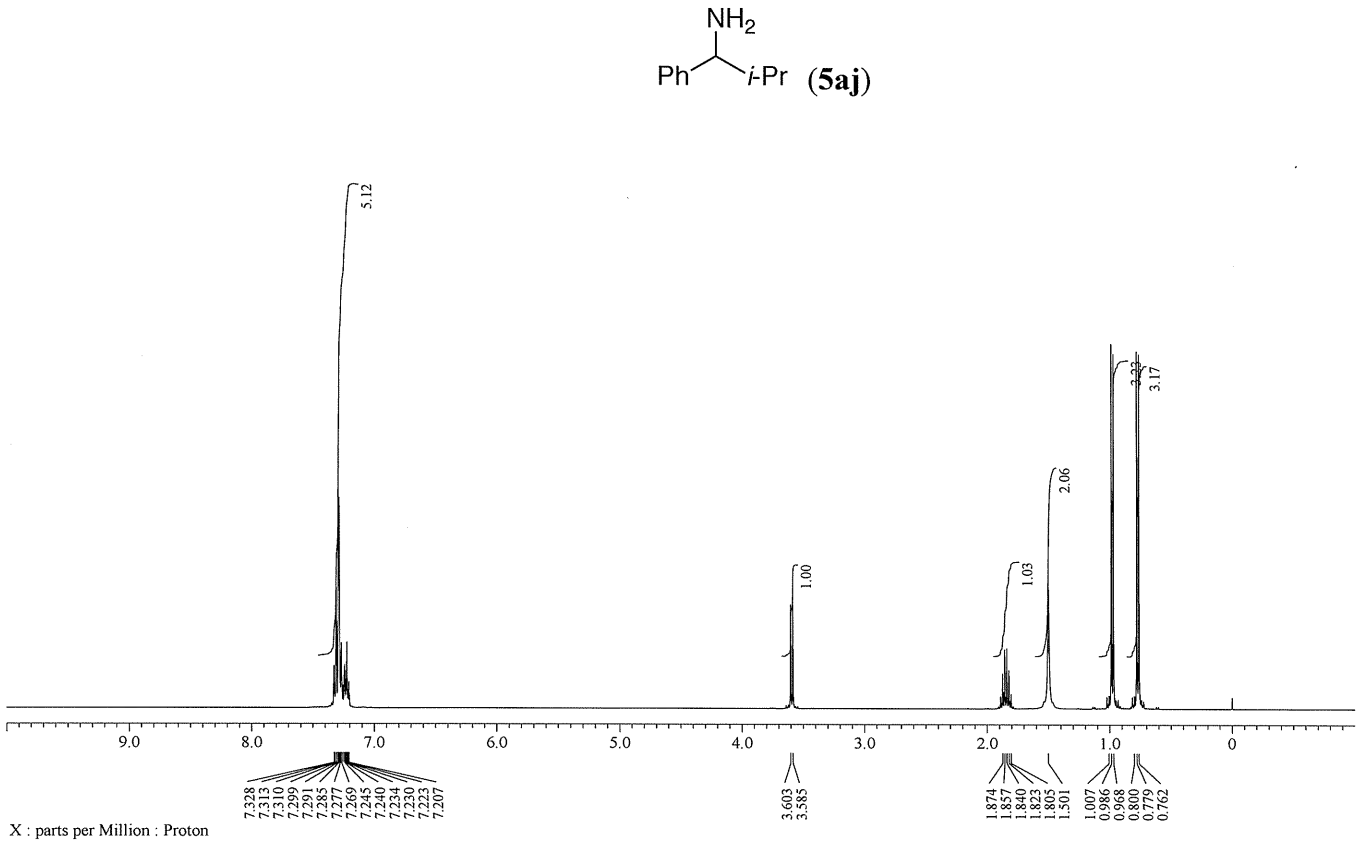
(5ab)



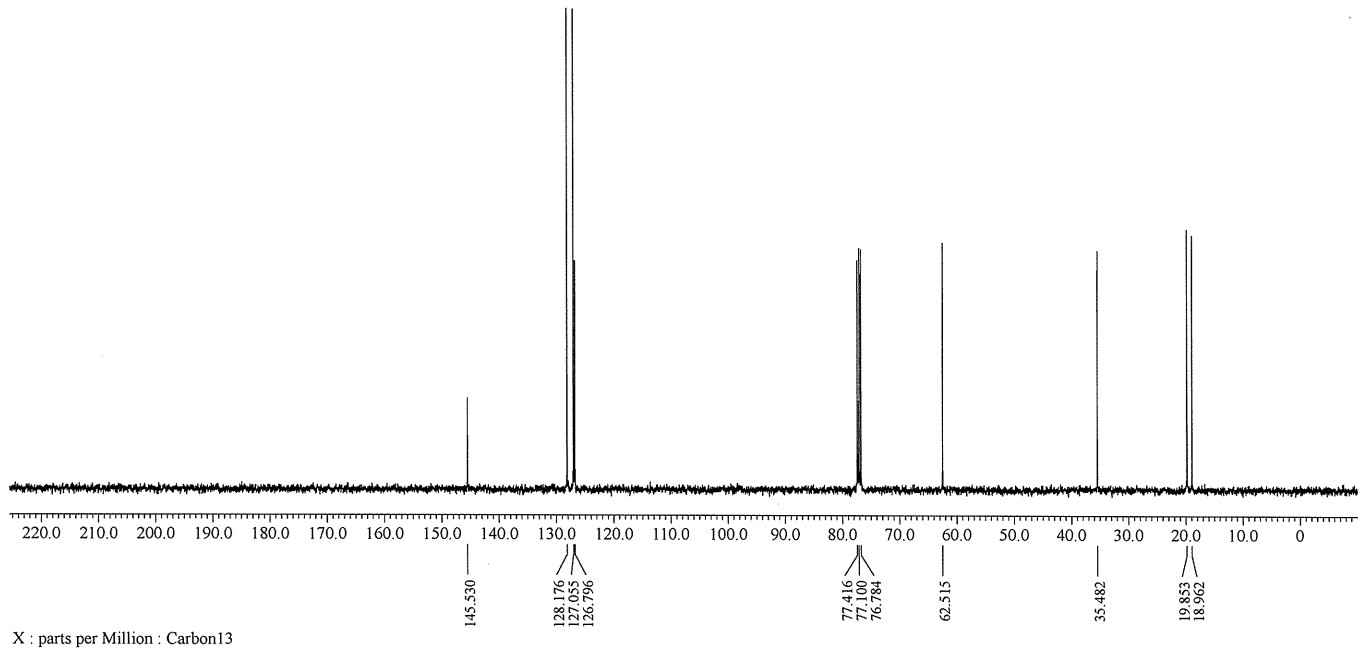
^{1}H NMR, 400 MHz, $CDCl_3$



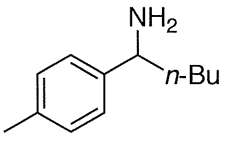
^{13}C NMR, 100 MHz, $CDCl_3$



^{1}H NMR, 400 MHz, $CDCl_3$



^{13}C NMR, 100 MHz, $CDCl_3$



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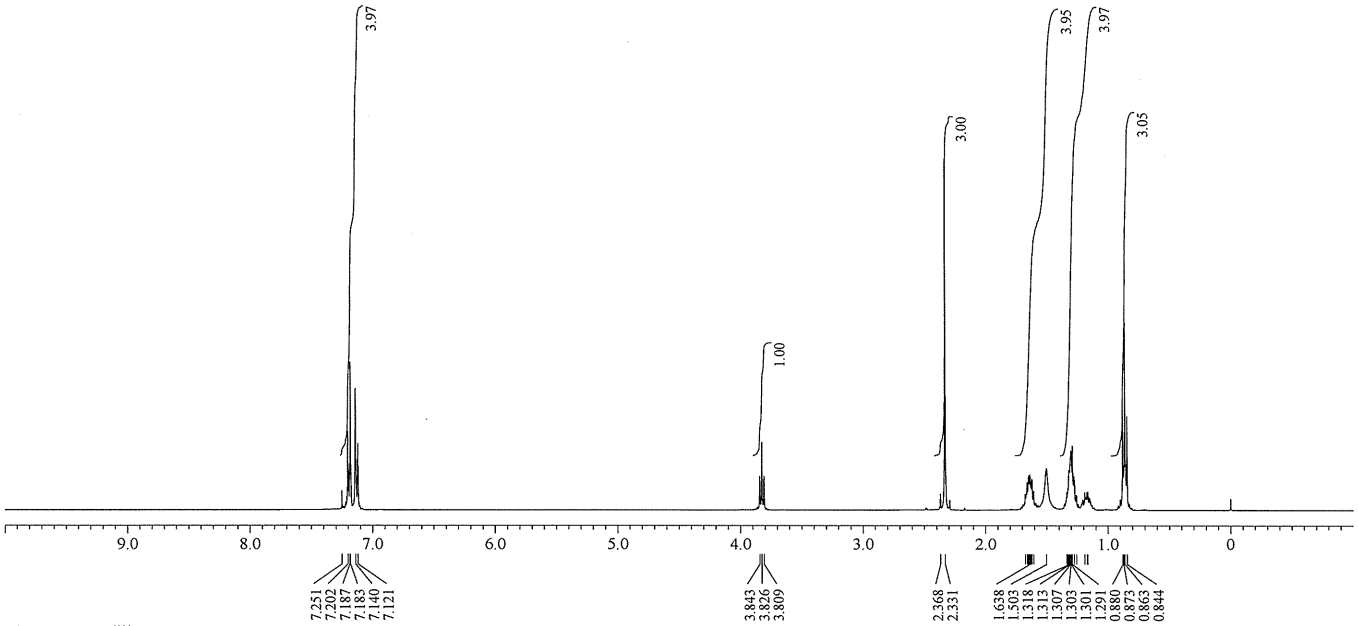
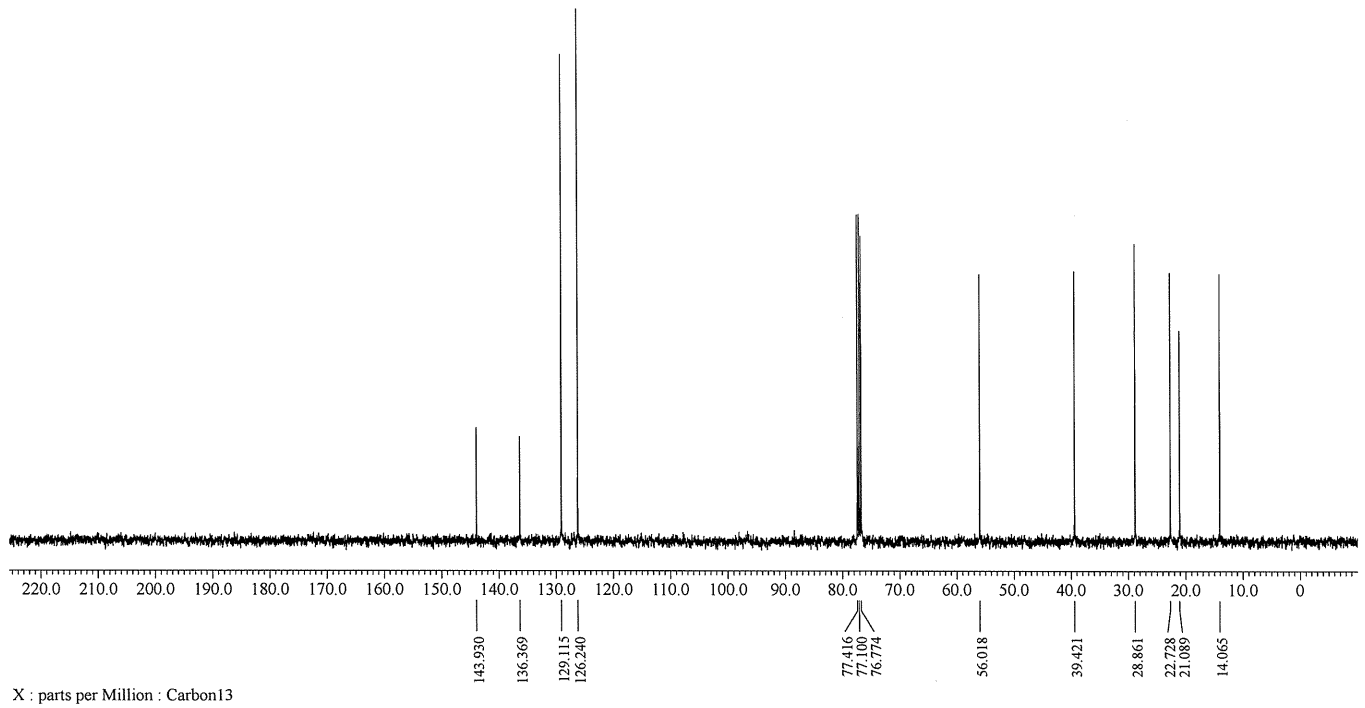
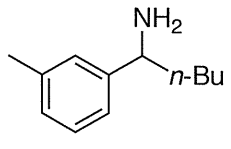


^{1}H NMR, 400 MHz, $CDCl_3$



^{13}C NMR, 100 MHz, $CDCl_3$



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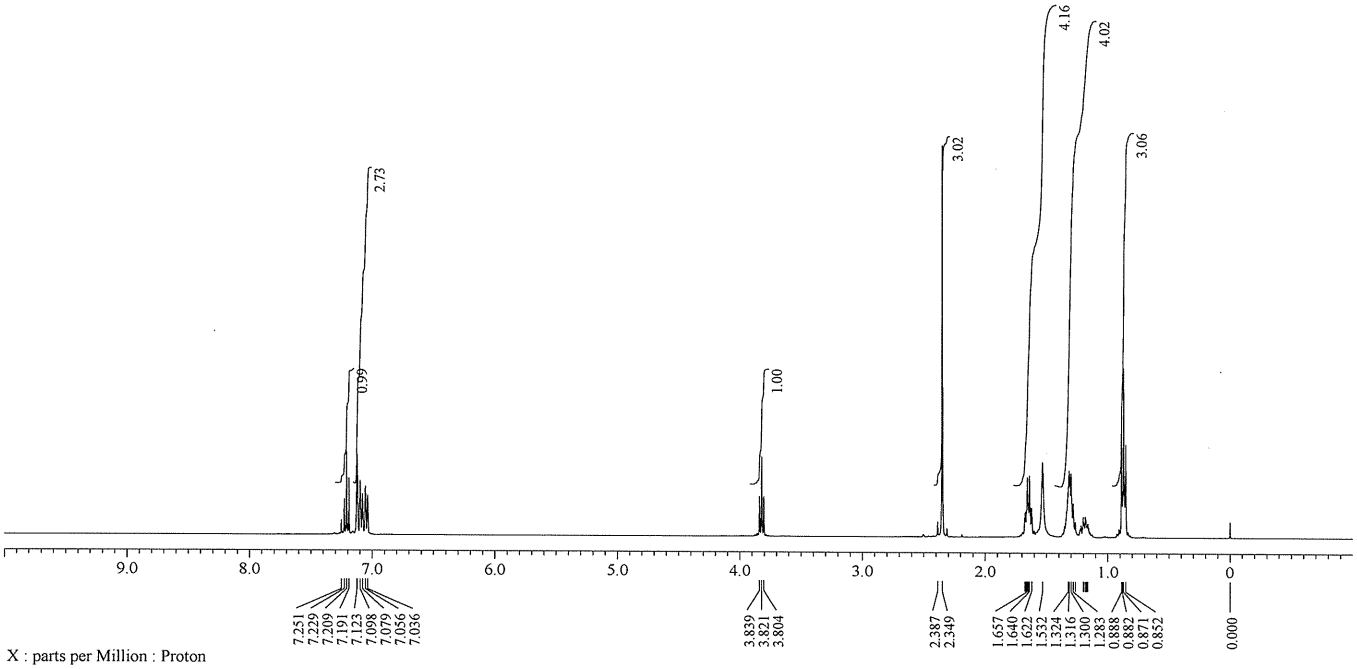
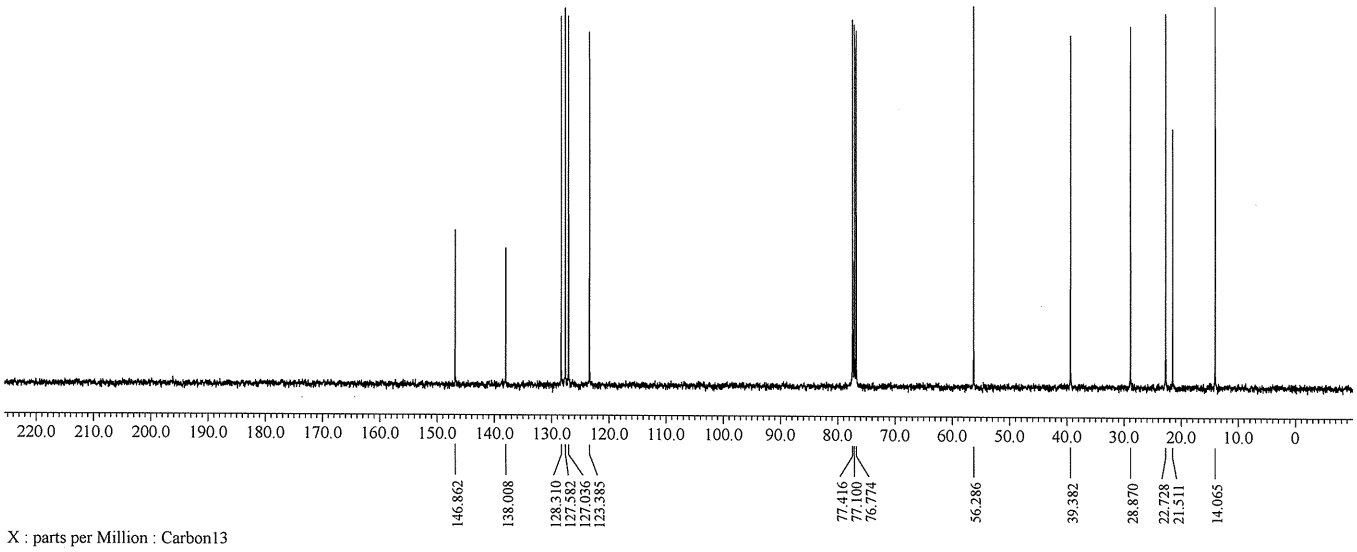
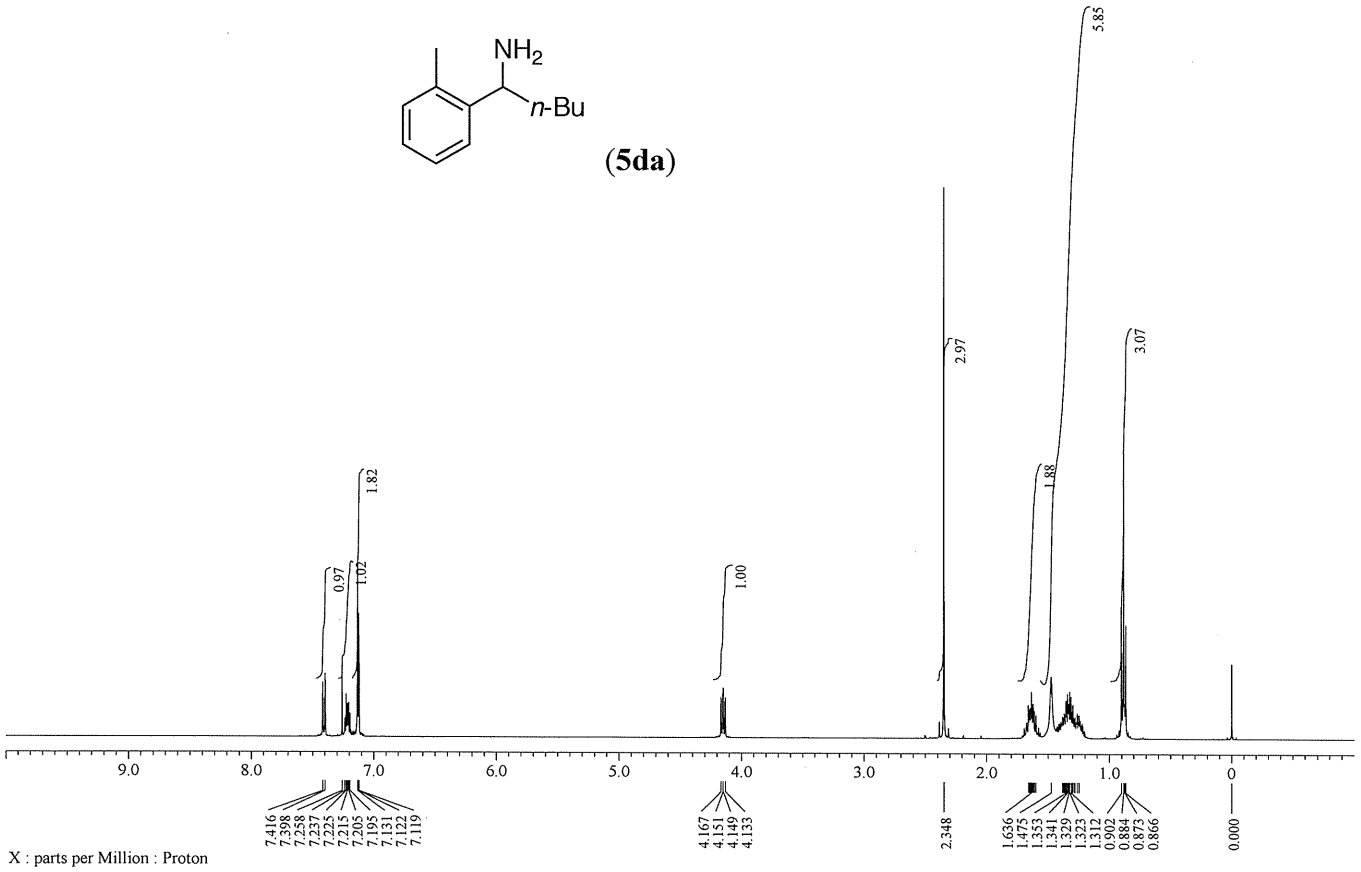


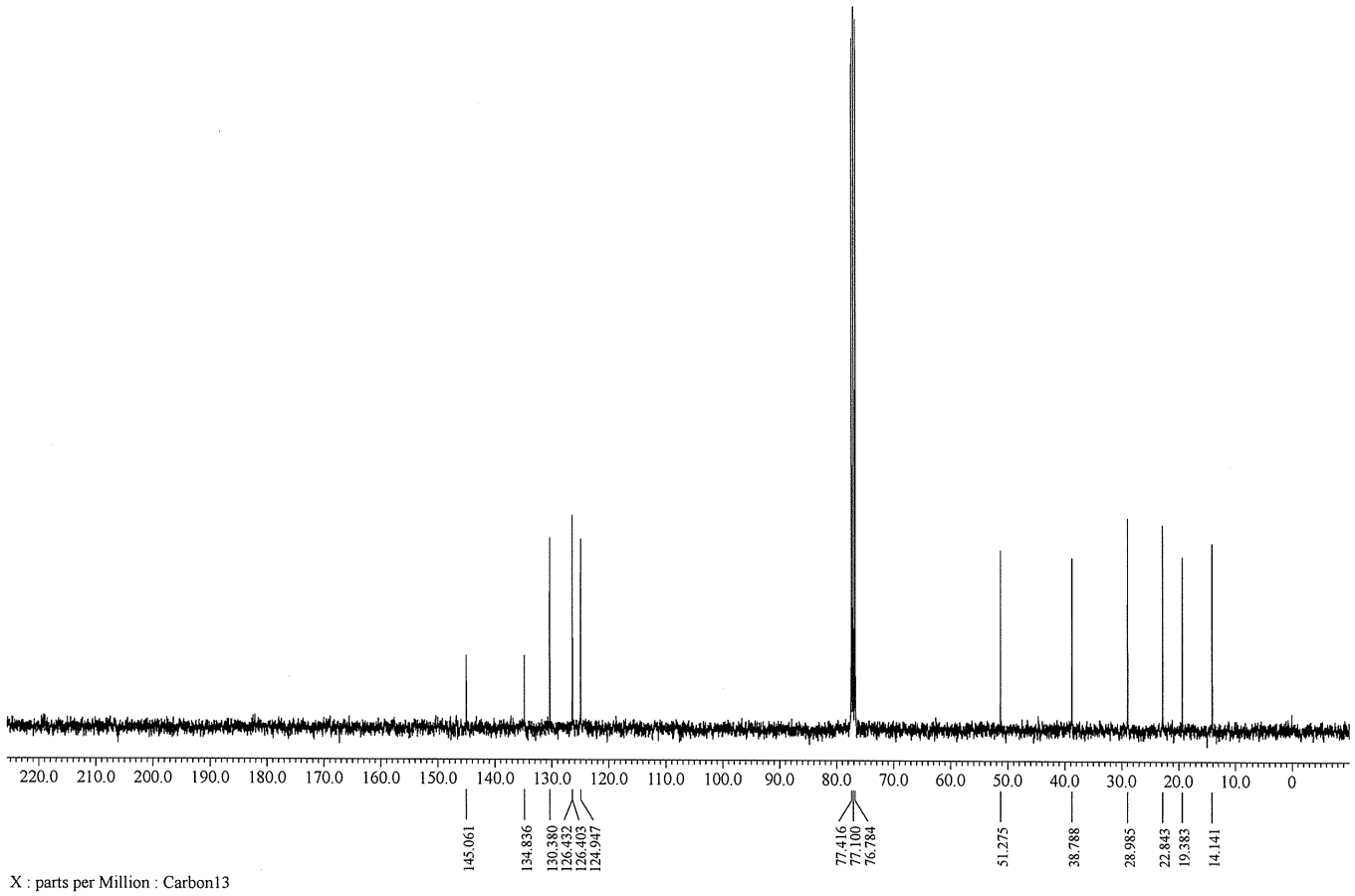
^{1}H NMR, 400 MHz, $CDCl_3$



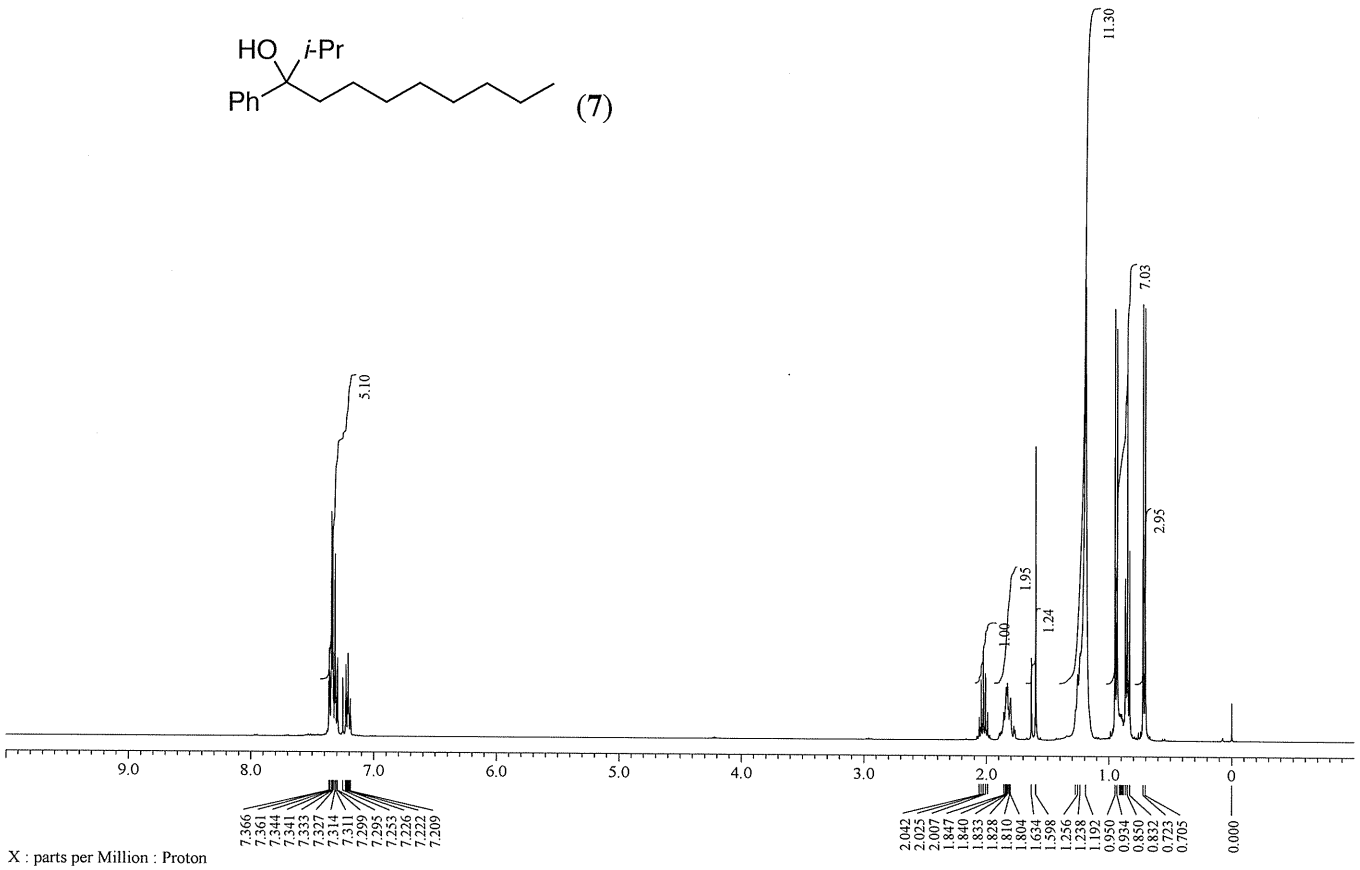
^{13}C NMR, 100 MHz, $CDCl_3$



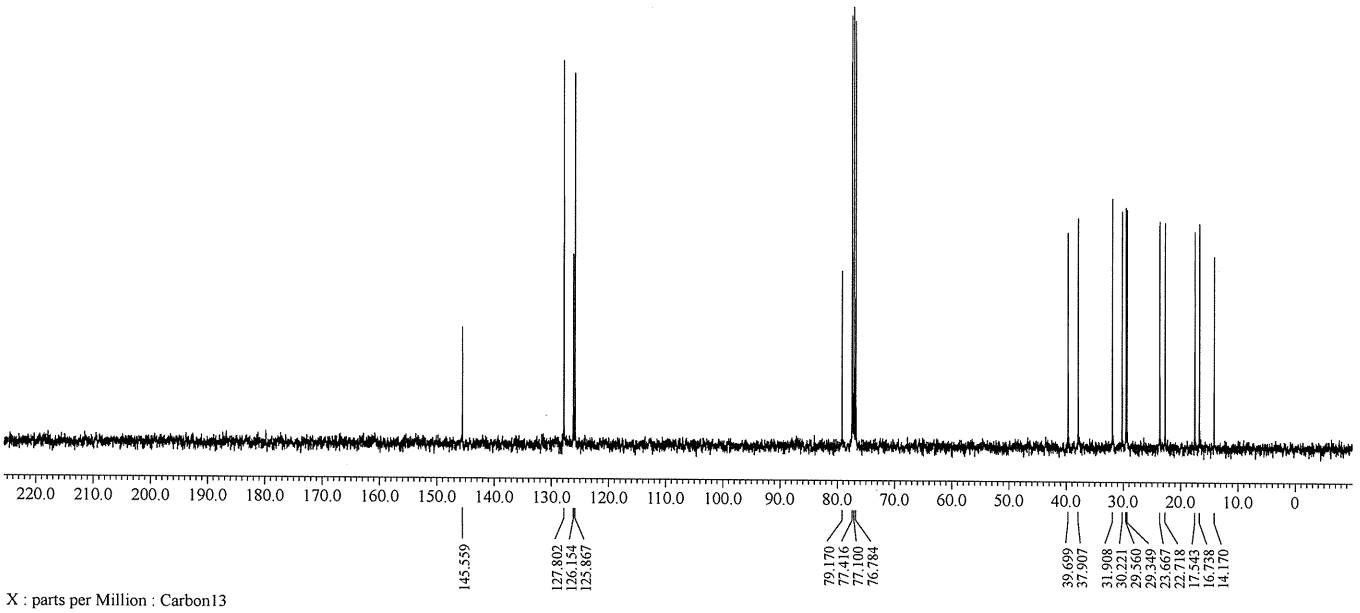
^{1}H NMR, 400 MHz, $CDCl_3$



^{13}C NMR, 100 MHz, $CDCl_3$



^{1}H NMR, 400 MHz, $CDCl_3$



^{13}C NMR, 100 MHz, $CDCl_3$