Electronic Supplementary Information

Aluminum porphyrins with quaternary ammonium halides as catalysts for copolymerization of cyclohexene oxide and CO_2: Metal–ligand cooperative catalysis

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Table of contents

[1] General methods.

Instrumentation. NMR spectra were recorded on a Bruker Ascend 500 (^{1}H: 500 MHz and ^{13}C: 126 MHz) or a JEOL-ECS400 spectrometer (^{1}H: 400 MHz and ^{13}C: 100 MHz). Size-exclusion chromatography (SEC) was carried out with two columns (Shodex KF-804L) using THF as an eluent at 1 mL/min at 40 °C, where molecular weights were calibrated by using standard polystyrene samples. Electrospray ionization (ESI) mass spectra were recorded on a Bruker micrOTOF. Matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectroscopic measurements were performed on a Bruker Autoflex III or a Shimadzu AXIMA-CFR plus mass spectrometer. IR spectra were recorded on a Shimadzu IRAffinity-1 spectrophotometer. Real-time IR measurements were performed on a Mettler Toledo ReactIR 45 and analyzed by iCIR.

Materials. Most reagents for the synthesis of the catalysts were purchased and used without further purification unless otherwise specified. Dry solvents were purchased or distilled over an appropriate drying agent or passed through solvent purification columns attached to a GlassContour solvent purification system. Cyclohexene oxide (CHO) was freshly distilled from CaH_2. Bis(triphenylphosphine)iminium chloride (PPNCl) was recrystallized from CH_2Cl_2/Et_2O under N_2, while PPNBr was prepared from PPNCl and NaBr in hot water and recrystallized from CH_2Cl_2/Et_2O under N_2.

Manipulation for polycarbonate synthesis. All the copolymerization reactions were performed in a 50-mL stainless steel autoclave. When the catalyst and CHO were put in the autoclave, standard glovebox and Schlenk techniques were used, respectively, under N_2 or Ar purified by passing through a hot column packed with BASF catalyst R3-11.

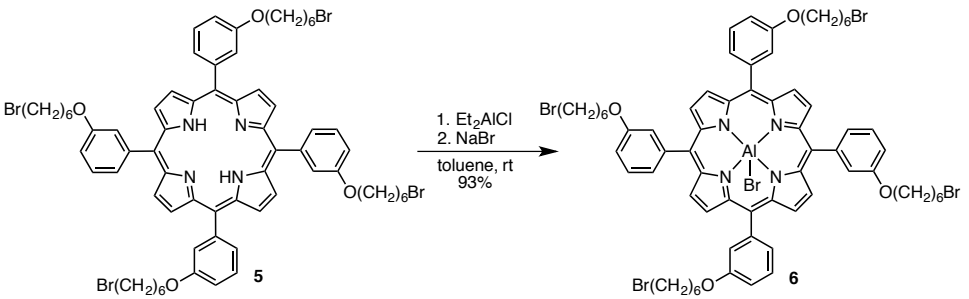
[2] Synthesis and characterizations of Al porphyrins.

Compounds **3-Cl**, **4-Br**, and **5** were prepared and characterized according to the previously reported methods.[S1]

References

(S1) (*a*) T. Ema, Y. Miyazaki, S. Koyama, Y. Yano and T. Sakai, *Chem. Commun.*, 2012, **48**, 4489; (*b*) T. Ema, Y. Miyazaki, J. Shimonishi, C. Maeda and J. Hasegawa, *J. Am. Chem. Soc*., 2014, **136**, 15270.

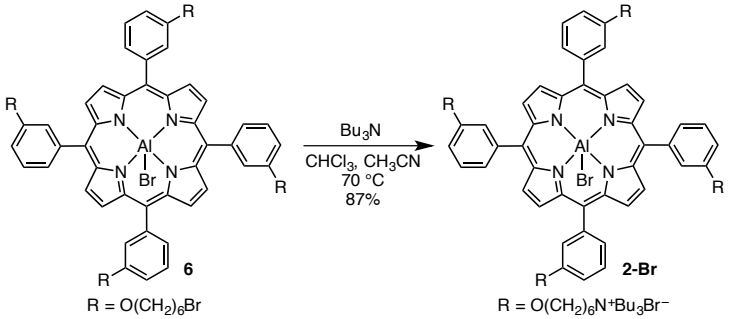
Synthesis of 6.



Et_2AlCl (0.87 M in hexane, 0.56 mL, 0.49 mmol) was slowly added to a solution of **5** (500 mg, 376 μmol) in dry toluene (11.3 mL), and the mixture was stirred at rt for 3 h. The mixture was diluted with $CHCl_3$, washed with 1 M NaBr aq., and dried over Na_2SO_4. The product was purified by silica gel column chromatography ($CHCl_3$/MeOH (10:1)), dissolved in $CHCl_3$, and washed with 3% HBr aq. and then 1 M NaBr aq. The solution was dried over Na_2SO_4 and evaporated to give **6** (503 mg, 93%) as a purple solid.

^{1}H NMR (DMSO-d_6, 400 MHz) δ 1.49 (m, 16H), 1.83 (m, 16H), 3.53 (t, J = 6.8 Hz, 8H), 4.21 (t, J = 6.2 Hz, 8H), 7.43–7.46 (m, 4H), 7.73 (s, 12H), 9.02 ppm (s, 8H); ^{13}C NMR (DMSO-d_6, 100 MHz, 60 °C) δ 24.6, 25.8, 28.4, 31.7, 44.9, 67.6, 114.0, 119.6, 120.8, 126.8, 127.6, 131.6, 142.0, 146.3, 157.0 ppm; HR-MS (ESI): m/z = 1355.2102. calcd for $C_{68}H_{72}N_4O_4AlBr_4$: 1355.2070 $[M–Br]^+$; IR (KBr) 2936, 2859, 1597, 1576, 1472, 1427, 1350, 1314, 1285, 1260, 1209, 1184, 1072, 1013, 802, 783, 723, 702 cm^{-1}.

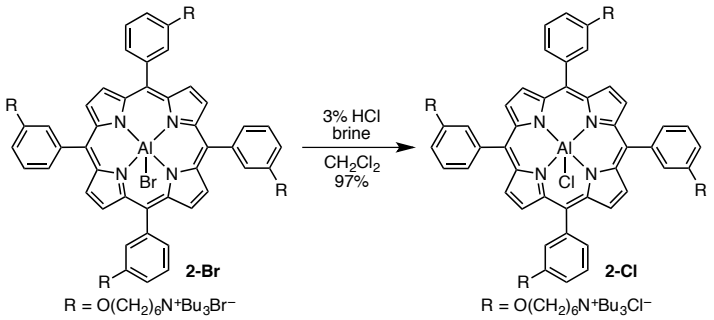
Synthesis of 2-Br.



A sealed tube containing **6** (95.8 mg, 66.7 μmol) and Bu_3N (0.67 mL, 2.8 mmol) in dry $CHCl_3$ (0.67 mL) and dry CH_3CN (0.67 mL) was heated at 70 °C for 1 week. After the solvents were evaporated, excess Bu_3N was removed by pipette, and the residue was precipitated with CH_2Cl_2/Et_2O. The crude product was dissolved in CH_2Cl_2, and the solution was vigorously washed with 3% HBr (×1) and 1 M NaBr aq. (×2), dried over Na_2SO_4, and evaporated to give **2-Br** (126 mg, 87%) as a purple solid.

^{1}H NMR (CD_3OD, 400 MHz, 60 °C) δ 1.00 (t, J = 7.6 Hz, 36H), 1.39–1.81 (m, 72H), 1.94 (m, 8H), 3.22–3.27 (m, 32H), 4.25 (t, J = 6.4 Hz, 8H), 7.42 (d, J = 7.9 Hz, 4H), 7.70 (t, J = 7.6 Hz, 4H), 7.77 (s, 8H), 9.10 ppm (s, 8H); ^{13}C NMR (CD_3OD, 100 MHz, 60 °C) δ 14.0, 20.7, 22.9, 24.9, 26.8, 27.2, 30.3, 59.5, 59.7, 69.1, 115.0, 121.7, 122.4, 128.5, 128.9, 132.9, 144.5, 149.1, 159.1 ppm; HR-MS (ESI): m/z = 1008.5728. calcd for $C_{116}H_{180}N_8O_4AlBr_3$: 1008.5724 $[M–2Br]^{2+}$; IR (KBr) 2959, 2936, 2874, 1595, 1576, 1472, 1423, 1383, 1350, 1285, 1260, 1184, 1167, 1069, 1011, 885, 800, 783, 721, 702 cm^{-1}.

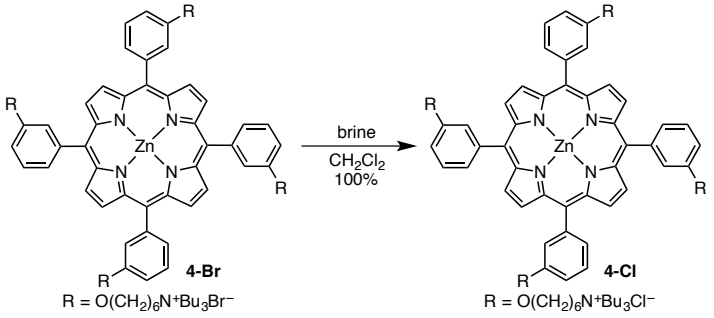
Synthesis of 2-Cl.



A solution of **2-Br** (127 mg, 58.3 μmol) in CH_2Cl_2 was vigorously washed with 3% HCl (×2) and brine (×1), dried over Na_2SO_4, and evaporated to give **2-Cl** (111 mg, 97%) as a blue-purple solid.

^{1}H NMR (CD_3OD, 400 MHz, 60 °C) δ 1.01 (t, J = 7.2 Hz, 36H), 1.34–1.78 (m, 72H), 1.95 (m, 8H), 3.22–3.27 (m, 32H), 4.25 (t, J = 5.8 Hz, 8H), 7.43 (d, J = 7.6 Hz, 4H), 7.71 (t, J = 7.6 Hz, 4H), 7.78 (s, 8H), 9.15 ppm (s, 8H); ^{13}C NMR (CD_3OD, 100 MHz, 60 °C) δ 14.0, 20.7, 22.9, 24.8, 26.9, 27.2, 30.3, 59.5, 59.6, 69.1, 115.0, 121.7, 122.4, 128.5, 128.9, 132.9, 144.4, 149.1, 159.1 ppm; HR-MS (ESI): m/z = 941.6517. calcd for $C_{116}H_{180}N_8O_4AlCl_3$: 941.6488 $[M–2Cl]^{2+}$; IR (KBr) 2959, 2936, 2874, 1593, 1576, 1472, 1423, 1385, 1350, 1312, 1287, 1260, 1184, 1169, 1069, 1009, 881, 799, 721, 702 cm^{-1}.

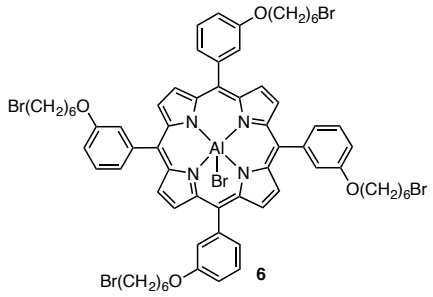
Synthesis of 4-Cl.

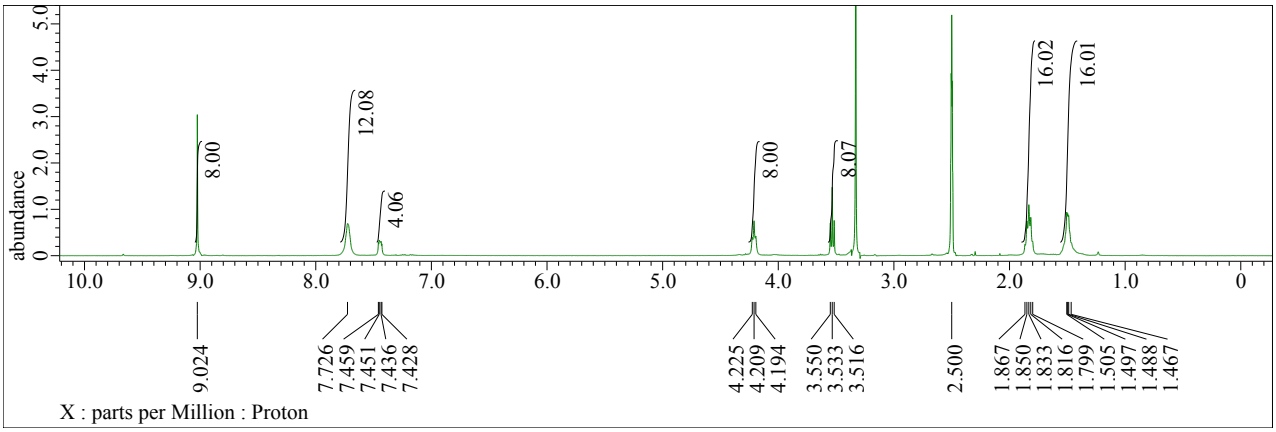


A solution of **4-Br** (56.1 mg, 26.3 μmol) in CH_2Cl_2 was vigorously washed with brine (×10), dried over Na_2SO_4, and evaporated. Recrystallization of the residue from CH_2Cl_2/Et_2O gave **4-Cl** (51.3 mg, 100%) as a blue-green solid.

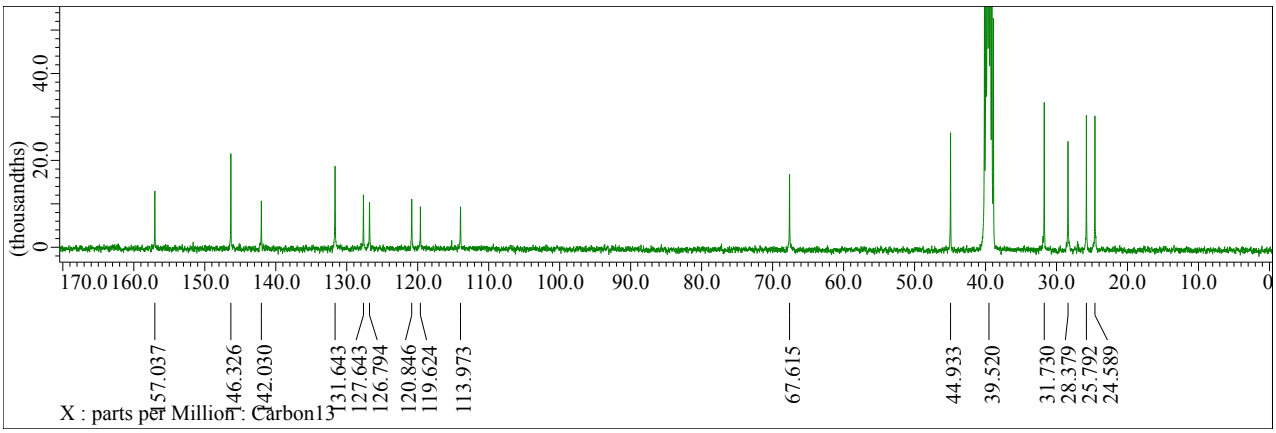
^{1}H NMR (CD_3OD, 400 MHz, 60 °C) δ 0.93 (t, J = 6.8 Hz, 36H), 1.22–1.69 (m, 72H), 1.87 (m, 8H), 3.10 (s, 32H), 4.19 (t, J = 5.8 Hz, 8H), 7.32 (dd, J = 2.0, 7.6 Hz, 4H), 7.62 (t, J = 7.6 Hz, 4H), 7.74–7.82 (m, 8H), 8.88 ppm (s, 8H); ^{13}C NMR (CD_3OD, 100 MHz, 60 °C) δ 13.8, 20.6, 22.8, 24.8, 26.7, 27.1, 30.2, 59.7, 59.8, 69.3, 114.7, 121.6, 122.9, 128.4, 128.8, 132.5, 146.1, 151.4, 158.8 ppm; HR-MS (ESI): m/z = 943.6397. calcd for $C_{116}H_{180}N_8O_4ZnCl_2$: 943.6394 $[M–2Cl]^{2+}$; IR (KBr) 2959, 2936, 2872, 1595, 1574, 1474, 1431, 1381, 1335, 1285, 1254, 1207, 1180, 1165, 1065, 1040, 1013, 995, 935, 878, 795, 745, 719, 702 cm^{-1}.

NMR spectra.

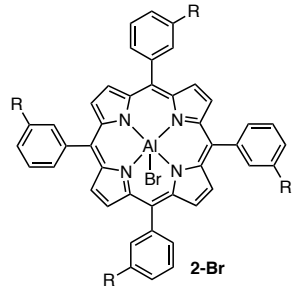


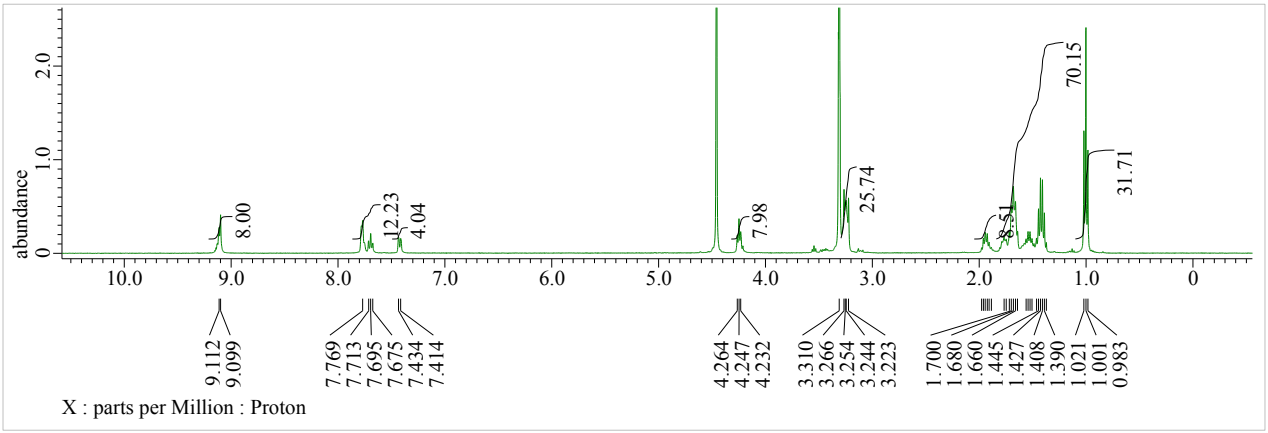


^{1}H NMR spectrum of **6** in DMSO-d_6

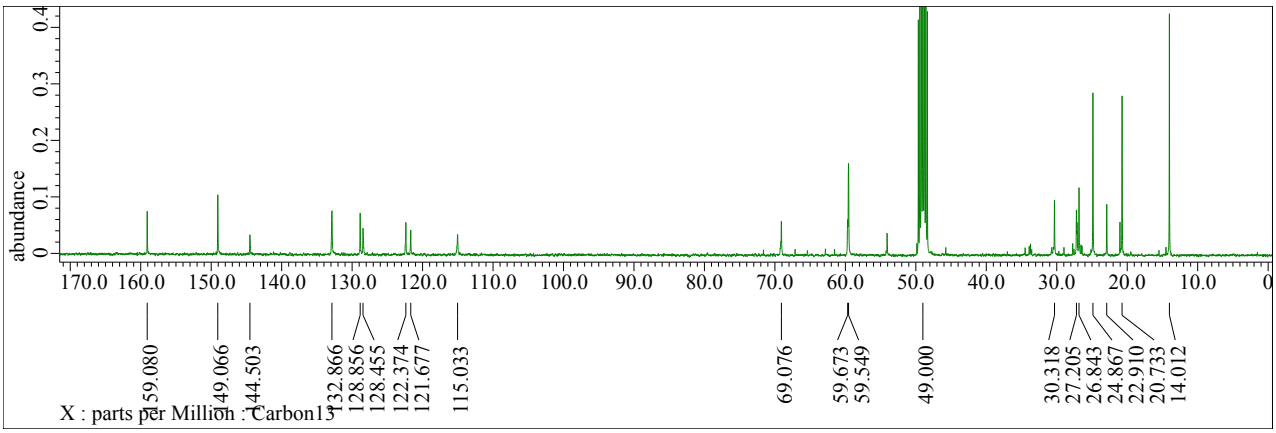


^{13}C NMR spectrum of **6** in DMSO-d_6 at 60 °C

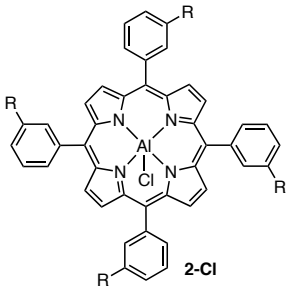




^{1}H NMR spectrum of **2-Br** in CD_3OD at 60 °C

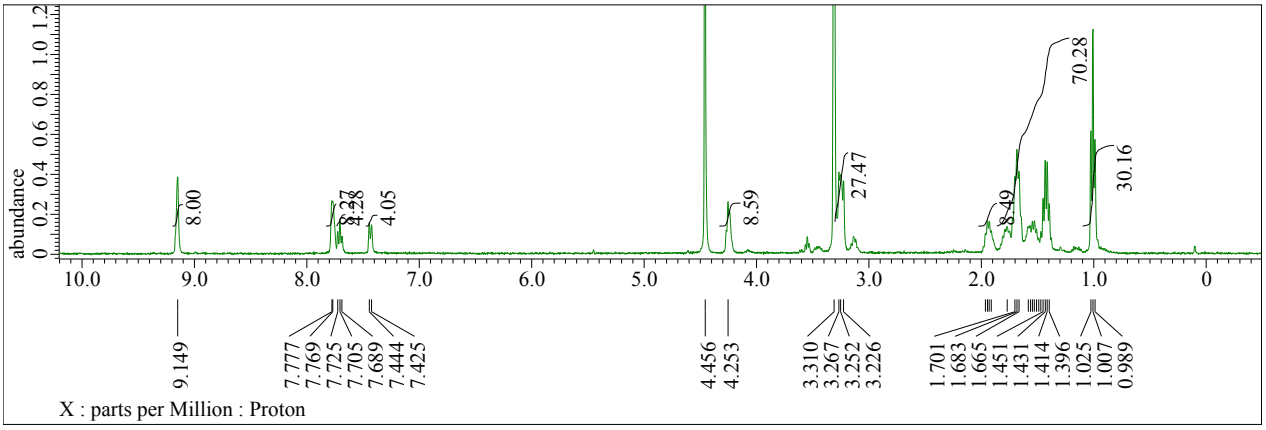


^{13}C NMR spectrum of **2-Br** in CD_3OD at 60 °C

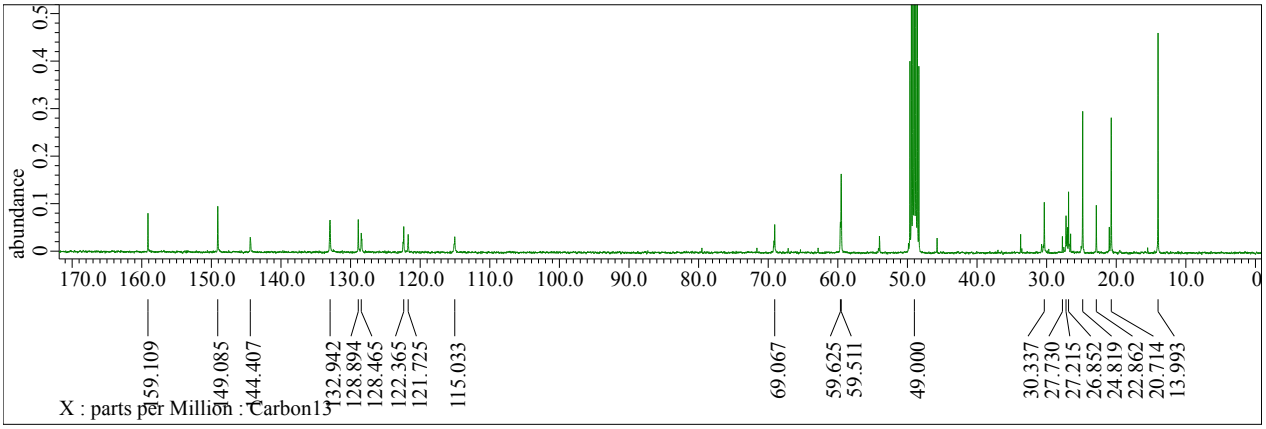


2-Cl

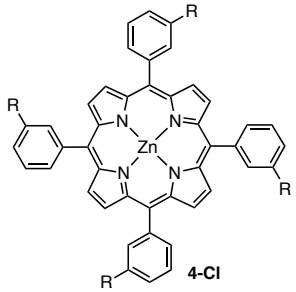
R = $O(CH_2)_6N^+Bu_3Cl^-$



^{1}H NMR spectrum of **2-Cl** in CD_3OD at 60 °C

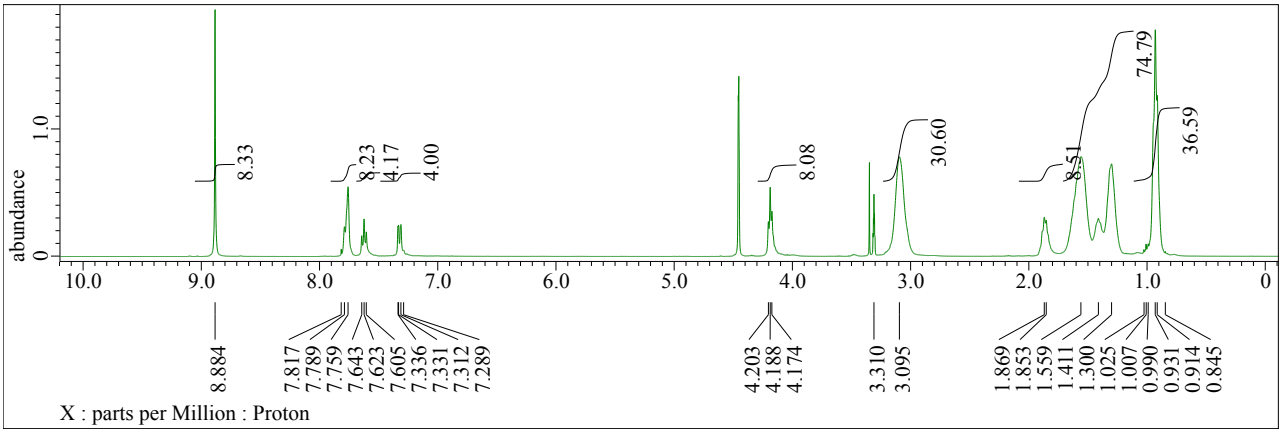


^{13}C NMR spectrum of **2-Cl** in CD_3OD at 60 °C

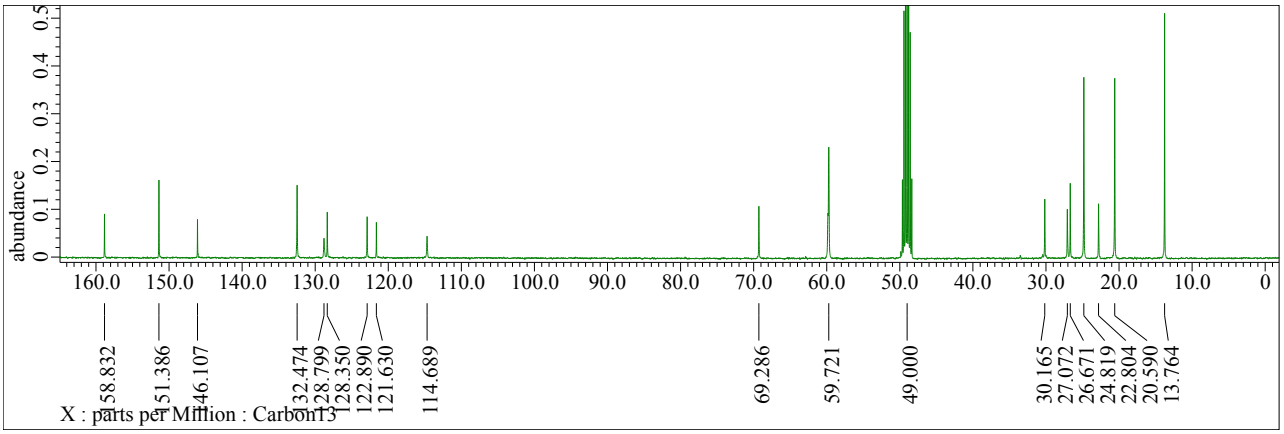


4-Cl

R = $O(CH_2)_6N^+Bu_3Cl^-$



^{1}H NMR spectrum of **4-Cl** in CD_3OD at 60 °C



^{13}C NMR spectrum of **4-Cl** in CD_3OD at 60 °C

[3] Copolymerization reactions.

General procedure. CHO was added to the catalyst (and co-catalyst if necessary) in an autoclave (preheated at 150 °C for 1 h and cooled down in vacuo) equipped with a Teflon stirring bar. The autoclave was then pressurized with 2.0 MPa of CO_2. The reaction mixture was stirred at specified temperature for a specified period of time. The reactor was cooled down to ambient temperature and vented in a fume hood. The resulting mixture was vacuumed to remove the residual CHO. The remaining mixture was dissolved in $CHCl_3$, and 0.5 M HCl in MeOH (0.2 mL) was added. Phenanthrene was added as an internal standard for the ^{1}H NMR measurement. The solution was then evaporated to dryness with heating. A small portion of the mixture was used for ^{1}H NMR and SEC analysis.

NMR analysis. TON and selectivity (carbonate linkages vs ether linkages and cyclic carbonate) were calculated from ^{1}H NMR spectra of the crude reaction mixture, using the integration of the methylene resonances for PCHC (4.65 ppm), ether linkage in the copolymer chain (3.45 ppm), and *trans*-CHC (4.0 ppm). TON of the catalyst for the PCHC formation was calculated as the number of moles of PCHC linkages divided by the number of moles of the catalyst, and the TOF was calculated as TON per hour, based on the relative integral to phenanthrene (internal standard).

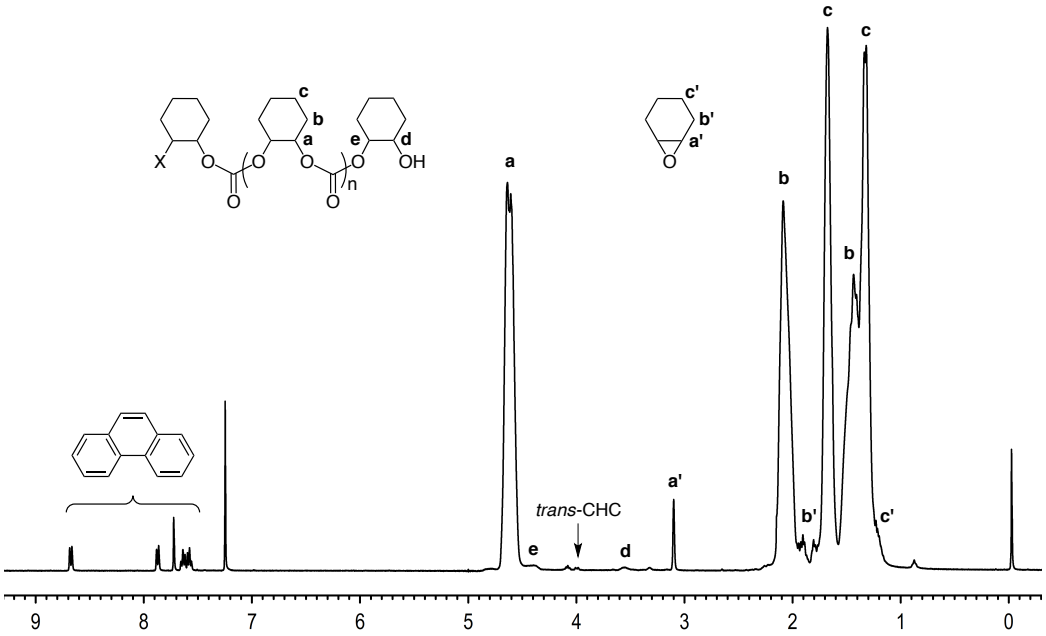
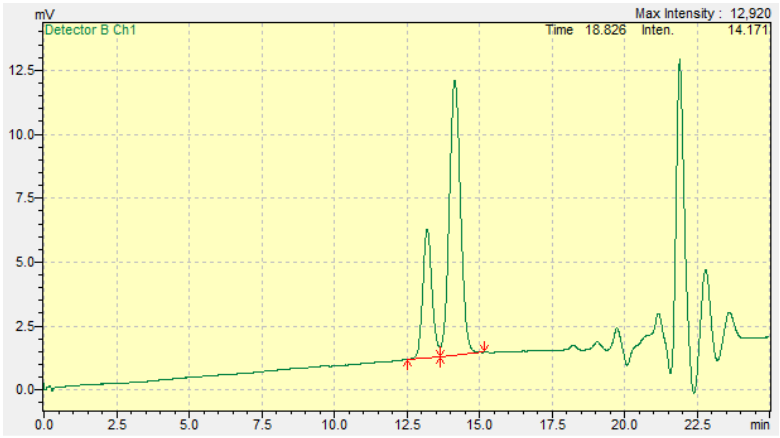


Fig. S1 Example of ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of as-prepared PCHC. Signals at 4.64 ppm are assigned to the methine groups of PCHC. Signals at 4.4 ppm and 3.6 ppm are assigned to the end-group H_e and H_d, respectively, which are hardly detected in the case of PCHC with molecular weight exceeding 60,000. A trace amount of *trans*-CHC is detected at 4.0 ppm. Residual CHO signals can also be seen.

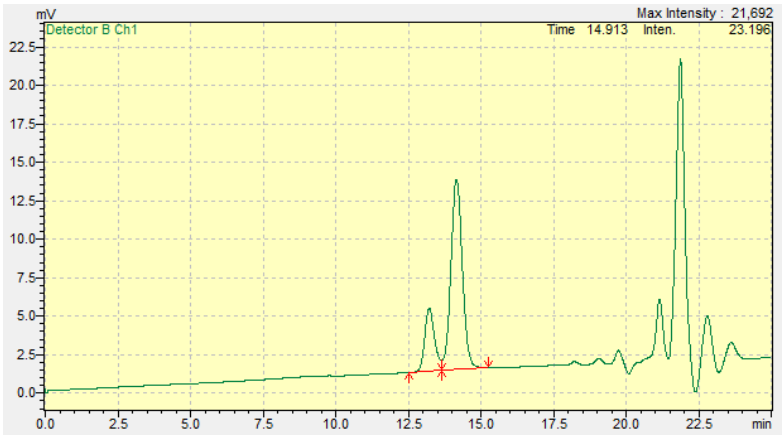
SEC charts.

Table 1, entry 1:



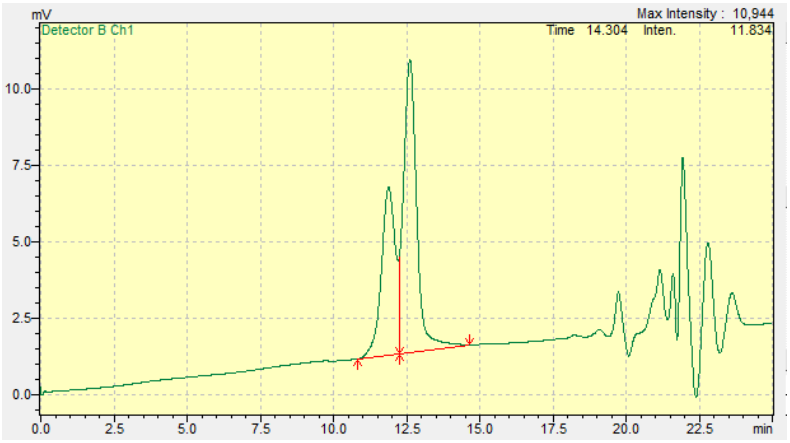
peak	M_n	M_w	M_w/M_n	%
1	68,355	69,575	1.01784	27.8058
2	31,662	32,347	1.02163	72.1942

Table 1, entry 2:



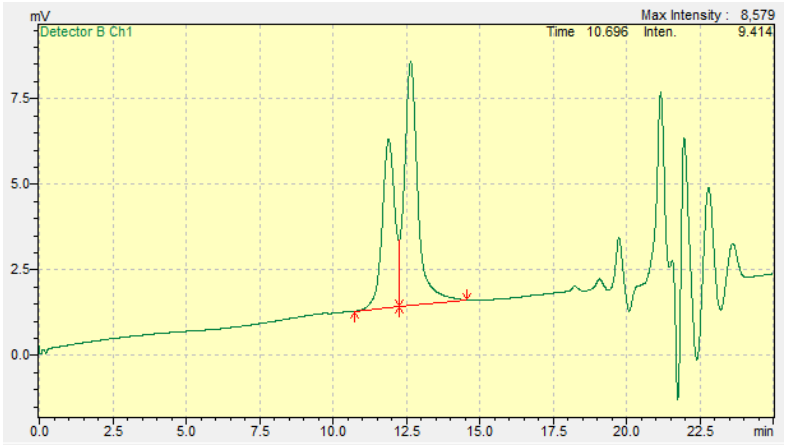
peak	M_n	M_w	M_w/M_n	%
1	66,549	67,866	1.01979	22.2695
2	31,486	32,228	1.02355	77.7305

Table 1, entry 3:



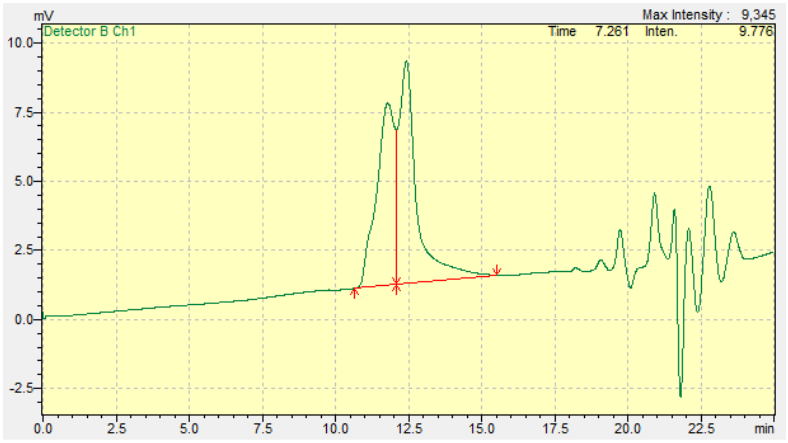
peak	M_n	M_w	M_w/M_n	%
1	231,820	244,539	1.05487	38.2428
2	106,426	113,841	1.06967	61.7572

Table 1, entry 4:



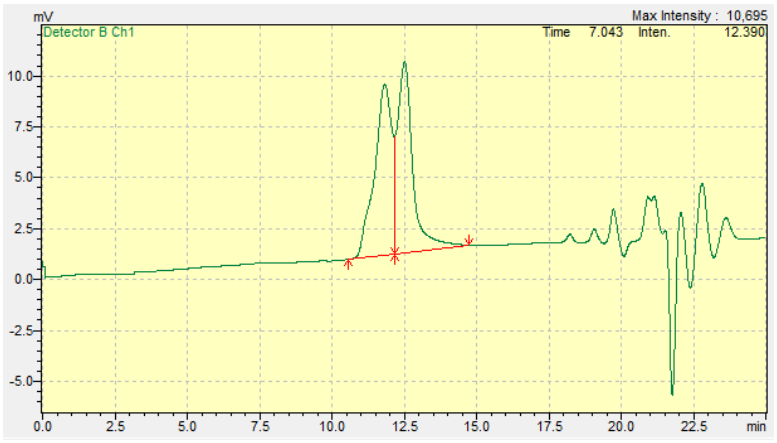
peak	M_n	M_w	M_w/M_n	%
1	228,598	238,695	1.04417	39.0340
2	100,776	108,793	1.07956	60.966

Table 1, entry 5:



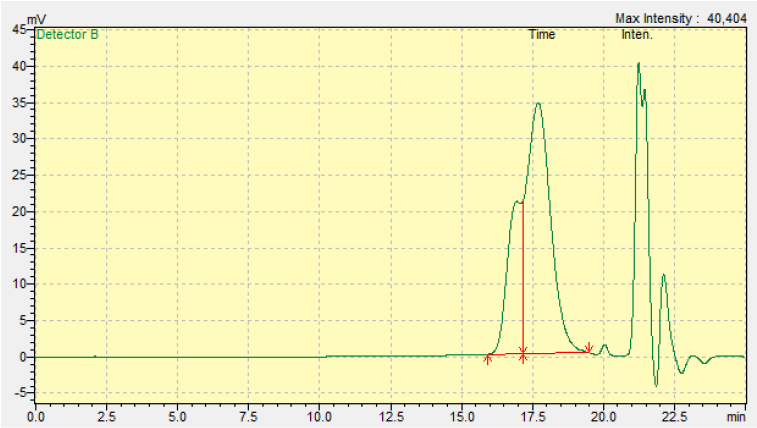
peak	M_n	M_w	M_w/M_n	%
1	280,528	305,196	1.08793	45.2750
2	96,227	122,303	1.27099	54.7250

Table 1, entry 6:



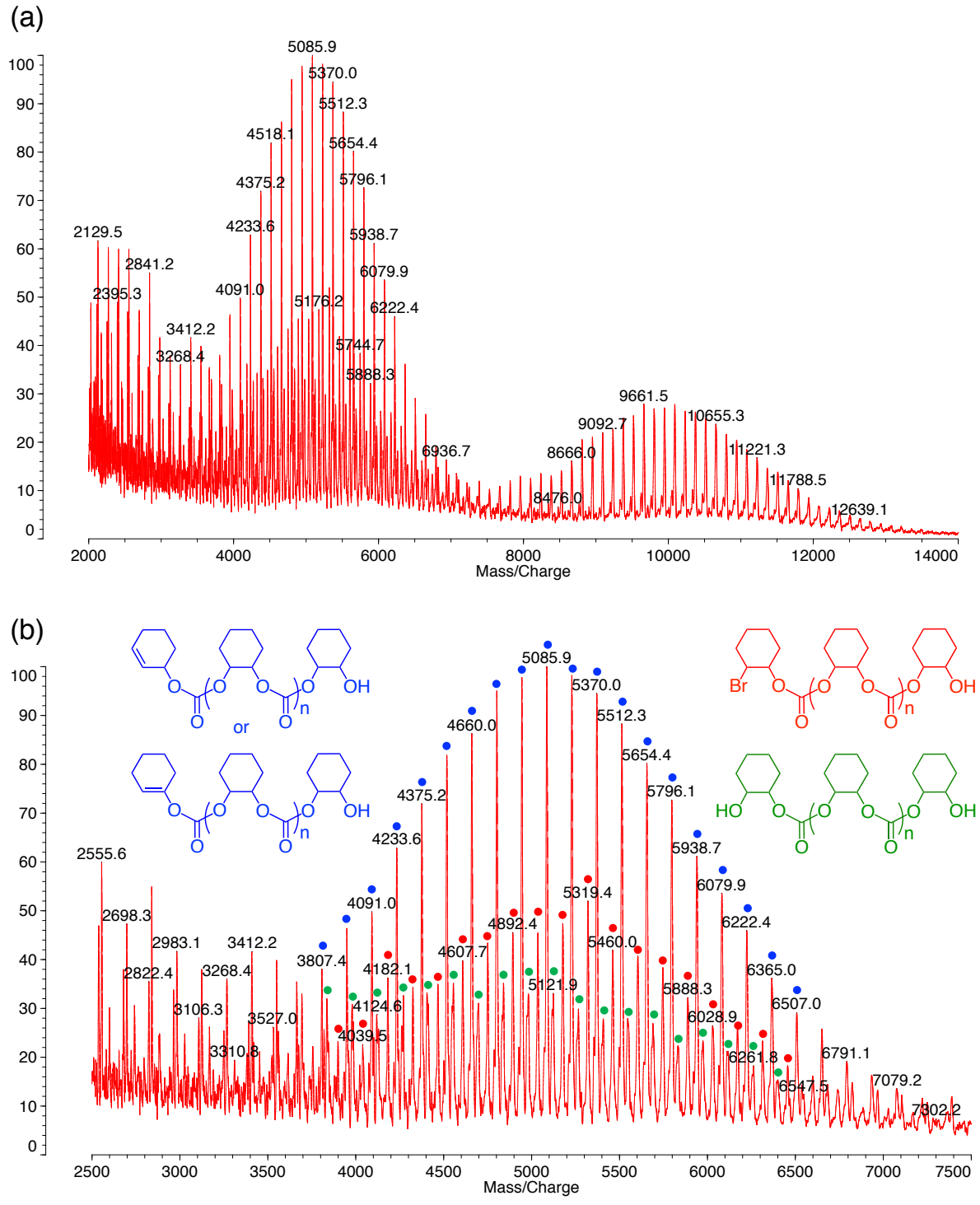
peak	M_n	M_w	M_w/M_n	%
1	263,075	286,476	1.08895	50.0933
2	107,744	120,742	1.12064	49.9067

Table 1, entry 7:



peak	M_n	M_w	M_w/M_n	%
1	3,928	4,057	1.03301	27.8884
2	1,615	1,833	1.13528	72.1116

MALDI-TOF mass spectrum of polymers.



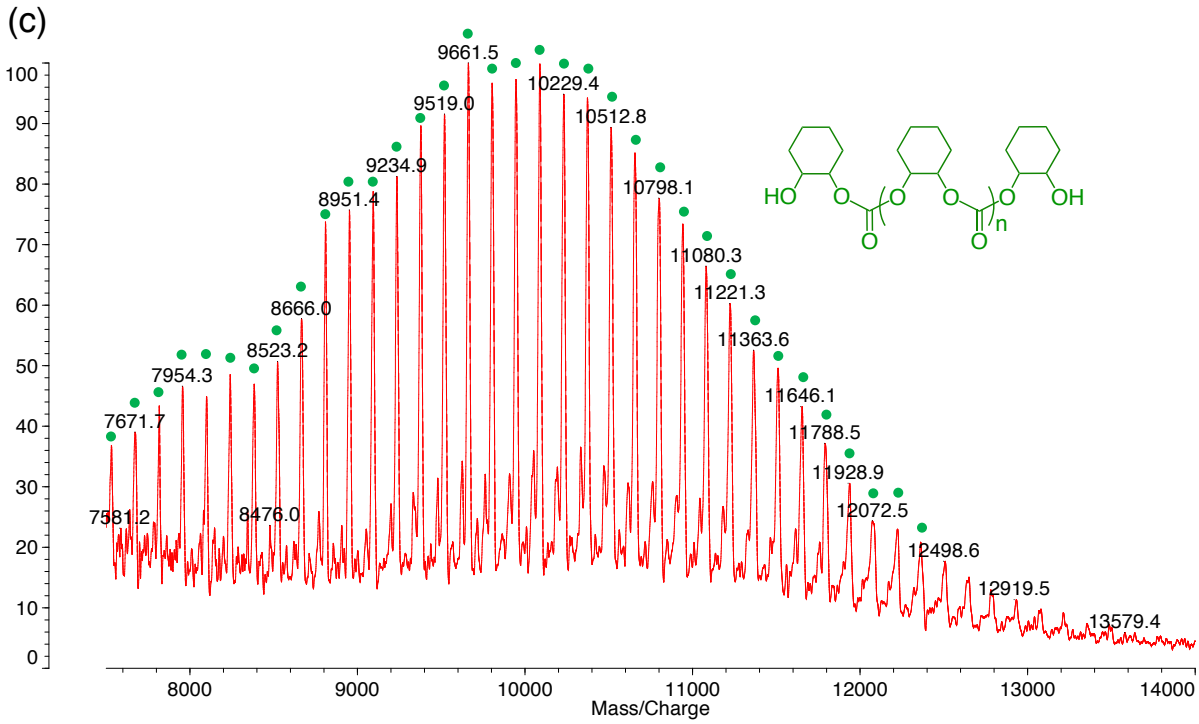


Fig. S2 The MALDI-TOF mass spectrum of PCHC synthesized with **2-Br**. Reaction conditions: CHO (10 mmol), **2-Br** (0.02 mol%), CO_2 (3.0 MPa), 70 °C, 14 h. Mass analysis conditions: dithranol (matrix), sodium trifluoroacetate (cation source), THF. (a) The whole spectrum. (b) The expanded spectrum of the lower-molecular-weight region. (c) The expanded spectrum of the higher-molecular-weight region. The peaks are assigned with the deduced polymer structures.

The MALDI-TOF mass spectrum of PCHC shows a bimodal molecular weight distribution. The lower-molecular-weight polymers have the OH group at one end and either OH, Br, or alkene at the other end, which suggests that the initiator, Br^-, can be regenerated from the chain end. On the other hand, the higher-molecular-weight polymers have the OH groups at both chain ends. This means that the higher-molecular-weight polymers were produced with cyclohexane-1,2-diol generated *in situ* by the reaction of CHO with a trace amount of water (impurity); cyclohexane-1,2-diol acted as a chain transfer agent to enable the polymer chain elongation on both sides, giving the higher-molecular-weight polymers that were approximately two-fold longer than the lower-molecular-weight polymers.

[4] Kinetic experiments.

Kinetic experiments with real-time IR. Since catalyst **2** was highly active, only a small amount of catalyst was enough for conducting the kinetic experiments. A solution of catalyst **2** in CH_2Cl_2 was prepared to take the catalyst more correctly. The reactor was equipped with a syringe port valve for liquid introduction, a valve for applying vacuum or inert gas and CO_2 introduction, as well as a pressure gauge and safety rupture disk. The reaction temperature was regulated by a standard oil bath. An autoclave (100 mL) equipped with IR probe, internal glass vial and magnetic stirring bar was charged with specified catalyst with or without co-catalyst. After flushed with N_2, diglyme was added via syringe to the autoclave while a slight countercurrent of N_2 was maintained. After addition of diglyme, the reaction vessel was heated to specified temperature and flushed with CO_2. A specified amount of CHO was then added to the autoclave through the syringe port valve. After sealing the reactor, the CO_2 pressure was immediately adjusted to the specified value, while low-frequency stirring was initiated to support CO_2 dissolution. This process was repeated several times until the CO_2 dissolution reached equilibrium with a constant pressure. Profiles of the absorbance height at 1750 cm^{-1} (PCHC, C=O stretching) were measured every 120 s (256 scans were integrated) and monitored during the reaction. After appropriate reaction time, the autoclave was cooled in a water bath for 30 min, and the pressure was then released.

Real-time IR data treatment. Background was measured before experiment under air. A calibration curve to demonstrate a linear response of absorbance to concentrations was obtained. The peak height of the polycarbonate signal at 1750 cm^{-1} was found to increase linearly with the concentration in the diglyme solution. Initial rates were determined as the slope of fits to plots of infrared absorption a.u. vs time (min) in the range of 3–10% CHO conversion.

Determination of reaction order.

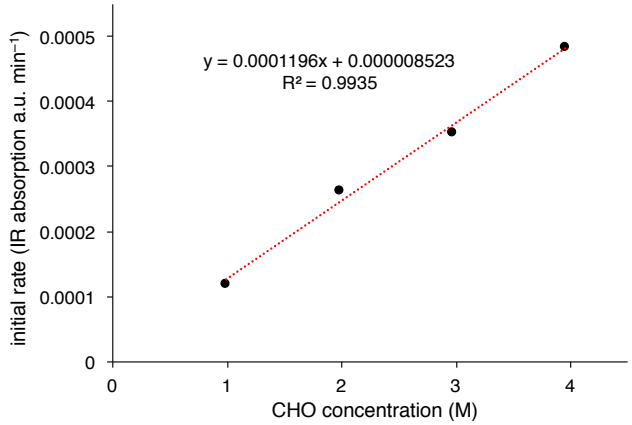


Fig. S3 Plot of initial rates of copolymerization vs different CHO concentrations (0.988, 1.98, 2.96, and 3.95 M) in diglyme at 68 °C with [**2-Br**] = 0.055 mM and 20 bar of CO_2.

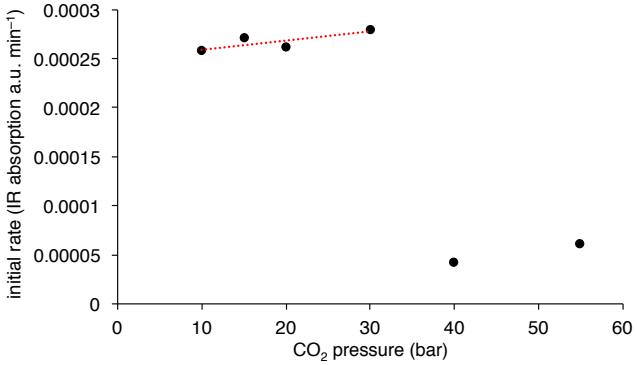


Fig. S4 Plot of initial rates of copolymerization vs different CO_2 pressures (10, 15, 20, 30, 40, and 55 bar) in diglyme at 68 °C with [**2-Br**] = 0.055 mM and [CHO] = 1.98 M. (The initial rates dropped at 40–55 bar presumably because of the precipitation of **2-Br**.)

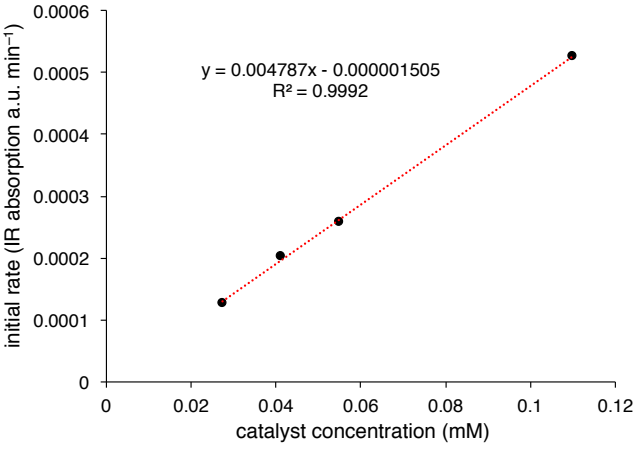


Fig. S5 Plot of initial rates of copolymerization vs different catalyst (**2-Br**) concentrations (0.0276, 0.0413, 0.0551, and 0.110 mM) in diglyme at 68 °C with initial [CHO] = 1.98 M and 20 bar of CO_2.

Arrhenius plot for the formation of PCHC with 1-Br/PPNBr.

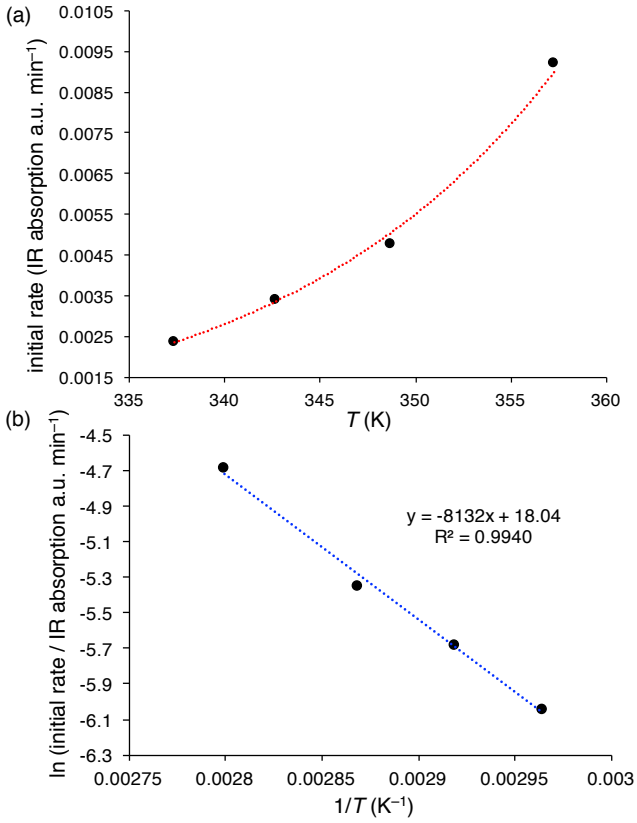


Fig. S6 (a) Plot of initial rates of copolymerization vs different reaction temperatures (337, 343, 349, and 357 K) in diglyme with [**1-Br**] = 2.40 mM, [PPNBr] = 4.80 mM, [CHO] = 4.94 M, and a CO_2 pressure of 20 bar. (b) Arrhenius plot for the formation of PCHC with **1-Br**/PPNBr.

Eyring plot for the formation of PCHC with 2-Br.

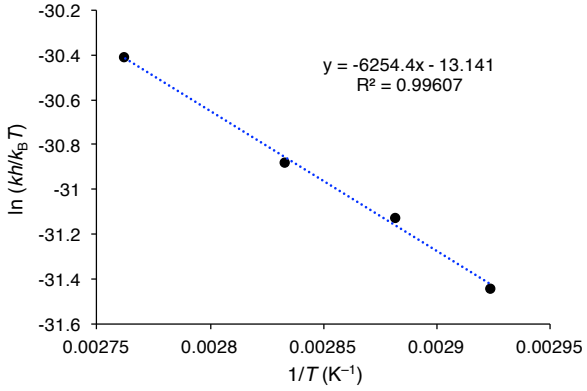


Fig. S7 Eyring plot for the formation of PCHC with **2-Br**.

[5] Computational details.

Monosubstituted Al^{III} complex **2'** and Mg^{II} complex **3'** (Fig. 3) were employed as model catalysts for **2-Br** and **3-Br**, respectively, while CHO was used as a substrate. DFT calculations were performed along the proposed reaction pathway (Scheme 2). Computations were performed with Gaussian 16 program[S2] at the ωB97XD[S3]/6-31G* level.[S4] The self-consistent reaction field (SCRF) method with the polarizable continuum model (PCM)[S5] was used to take into account of the solvation effect (Et_2O). Harmonic frequency and normal mode were calculated to verify the transition-state structures. Natural population analysis (NPA)[S6] was done to calculate the natural atomic charges.

References

(S2) *Gaussian 16*, *Revision A.03*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford, CT, 2016.

(S3) J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615.

(S4) (*a*) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257; (*b*) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213.

(S5) (*a*) S. Miertuš, E. Scrocco and J. Tomasi, *Chem. Phys.*, 1981, **55**, 117; (*b*) B. Mennucci and J. Tomasi, *J. Chem. Phys.*, 1997, **106**, 5151; (*c*) R. Cammi, B. Mennucci and J. Tomasi, *J. Phys. Chem. A*, 2000, **104**, 5631.

(S6) (*a*) A. E. Reed and F. Weinhold, *J. Chem. Phys.*, 1983, **78**, 4066; (*b*) A. E. Reed, R. B. Weinstock and F. Weinhold, *J. Chem. Phys.*, 1985, **83**, 735.

[6] Intermediate and transition-state structures.

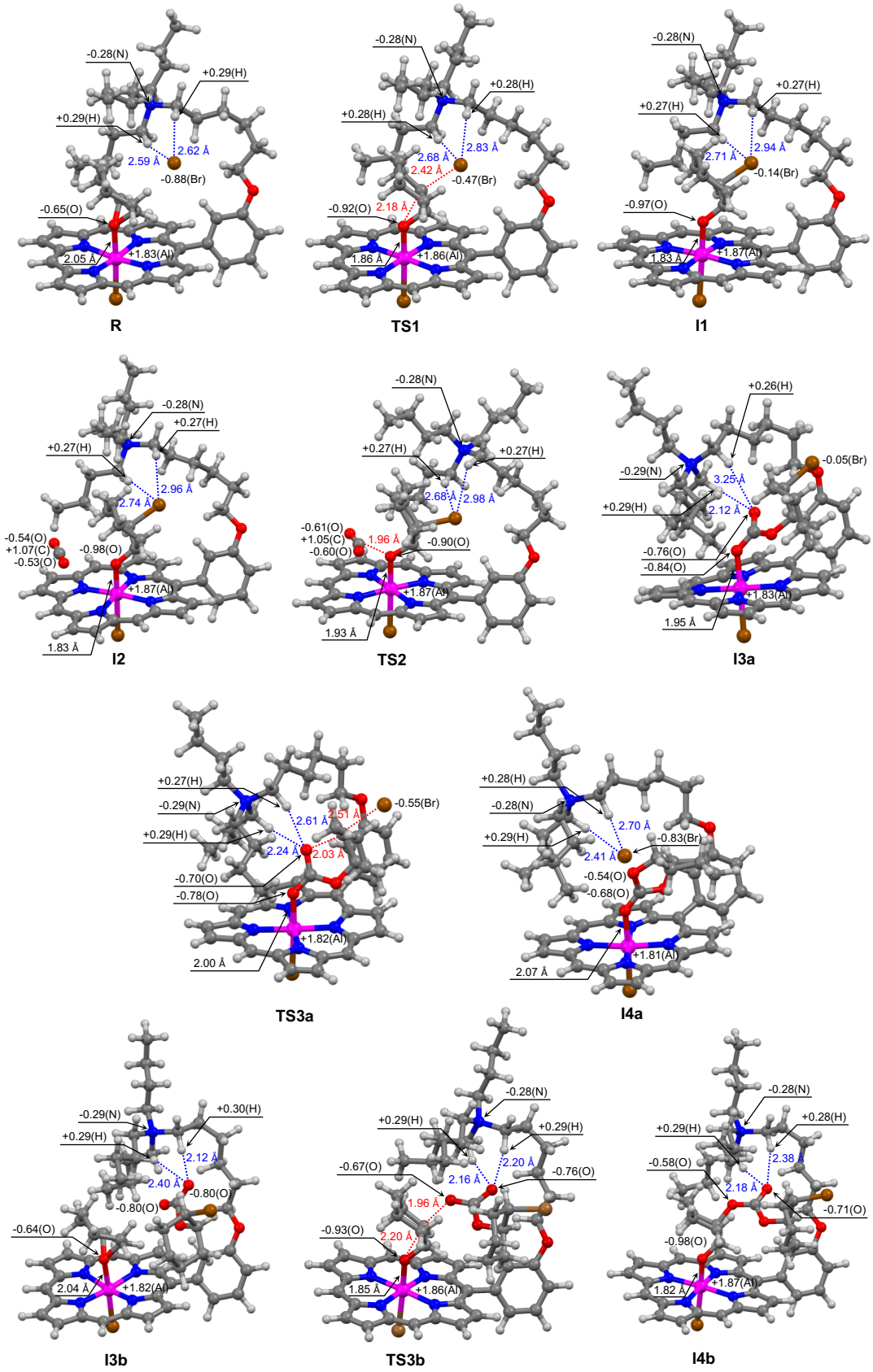


Fig. S8 Optimized intermediate and transition-state structures with Al^{III} complex **2'** in the potential energy profile (Fig. 3).

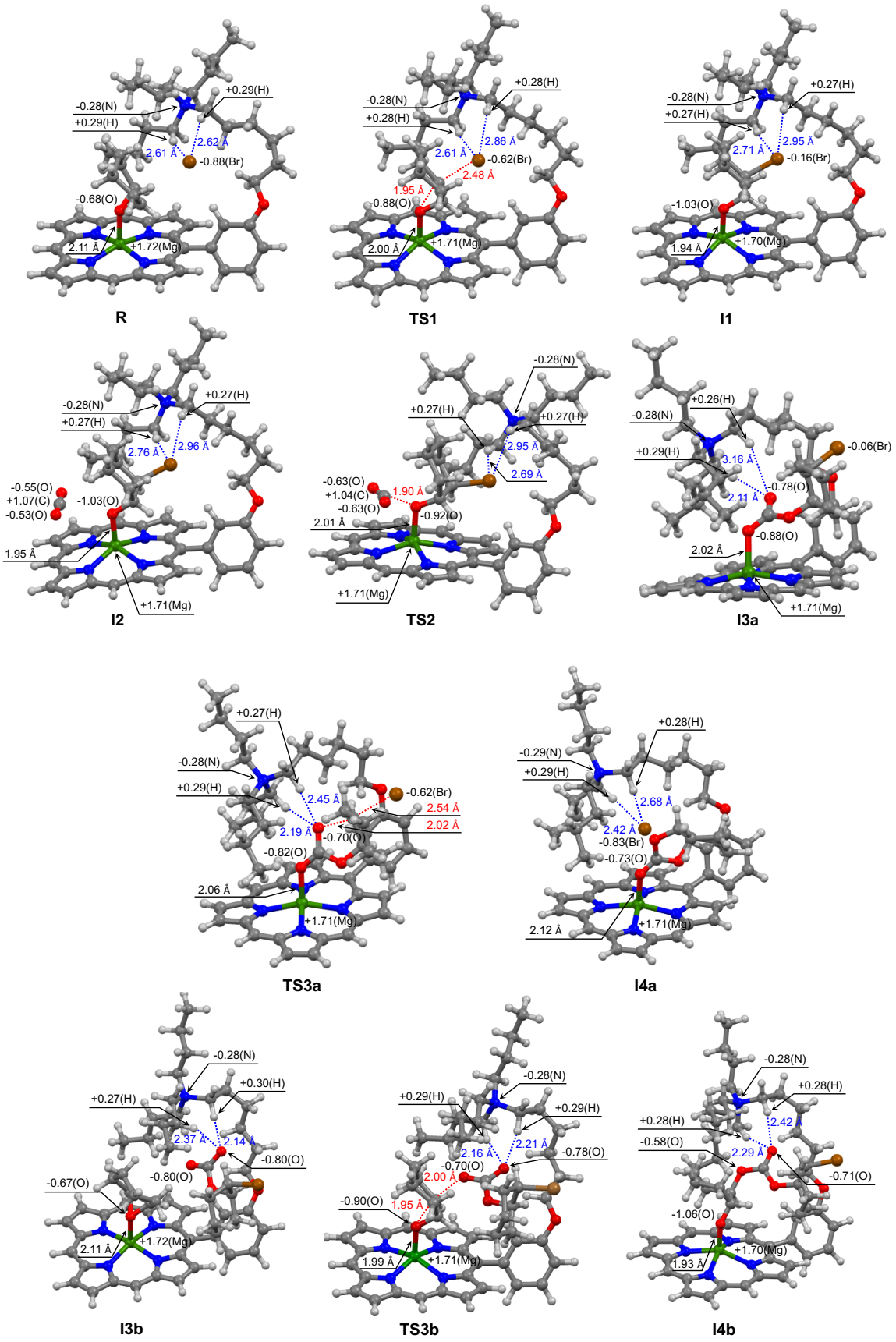


Fig. S9 Optimized intermediate and transition-state structures with Mg^{II} complex **3'** in the potential energy profile (Fig. 3).

[7] Comparison between 1,2-diaxial and 1,2-diequatorial conformations.

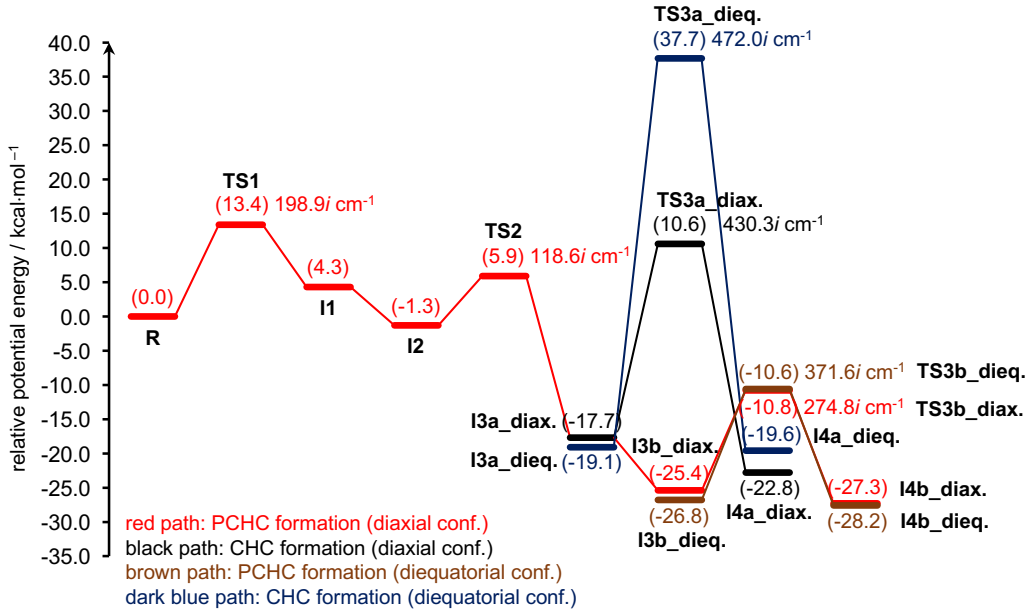


Fig. S10 Potential energy profiles for comparison between 1,2-diaxial and 1,2-diequatorial conformations with Al^{III} complex **2'**. Computations were performed at the ωB97XD/6-31G* level with the SCRF method (Et_2O).

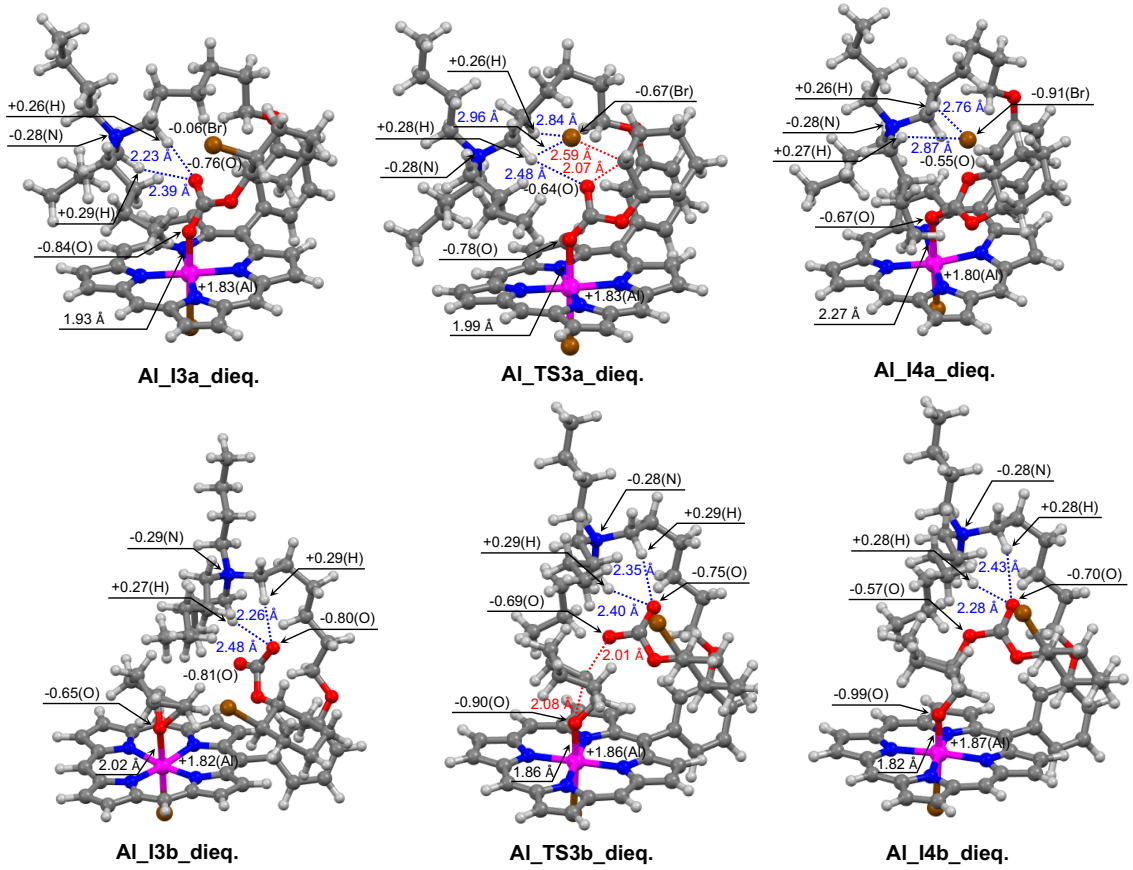


Fig. S11 Optimized intermediate and transition-state structures in the 1,2-diequatorial conformations with Al^{III} complex **2'** (Fig. S10).

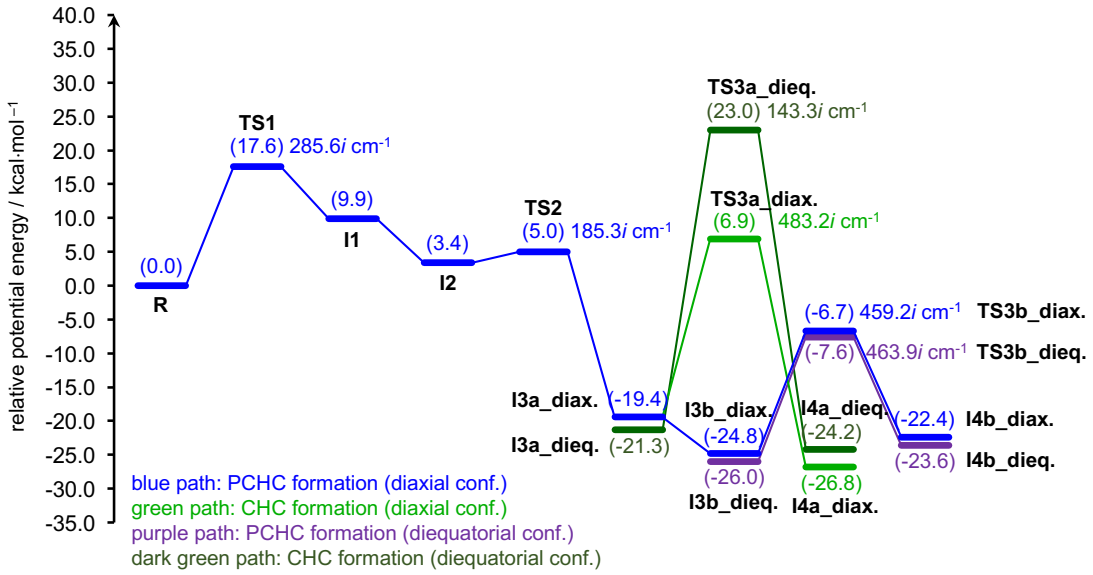


Fig. S12 Potential energy profiles for comparison between 1,2-diaxial and 1,2-diequatorial conformations with Mg^{II} complex **3'**. Computations were performed at the ωB97XD/6-31G* level with the SCRF method (Et_2O).

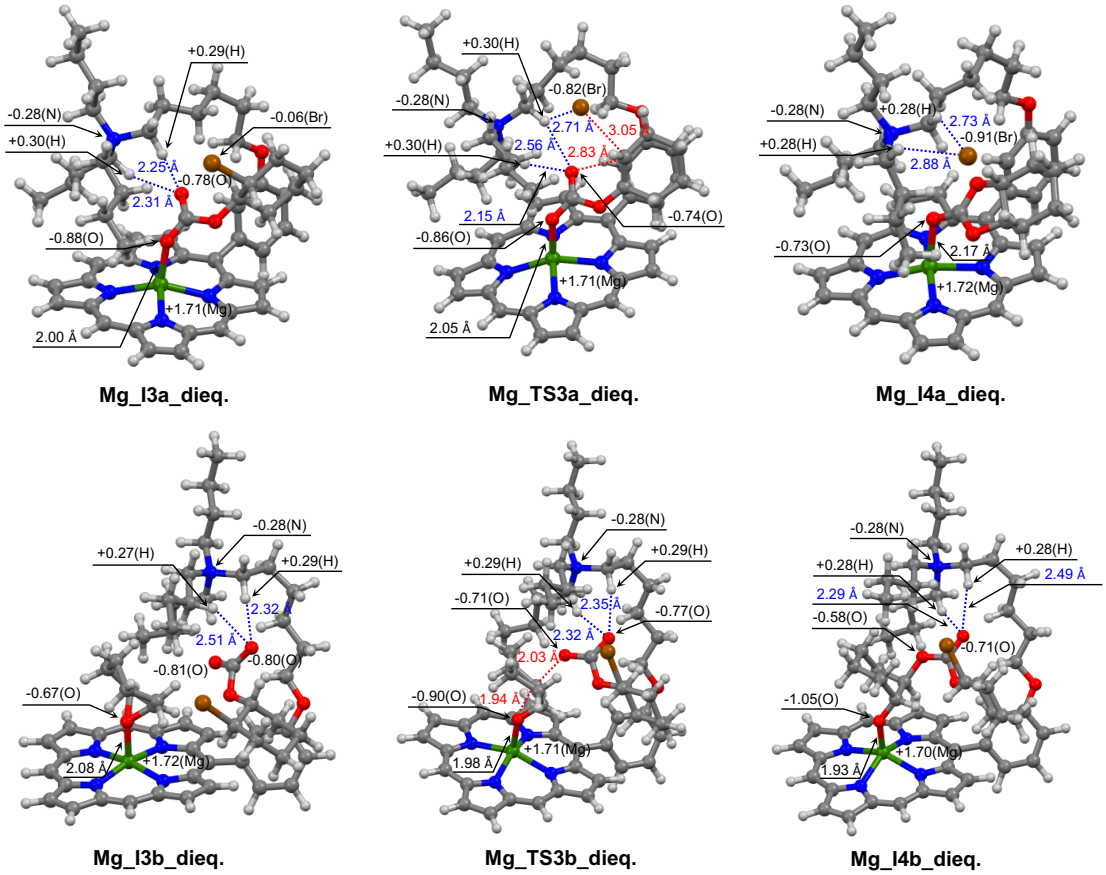


Fig. S13 Optimized intermediate and transition-state structures in the 1,2-diequatorial conformations with Mg^{II} complex **3'** (Fig. S12).

The 1,2-diaxial and 1,2-diequatorial conformations are compared. The intermediate and transition-state structures in the 1,2-diaxial conformations with Al^{III} complex **2'** are shown in Fig. S8, while the corresponding 1,2-diequatorial conformations are shown in Fig. S11. The energy differences between the 1,2-diaxial and 1,2-diequatorial conformations in **I3a**, **I3b**, **TS3b**, and **I4b** are 1.4, 1.4, 0.2, and 0.9 kcal mol^{-1}, respectively (Fig. S10). The energy barrier in the CHC formation step is much higher in the 1,2-diequatorial conformation (E_a = 56.8 kcal mol^{-1}) than in the 1,2-diaxial conformation (E_a = 28.3 kcal mol^{-1}). This is because the front-side attack occurs in the 1,2-diequatorial conformation (Fig. S11). Importantly, the activation energy in the carbonate linkage formation step (**TS3b**) is lower in the 1,2-diaxial conformation (E_a = 14.6 kcal mol^{-1}) than in the 1,2-diequatorial conformation (E_a = 16.2 kcal mol^{-1}) (Fig. S10).

The intermediate and transition-state structures in the 1,2-diaxial conformations with Mg^{II} complex **3'** are shown in Fig. S9, while the corresponding 1,2-diequatorial conformations are shown in Fig. S13. The energy differences between the 1,2-diaxial and 1,2-diequatorial conformations in **I3a**, **I3b**, **TS3b**, and **I4b** are 1.9, 1.2, 0.9, and 1.2 kcal mol^{-1}, respectively (Fig. S12). The energy barrier in the CHC formation step is again much higher in the 1,2-diequatorial conformation (E_a = 44.3 kcal mol^{-1}) than in the 1,2-diaxial conformation (E_a = 26.3 kcal mol^{-1}). In the carbonate linkage formation step (**TS3b**), the activation energy is slightly lower in the 1,2-diaxial conformation (E_a = 18.1 kcal mol^{-1}) than in the 1,2-diequatorial conformation (E_a = 18.4 kcal mol^{-1}) (Fig. S12).

[8] Energy for ring flip from 1,2-diaxial to 1,2-diequatorial conformations.

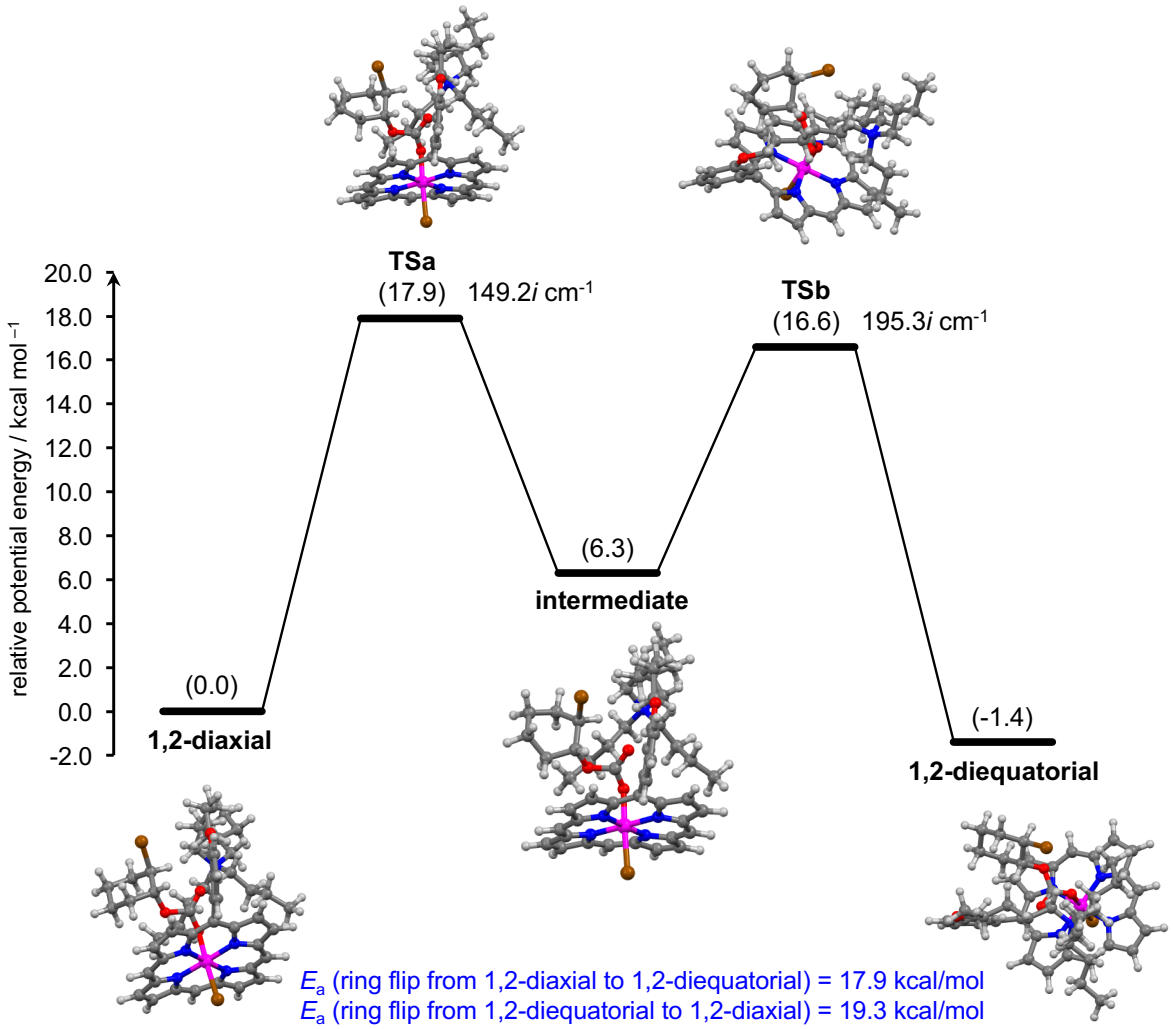


Fig. S14. Potential energy profile for the ring flip from 1,2-diaxial to 1,2-diequatorial conformations in intermediate **I3a** with Al^{III} complex **2'**. Computations were performed at the ωB97XD/6-31G* level with the SCRF method (Et_2O).

The 1,2-diaxial conformation can be converted into the 1,2-diequatorial conformation by the ring flip. We have examined the energy barrier for the ring-flip process in intermediate **I3a** with Al^{III} complex **2'** (Fig. S14). The energy barrier for the conversion of the 1,2-diaxial conformation into the 1,2-diequatorial conformation is 17.9 kcal mol^{-1}, and that for the backward conformational change is 19.3 kcal mol^{-1}. These energy barriers are greater than that (E_a = 14.6 kcal mol^{-1}) for the carbonate linkage formation (**TS3b** in Fig. 3). Therefore, these results suggest that the terminal carbonate linkage is formed prior to the conformational change.

[9] Binding energies of Al^{III} and Mg^{II} porphyrins for axial ligands.

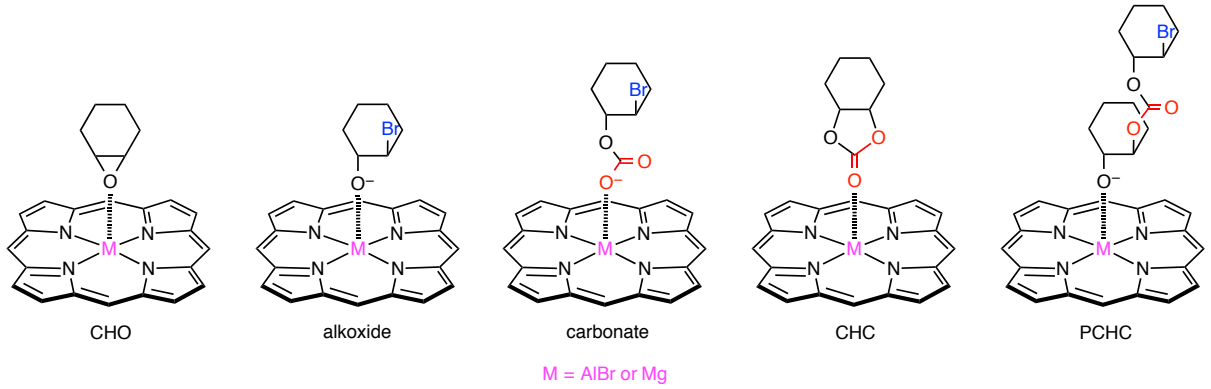


Fig. S15 Al^{III} and Mg^{II} porphyrins complexed with CHO, alkoxide, carbonate, CHC, and PCHC.

Table S1. Binding energies of Al^{III} and Mg^{II} porphyrins for axial ligands.

	binding energy (*BE*) (kcal mol^{-1}) [a]				
	CHO	alkoxide	carbonate	CHC	PCHC
Al^{III} porphyrin	–22.3	–58.7	–34.0	–16.6	–59.5
Mg^{II} porphyrin	–20.9	–49.5	–32.7	–19.2	–53.4
$\Delta BE_{Al–Mg}$ [b]	**–1.4**	**–9.2**	**–1.3**	**2.6**	**–6.1**

[a] The binding energy is defined as follows: $BE = E_{complex} - E_{porphyrin} - E_{ligand}$.

[b] A negative value of $\Delta BE_{Al–Mg}$ means that the Al^{III} complex is more stable than the corresponding Mg^{II} complex.

Simple models were used to estimate the relative binding abilities of Al^{III} and Mg^{II} porphyrins for neutral or anionic ligands such as CHO, alkoxide, carbonate, CHC, and PCHC (Fig. S15). Calculated binding energies of Al^{III} and Mg^{II} porphyrins for the ligands are listed in Table S1. Al^{III} porphyrin binds alkoxide and PCHC much more strongly than Mg^{II} porphyrin. This is considered to result from the intrinsic nature of the metal centers such as Lewis acidity and ionic radius, and the same trend can be expected for bifunctional Al^{III} complex **2'** and Mg^{II} complex **3'**. This accounts partly for the energy differences between **2'** and **3'** in the potential energy profiles (Fig. 3), where Al^{III} complex **2'** stabilizes anionic species in **TS1**, **I1**, **I2**, **TS3b**, and **I4b** more effectively than Mg^{II} complex **3'**.

[10] Energy for the dissociation of the carbonate anion from the Al atom.

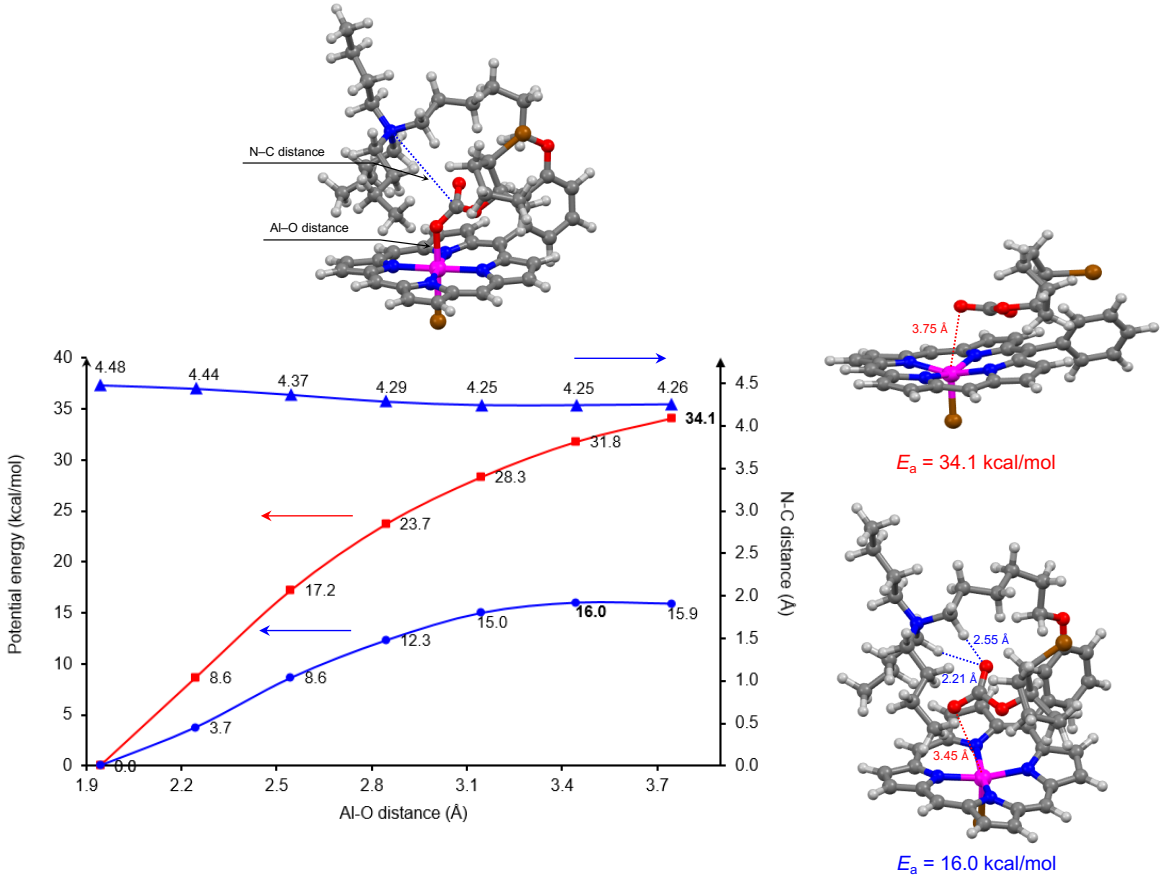


Fig. S16 Potential energy of intermediate **I3a** with a scan of the Al–O distance. The potential energies for Al^{III} porphyrins with and without the quaternary ammonium cation are shown by blue circle and red square, respectively, where the N–C distance in the former case is shown by blue triangle. Computations were performed at the ωB97XD/6-31G* level with the SCRF method (Et_2O). The structures of Al^{III} complex **2'** at the Al–O distance of 3.45 Å and Al^{III} 5-phenylporphyrin complex at the Al–O distance of 3.75 Å are shown on the right hand.

The tethered quaternary ammonium cation may promote the dissociation of the carbonate anion from the Al atom in **I3a**, facilitating the replacement with CHO. We compared the potential energies between Al^{III} complex **2'** and Al^{III} 5-phenylporphyrin by scanning the Al–O bond distance. As shown in Fig. S16, **2'** has a lower energy barrier (E_a = 16.0 kcal mol^{-1}) than Al^{III} 5-phenylporphyrin (E_a = 34.1 kcal mol^{-1}), which indicates that the carbonate anion dissociates more easily in **2'**. Fig. S16 also indicates that the N–C distance changes slightly upon the Al–O bond dissociation. Obviously, the carbonate anion is well solvated and stabilized by the tethered quaternary ammonium cation.

[11] Cartesian coordinates.

R_Al cat. 2'

C	1.3920	1.7090	-1.3760
C	0.3960	1.9050	-2.3980
N	1.9600	0.4690	-1.5100
C	1.3510	-0.1140	-2.5900
C	0.3750	0.7760	-3.1490
C	1.7370	2.6660	-0.4160
H	-0.1950	2.8000	-2.5220
C	5.2940	0.7190	2.2440
C	2.7550	2.4910	0.5260
H	-0.2390	0.5520	-4.0120
N	3.5330	1.3690	0.6620
C	3.0990	3.4500	1.5460
C	4.3610	1.6060	1.7240
C	4.1020	2.9050	2.2770
C	5.5160	-0.5710	1.7960
N	4.8530	-1.1700	0.7610
C	5.3570	-2.4370	0.6720
C	6.4650	-1.4860	2.3760
C	6.3660	-2.6450	1.6800
C	1.6050	-1.3890	-3.0740
C	2.4960	-2.2970	-2.5270
N	3.2760	-2.0660	-1.4280
C	4.0050	-3.2070	-1.2360
C	2.7310	-3.6230	-3.0360
C	3.6610	-4.1910	-2.2290
C	4.9640	-3.3930	-0.2510
H	2.6210	4.4090	1.6820
H	4.6180	3.3280	3.1290
H	7.1150	-1.2520	3.2100
H	6.9140	-3.5670	1.8200
H	2.2440	-4.0470	-3.9050
H	4.1000	-5.1780	-2.2940
C	-5.8230	2.1870	0.4590

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C -3.2770 4.0240 0.0690
C 0.9570 3.9360 -0.3820
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H -3.2650 -4.7950 4.5650
O -2.4510 5.1640 0.2990
H -0.8630 2.9460 0.2060
H 2.6330 5.1690 -0.9280
H 1.3320 7.2860 -0.8020
H -1.0880 7.2210 -0.2200
C -5.1300 1.0520 -0.3010
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C -2.9250 -2.7410 -1.2810
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H -5.7450 -2.7940 -1.6070
H -5.6120 -1.1200 -2.1320
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H 5.8850 1.0620 3.0870
H 5.4610 -4.3570 -0.2140
Al 3.4930 -0.3090 -0.4600

Br 5.1790 0.4930 -2.0080
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C 0.0020 -2.7160 2.6690
C 1.1920 -2.1360 3.4370
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O 2.1310 -1.0540 0.8780
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H -0.1700 -3.7630 2.9430
H -0.8950 -2.1450 2.9460
H 1.0740 -2.3170 4.5100
H 2.1190 -2.6330 3.1240
H 0.4570 -0.1090 3.6600
H 2.2240 -0.2150 3.5960

TS1_Al cat. 2'
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N 1.9700 0.3760 -1.3880
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C 0.2960 0.8090 -2.9010
C 2.1020 2.6090 -0.3570
H 0.0340 2.9120 -2.3410
C 5.5570 0.2990 2.1430
C 3.1400 2.3320 0.5410
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C 5.6560 -1.0010 1.6690

N 4.8890 -1.5380 0.6790
C 5.3120 -2.8230 0.5170
C 6.5960 -1.9820 2.1570
C 6.3850 -3.1120 1.4390
C 1.3030 -1.4760 -2.8570
C 2.1820 -2.4500 -2.4070
N 3.0850 -2.2880 -1.3970
C 3.7620 -3.4670 -1.2920
C 2.2870 -3.7800 -2.9570
C 3.2640 -4.4130 -2.2620
C 4.7930 -3.7270 -0.4000
H 3.3180 4.2830 1.6460
H 5.2340 2.9850 3.0220
H 7.3210 -1.8060 2.9420
H 6.8960 -4.0630 1.5120
H 1.6950 -4.1590 -3.7800
H 3.6390 -5.4200 -2.3900
C -4.9740 2.5390 0.4370
C -4.9670 3.8330 -0.3830
C -4.0610 4.9200 0.2030
C -2.6120 4.4510 0.2660
C 1.4960 3.9720 -0.3290
C 0.1500 4.1100 0.0290
C -0.4460 5.3720 0.0230
C 0.3140 6.5040 -0.2870
C 1.6520 6.3620 -0.6210
C 2.2460 5.1010 -0.6600
C -10.1430 -1.1250 -1.7250
C -8.6690 -1.2720 -2.0950
C -7.7600 -1.2440 -0.8610
H -3.4710 -2.1570 1.7190
C -5.4540 -2.3450 0.8150
C -4.5140 -2.3140 2.0160
C -4.6450 -3.6300 2.7910
C -3.9100 -3.5980 4.1290
H -5.7080 -3.8420 2.9660

H -4.0150 -4.5530 4.6520
O -1.7610 5.5870 0.2950
H -0.4050 3.2190 0.3080
H 3.2860 4.9880 -0.9500
H 2.2360 7.2410 -0.8760
H -0.1680 7.4760 -0.2770
C -5.3730 1.3160 -0.3920
C -5.3680 0.0860 0.5050
N -5.2590 -1.2480 -0.2060
C -3.8850 -1.3370 -0.8640
C -1.4390 -3.9960 -2.2130
C -2.0920 -2.6310 -2.0220
C -3.3990 -2.7320 -1.2260
H -0.5030 -3.9040 -2.7690
H -2.2930 -2.1680 -2.9960
H -3.2160 -3.3230 -0.3210
H -4.6400 1.2130 -1.1990
H -6.3540 1.4630 -0.8590
H -6.2700 0.0460 1.1200
H -4.5060 0.1290 1.1720
C -6.3060 -1.3820 -1.2920
H -3.9720 2.3380 0.8300
H -5.6350 2.6480 1.3060
H -4.6160 3.6120 -1.4010
H -5.9890 4.2150 -0.4870
H -4.4070 5.2240 1.1990
H -4.1020 5.8080 -0.4380
H -2.3800 3.8480 -0.6250
H -2.4220 3.8220 1.1440
H -8.5160 -2.2140 -2.6370
H -7.9200 -0.3010 -0.3270
H -10.3260 -0.1730 -1.2140
H -10.7740 -1.1530 -2.6180
H -10.4650 -1.9320 -1.0590
H -8.3780 -0.4650 -2.7790
H -8.0550 -2.0550 -0.1880

H -5.3730 -3.2900 0.2760
H -6.4830 -2.2550 1.1680
H -4.7750 -1.4820 2.6770
H -4.2610 -4.4520 2.1740
H -4.3100 -2.8110 4.7780
H -2.8430 -3.4050 3.9890
H -3.1760 -0.8460 -0.1920
H -3.9450 -0.7280 -1.7680
H -2.0980 -4.6790 -2.7610
H -1.2030 -4.4540 -1.2460
H -1.3910 -1.9630 -1.5060
H -4.1380 -3.2810 -1.8230
H -6.1410 -2.3570 -1.7580
H -6.0690 -0.6170 -2.0340
H 0.6350 -1.7490 -3.6690
H 6.2320 0.5850 2.9440
H 5.2380 -4.7170 -0.4280
Al 3.4050 -0.5920 -0.3280
Br 5.1040 0.1160 -2.0610
C 1.2520 -0.3630 1.6030
C 0.0350 -0.8680 0.8780
C -0.4660 -2.2280 1.2500
C -0.4930 -2.4570 2.7620
C 0.8400 -2.0770 3.4140
C 1.2070 -0.6240 3.1070
O 2.1940 -1.1550 0.9660
H 1.3790 0.7110 1.4220
Br -1.7470 0.6410 1.5160
H -0.0200 -0.5830 -0.1670
H -1.4400 -2.4180 0.7910
H 0.2450 -2.9200 0.7750
H -0.7370 -3.5060 2.9630
H -1.2960 -1.8410 3.1890
H 0.7800 -2.2340 4.4970
H 1.6330 -2.7310 3.0330
H 0.4760 0.0550 3.5650

H 2.1940 -0.3780 3.5140

I1_Al cat. 2'

C 1.5800 1.6820 -1.2580
C 0.5270 1.9720 -2.2050
N 1.9640 0.3770 -1.3860
C 1.1970 -0.1640 -2.3770
C 0.2880 0.8250 -2.8910
C 2.1300 2.6100 -0.3610
H 0.0530 2.9330 -2.3360
C 5.5530 0.2600 2.1450
C 3.1670 2.3220 0.5360
H -0.4240 0.6560 -3.6900
N 3.7820 1.1110 0.6750
C 3.7060 3.2560 1.5000
C 4.6980 1.2500 1.6760
C 4.6590 2.5910 2.1990
C 5.6300 -1.0440 1.6780
N 4.8530 -1.5750 0.6930
C 5.2630 -2.8630 0.5290
C 6.5620 -2.0350 2.1650
C 6.3360 -3.1640 1.4490
C 1.2720 -1.4710 -2.8470
C 2.1410 -2.4540 -2.3980
N 3.0440 -2.3040 -1.3880
C 3.7090 -3.4890 -1.2830
C 2.2330 -3.7850 -2.9510
C 3.2040 -4.4280 -2.2570
C 4.7360 -3.7610 -0.3890
H 3.3870 4.2810 1.6230
H 5.2840 2.9600 3.0010
H 7.2920 -1.8660 2.9460
H 6.8380 -4.1200 1.5210
H 1.6400 -4.1550 -3.7770
H 3.5690 -5.4390 -2.3870
C -4.8640 2.5500 0.4720

C -4.9030 3.8600 -0.3180
C -4.0000 4.9510 0.2660
C -2.5480 4.4900 0.3090
C 1.5420 3.9800 -0.3340
C 0.2010 4.1330 0.0360
C -0.3850 5.3990 0.0310
C 0.3810 6.5230 -0.2900
C 1.7150 6.3670 -0.6360
C 2.2980 5.1010 -0.6760
C -10.1540 -0.9770 -1.6860
C -8.6860 -1.1510 -2.0670
C -7.7690 -1.1510 -0.8380
H -3.4910 -2.1940 1.7130
C -5.4750 -2.3260 0.8050
C -4.5370 -2.3300 2.0070
C -4.6960 -3.6540 2.7630
C -3.9650 -3.6570 4.1030
H -5.7630 -3.8470 2.9320
H -4.0930 -4.6170 4.6120
O -1.6970 5.6240 0.3140
H -0.3570 3.2460 0.3190
H 3.3340 4.9790 -0.9750
H 2.3040 7.2410 -0.8990
H -0.0920 7.5000 -0.2800
C -5.3420 1.3510 -0.3500
C -5.3400 0.1070 0.5310
N -5.2630 -1.2160 -0.2010
C -3.8960 -1.3200 -0.8690
C -1.5000 -3.9900 -2.2820
C -2.1340 -2.6200 -2.0660
C -3.4380 -2.7160 -1.2640
H -0.5680 -3.9010 -2.8440
H -2.3350 -2.1390 -3.0310
H -3.2600 -3.3300 -0.3740
H -4.6540 1.2370 -1.1940
H -6.3380 1.5350 -0.7680

H -6.2330 0.0740 1.1600
H -4.4700 0.1260 1.1880
C -6.3210 -1.3140 -1.2810
H -3.8360 2.3280 0.7810
H -5.4530 2.6490 1.3930
H -4.5770 3.6650 -1.3500
H -5.9340 4.2240 -0.3830
H -4.3370 5.2450 1.2670
H -4.0540 5.8420 -0.3680
H -2.3290 3.8770 -0.5790
H -2.3450 3.8720 1.1930
H -8.5550 -2.0910 -2.6170
H -7.9070 -0.2090 -0.2950
H -10.3150 -0.0250 -1.1680
H -10.7920 -0.9890 -2.5740
H -10.4870 -1.7820 -1.0210
H -8.3840 -0.3450 -2.7470
H -8.0760 -1.9620 -0.1710
H -5.4070 -3.2640 0.2500
H -6.5020 -2.2260 1.1570
H -4.7830 -1.5020 2.6800
H -4.3270 -4.4740 2.1340
H -4.3500 -2.8720 4.7620
H -2.8930 -3.4860 3.9680
H -3.1740 -0.8610 -0.1910
H -3.9460 -0.6890 -1.7580
H -2.1730 -4.6580 -2.8330
H -1.2610 -4.4630 -1.3230
H -1.4200 -1.9720 -1.5430
H -4.1910 -3.2370 -1.8680
H -6.1790 -2.2860 -1.7590
H -6.0720 -0.5460 -2.0160
H 0.6000 -1.7380 -3.6580
H 6.2360 0.5400 2.9420
H 5.1710 -4.7560 -0.4190
Al 3.3620 -0.6180 -0.2970

Br 5.0920 0.0650 -2.0430
C 1.1880 -0.3600 1.5710
C -0.1470 -0.7290 0.8950
C -0.5740 -2.1520 1.2130
C -0.5930 -2.4380 2.7150
C 0.7460 -2.0830 3.3700
C 1.1330 -0.6310 3.0810
O 2.1490 -1.1450 0.9710
H 1.3530 0.7170 1.4200
Br -1.5810 0.5700 1.4720
H -0.0900 -0.5390 -0.1750
H -1.5430 -2.3820 0.7570
H 0.1700 -2.7900 0.7210
H -0.8310 -3.4960 2.8790
H -1.3950 -1.8490 3.1800
H 0.6890 -2.2570 4.4510
H 1.5280 -2.7390 2.9730
H 0.4160 0.0520 3.5550
H 2.1240 -0.4090 3.4920

I2_Al cat. 2'
C 1.3360 2.0010 -1.2070
C 0.2460 2.2890 -2.1130
N 1.7570 0.7140 -1.3970
C 0.9740 0.1830 -2.3790
C 0.0150 1.1570 -2.8250
C 1.8680 2.9050 -0.2750
H -0.2580 3.2400 -2.1990
C 5.3630 0.5320 2.1060
C 2.9100 2.6020 0.6110
H -0.7170 0.9940 -3.6060
N 3.5730 1.4100 0.6780
C 3.3890 3.4840 1.6530
C 4.4580 1.5110 1.7090
C 4.3480 2.8050 2.3300
C 5.5460 -0.7040 1.5050

N 4.8170 -1.1880 0.4600
C 5.3630 -2.3910 0.1320
C 6.5790 -1.6450 1.8670
C 6.4730 -2.6880 1.0080
C 1.0970 -1.0930 -2.9200
C 2.0670 -2.0290 -2.5970
N 3.0160 -1.8770 -1.6310
C 3.8180 -2.9780 -1.6990
C 2.2630 -3.2810 -3.2910
C 3.3530 -3.8660 -2.7380
C 4.9150 -3.2250 -0.8840
H 3.0260 4.4840 1.8390
H 4.9360 3.1380 3.1760
H 7.2950 -1.5010 2.6670
H 7.0770 -3.5840 0.9560
H 1.6510 -3.6370 -4.1100
H 3.8180 -4.8080 -2.9980
C -5.0460 2.4620 0.3980
C -5.1350 3.7780 -0.3780
C -4.3470 4.9180 0.2750
C -2.8740 4.5460 0.3960
C 1.2330 4.2500 -0.1750
C -0.1170 4.3330 0.1840
C -0.7570 5.5720 0.2210
C -0.0320 6.7400 -0.0300
C 1.3140 6.6540 -0.3540
C 1.9490 5.4160 -0.4470
C -10.1070 -1.2940 -1.9050
C -8.6200 -1.3850 -2.2370
C -7.7460 -1.3660 -0.9770
H -3.5200 -2.1780 1.7220
C -5.4660 -2.4220 0.7590
C -4.5650 -2.3670 1.9880
C -4.6710 -3.6880 2.7570
C -3.9370 -3.6430 4.0950
H -5.7290 -3.9230 2.9290

H -4.0260 -4.6000 4.6180
O -2.0860 5.7230 0.4730
H -0.6390 3.4130 0.4230
H 2.9930 5.3490 -0.7350
H 1.8720 7.5620 -0.5620
H -0.5440 7.6960 0.0150
C -5.4410 1.2440 -0.4390
C -5.4140 0.0090 0.4520
N -5.2630 -1.3200 -0.2580
C -3.8710 -1.3810 -0.8790
C -1.3200 -3.9780 -2.1540
C -2.0100 -2.6290 -1.9790
C -3.3460 -2.7630 -1.2370
H -0.3560 -3.8560 -2.6550
H -2.1820 -2.1610 -2.9560
H -3.1850 -3.3600 -0.3320
H -4.7210 1.1560 -1.2600
H -6.4310 1.3820 -0.8890
H -6.3220 -0.0530 1.0560
H -4.5640 0.0700 1.1340
C -6.2790 -1.4720 -1.3710
H -4.0150 2.2910 0.7300
H -5.6610 2.5220 1.3050
H -4.7390 3.6240 -1.3920
H -6.1860 4.0670 -0.4960
H -4.7620 5.1690 1.2580
H -4.4230 5.8150 -0.3490
H -2.5730 3.9690 -0.4910
H -2.6840 3.9190 1.2760
H -8.4230 -2.3050 -2.8010
H -7.9380 -0.4370 -0.4290
H -10.3340 -0.3670 -1.3680
H -10.7120 -1.3120 -2.8170
H -10.4230 -2.1340 -1.2750
H -8.3360 -0.5490 -2.8890
H -8.0440 -2.1960 -0.3300

H -5.3450 -3.3650 0.2220
H -6.5080 -2.3570 1.0760
H -4.8720 -1.5470 2.6440
H -4.2670 -4.4990 2.1380
H -4.3500 -2.8640 4.7440
H -2.8730 -3.4330 3.9530
H -3.1910 -0.8830 -0.1840
H -3.9150 -0.7630 -1.7780
H -1.9340 -4.6660 -2.7450
H -1.1240 -4.4420 -1.1820
H -1.3440 -1.9550 -1.4290
H -4.0520 -3.3170 -1.8660
H -6.0820 -2.4420 -1.8340
H -6.0370 -0.7010 -2.1050
H 0.4010 -1.3580 -3.7120
H 6.0160 0.7780 2.9380
H 5.4560 -4.1520 -1.0450
Al 3.2380 -0.2700 -0.4140
Br 4.8840 0.6630 -2.1450
C 1.1120 -0.1980 1.4900
C -0.2460 -0.6260 0.9040
C -0.6160 -2.0450 1.2920
C -0.5410 -2.2850 2.8000
C 0.8170 -1.8660 3.3760
C 1.1570 -0.4220 3.0060
O 2.0710 -0.9530 0.8380
H 1.2200 0.8800 1.3100
Br -1.6870 0.6490 1.5160
H -0.2480 -0.4670 -0.1730
H -1.6010 -2.3180 0.9000
H 0.1140 -2.6760 0.7740
H -0.7330 -3.3450 3.0070
H -1.3390 -1.7120 3.2930
H 0.8120 -1.9920 4.4650
H 1.6010 -2.5200 2.9820
H 0.4560 0.2650 3.4980

H 2.1660 -0.1650 3.3460
C 2.4340 -4.2340 0.9740
O 1.6250 -4.4160 0.1540
O 3.2280 -4.1060 1.8150

TS2_Al cat. 2'
C 1.5070 1.8560 -1.3050
C 0.4610 2.1790 -2.2440
N 1.8280 0.5290 -1.4110
C 1.0180 0.0110 -2.3830
C 0.1530 1.0330 -2.9020
C 2.0900 2.7700 -0.4180
H 0.0290 3.1600 -2.3800
C 5.6300 0.3810 1.8740
C 3.1440 2.4560 0.4500
H -0.5790 0.8840 -3.6850
N 3.7540 1.2380 0.5460
C 3.7340 3.3740 1.3970
C 4.7300 1.3660 1.4920
C 4.7230 2.6990 2.0330
C 5.6860 -0.9120 1.3790
N 4.8230 -1.4430 0.4650
C 5.2360 -2.7260 0.2480
C 6.6700 -1.8930 1.7610
C 6.3920 -3.0180 1.0570
C 1.0090 -1.3100 -2.8140
C 1.8680 -2.3110 -2.3860
N 2.8510 -2.1600 -1.4520
C 3.5120 -3.3540 -1.3950
C 1.8880 -3.6530 -2.9160
C 2.9090 -4.2990 -2.3020
C 4.6250 -3.6250 -0.6150
H 3.4280 4.3990 1.5470
H 5.3950 3.0570 2.8020
H 7.4630 -1.7230 2.4770
H 6.9090 -3.9690 1.0720

H 1.2170 -4.0280 -3.6780
H 3.2480 -5.3160 -2.4460
C -4.8960 2.4790 0.8510
C -4.9620 3.8310 0.1260
C -4.0280 4.9040 0.6930
C -2.5670 4.4890 0.5650
C 1.4890 4.1330 -0.3300
C 0.1610 4.2380 0.0970
C -0.4530 5.4850 0.1930
C 0.2730 6.6420 -0.1030
C 1.5930 6.5340 -0.5180
C 2.2050 5.2870 -0.6450
C -10.3310 -0.5010 -1.2020
C -8.9070 -0.6570 -1.7300
C -7.9080 -0.9420 -0.6040
H -3.5710 -2.8780 1.2590
C -5.6230 -2.4350 0.7130
C -4.5420 -2.7370 1.7410
C -4.9100 -4.0140 2.5050
C -3.8500 -4.4010 3.5330
H -5.8760 -3.8740 3.0040
H -4.1430 -5.3070 4.0710
O -1.7540 5.6530 0.5560
H -0.3670 3.3260 0.3460
H 3.2310 5.2070 -0.9910
H 2.1500 7.4340 -0.7600
H -0.2150 7.6080 -0.0170
C -5.2900 1.3280 -0.0800
C -5.2930 0.0080 0.6780
N -5.3810 -1.2410 -0.1840
C -4.0760 -1.3770 -0.9530
C -2.0670 -3.9220 -3.0420
C -2.4580 -2.6070 -2.3750
C -3.7940 -2.7120 -1.6260
H -1.1220 -3.8140 -3.5810
H -2.5250 -1.8140 -3.1290

H -3.7240 -3.5200 -0.8900
H -4.5590 1.3020 -0.8960
H -6.2710 1.5300 -0.5240
H -6.1240 -0.0320 1.3860
H -4.3640 -0.0840 1.2430
C -6.5140 -1.1420 -1.1840
H -3.8810 2.2830 1.2140
H -5.5410 2.4960 1.7380
H -4.7020 3.6830 -0.9310
H -5.9950 4.1980 0.1360
H -4.2700 5.1240 1.7390
H -4.1660 5.8310 0.1270
H -2.4160 3.9350 -0.3740
H -2.2620 3.8290 1.3880
H -8.8720 -1.4700 -2.4660
H -7.9250 -0.1050 0.1030
H -10.3920 0.3130 -0.4710
H -11.0280 -0.2760 -2.0150
H -10.6720 -1.4190 -0.7110
H -8.6060 0.2560 -2.2570
H -8.2350 -1.8340 -0.0590
H -5.7710 -3.2890 0.0490
H -6.5690 -2.2450 1.2240
H -4.4320 -1.9120 2.4520
H -5.0420 -4.8360 1.7900
H -3.7040 -3.6040 4.2700
H -2.8860 -4.5940 3.0500
H -3.2770 -1.1290 -0.2560
H -4.0890 -0.5880 -1.7070
H -2.8290 -4.2450 -3.7590
H -1.9380 -4.7170 -2.2990
H -1.6670 -2.3020 -1.6770
H -4.5830 -2.9840 -2.3360
H -6.4820 -2.0600 -1.7740
H -6.2580 -0.3150 -1.8500
H 0.2900 -1.5700 -3.5860

H 6.3690 0.6550 2.6210
H 5.0540 -4.6190 -0.6850
Al 3.2910 -0.4760 -0.4200
Br 4.8930 0.2050 -2.2650
C 1.0530 -0.1830 1.4260
C -0.1950 -0.7250 0.7050
C -0.7910 -1.9540 1.3610
C -1.1280 -1.7200 2.8330
C 0.1210 -1.2760 3.5990
C 0.8100 -0.0720 2.9420
O 2.1340 -0.9880 1.0440
H 1.2240 0.8380 1.0760
Br -1.5670 0.7450 0.6220
H 0.0280 -0.8930 -0.3440
H -1.6580 -2.3070 0.7930
H -0.0210 -2.7300 1.2770
H -1.5370 -2.6350 3.2730
H -1.9080 -0.9500 2.9060
H -0.1430 -1.0180 4.6310
H 0.8100 -2.1230 3.6690
H 0.1710 0.8080 3.0900
H 1.7680 0.1360 3.4260
C 2.6960 -2.4840 2.1810
O 2.2430 -3.4260 1.6190
O 3.2860 -1.9690 3.0710

I3a_Al cat. 2' (1,2-diaxial conformation)
C 2.0360 0.9840 -2.4170
C 1.6690 0.9570 -3.8120
N 2.3650 -0.2710 -1.9990
C 2.2220 -1.0920 -3.0780
C 1.8250 -0.3250 -4.2310
C 2.1040 2.1440 -1.6400
H 1.3680 1.8200 -4.3890
C 3.9120 0.8110 2.6410
C 2.6850 2.1910 -0.3690

H 1.6650 -0.7330 -5.2210
N 3.0680 1.1020 0.3620
C 2.9760 3.3990 0.3610
C 3.5750 1.5810 1.5340
C 3.5710 3.0190 1.5210
C 3.7480 -0.5620 2.7460
N 3.3050 -1.3830 1.7480
C 3.2990 -2.6480 2.2600
C 4.0130 -1.3330 3.9360
C 3.7250 -2.6250 3.6370
C 2.3110 -2.4790 -3.0460
C 2.4420 -3.2500 -1.9000
N 2.6140 -2.7620 -0.6360
C 2.6860 -3.8440 0.1920
C 2.3770 -4.6900 -1.8660
C 2.5110 -5.0570 -0.5660
C 2.9710 -3.7960 1.5510
H 2.7700 4.4010 0.0120
H 3.9390 3.6470 2.3220
H 4.3760 -0.9210 4.8690
H 3.8010 -3.4970 4.2740
H 2.2480 -5.3220 -2.7360
H 2.5200 -6.0550 -0.1450
C -4.4090 1.2010 -0.4410
C -5.0030 2.1100 -1.5160
C -4.2570 3.4460 -1.6470
C -2.7580 3.2310 -1.7840
C 1.3820 3.3560 -2.1300
C -0.0110 3.3050 -2.0060
C -0.7920 4.4010 -2.3690
C -0.1750 5.5490 -2.8790
C 1.2060 5.5860 -3.0130
C 1.9970 4.4950 -2.6410
C -8.1710 -4.7680 0.1490
C -6.9240 -4.4320 -0.6670
C -6.0060 -3.4470 0.0650

H -1.0410 -2.0320 0.6850
C -2.9200 -3.1140 0.7870
C -1.7300 -2.4250 1.4360
C -0.9420 -3.3840 2.3360
C 0.0130 -2.6050 3.2400
H -1.6270 -3.9860 2.9470
H 0.6690 -3.2770 3.8010
O -2.1460 4.4250 -2.2530
H -0.4490 2.4000 -1.5990
H 3.0770 4.5330 -2.7450
H 1.6760 6.4780 -3.4150
H -0.7910 6.3970 -3.1620
C -5.1680 -0.1110 -0.2240
C -4.3400 -1.1050 0.6040
N -3.7260 -2.2530 -0.1720
C -2.8380 -1.6890 -1.2680
C -0.7770 -3.0040 -4.2400
C -1.3260 -2.0060 -3.2250
C -2.0910 -2.7160 -2.1040
H -0.1750 -2.4990 -5.0010
H -1.9920 -1.2980 -3.7360
H -1.3750 -3.2770 -1.4930
H -5.4670 -0.5410 -1.1860
H -6.1050 0.0850 0.3080
H -4.9180 -1.5590 1.4090
H -3.5030 -0.5800 1.0630
C -4.8010 -3.1170 -0.8070
H -3.3700 0.9710 -0.7040
H -4.3630 1.7450 0.5100
H -4.9710 1.5850 -2.4820
H -6.0610 2.3060 -1.3020
H -4.4460 4.0730 -0.7670
H -4.6260 3.9890 -2.5240
H -2.5460 2.4130 -2.4890
H -2.3300 2.9580 -0.8130
H -6.3690 -5.3520 -0.8890

H -6.5750 -2.5400 0.2950
H -8.7530 -3.8650 0.3650
H -8.8160 -5.4630 -0.3960
H -7.9030 -5.2330 1.1040
H -7.2200 -4.0020 -1.6320
H -5.6960 -3.8910 1.0180
H -2.5920 -3.9850 0.2160
H -3.6220 -3.4610 1.5480
H -2.0670 -1.5830 2.0480
H -0.3730 -4.0810 1.7080
H -0.5470 -2.0000 3.9630
H 0.6410 -1.9330 2.6470
H -2.1350 -0.9920 -0.8040
H -3.5000 -1.1080 -1.9140
H -1.5920 -3.5320 -4.7490
H -0.1430 -3.7500 -3.7490
H -0.5140 -1.4150 -2.7890
H -2.7840 -3.4390 -2.5500
H -4.3060 -4.0370 -1.1190
H -5.1280 -2.6010 -1.7120
H 2.1890 -3.0040 -3.9870
H 4.2840 1.3350 3.5160
H 3.0110 -4.7400 2.0860
C 0.1570 0.2040 0.4620
O -0.7680 0.5470 -0.2840
O 0.9470 -0.7760 0.2910
Al 2.8550 -0.8330 -0.1310
Br 5.2720 -0.9570 -0.7620
C -0.3330 2.0890 1.8550
C -1.7990 1.7650 2.1700
C -1.9800 1.0640 3.5080
C -1.2830 1.7890 4.6610
C 0.1940 2.0290 4.3350
C 0.3530 2.7950 3.0190
O 0.3710 0.8620 1.6400
H -0.2740 2.6920 0.9430

Br -2.8260 3.4530 2.1080
H -2.2160 1.1900 1.3470
H -3.0450 0.9130 3.7110
H -1.5230 0.0720 3.3920
H -1.3850 1.1990 5.5780
H -1.7840 2.7500 4.8400
H 0.6740 2.5880 5.1460
H 0.7150 1.0670 4.2560
H -0.0900 3.7930 3.1120
H 1.4070 2.9260 2.7690

TS3a_Al cat. 2' (1,2-diaxial conformation)

C 1.8650 0.9990 -2.3620
C 1.3750 0.9590 -3.7240
N 2.2380 -0.2450 -1.9660
C 2.0090 -1.0790 -3.0280
C 1.5020 -0.3270 -4.1420
C 1.9820 2.1720 -1.6060
H 1.0220 1.8160 -4.2760
C 4.2340 0.9020 2.4810
C 2.6770 2.2370 -0.3970
H 1.2620 -0.7380 -5.1120
N 3.2050 1.1670 0.2730
C 2.9280 3.4510 0.3490
C 3.7570 1.6600 1.4180
C 3.6260 3.0930 1.4570
C 4.1400 -0.4750 2.5960
N 3.6180 -1.3110 1.6500
C 3.6960 -2.5760 2.1650
C 4.5430 -1.2350 3.7550
C 4.2580 -2.5300 3.4930
C 2.1070 -2.4630 -2.9950
C 2.3700 -3.2240 -1.8670
N 2.6900 -2.7230 -0.6370
C 2.8760 -3.7960 0.1830
C 2.3310 -4.6630 -1.8170

C 2.6310 -5.0180 -0.5390
C 3.3220 -3.7340 1.4990
H 2.6060 4.4350 0.0480
H 3.9960 3.7240 2.2470
H 4.9860 -0.8080 4.6480
H 4.4200 -3.3970 4.1190
H 2.1070 -5.3050 -2.6580
H 2.7060 -6.0070 -0.1100
C -4.4010 1.1200 -0.2200
C -5.1080 1.9890 -1.2650
C -4.4130 3.3390 -1.5080
C -2.9260 3.1510 -1.7280
C 1.2150 3.3710 -2.0600
C -0.1760 3.2840 -1.9540
C -0.9840 4.3600 -2.3130
C -0.3930 5.5290 -2.7970
C 0.9920 5.6060 -2.9090
C 1.8070 4.5330 -2.5430
C -8.4370 -4.4770 0.2740
C -7.1670 -4.2420 -0.5450
C -6.1510 -3.3660 0.2050
H -1.2210 -2.1550 0.9550
C -3.0210 -3.3610 0.8260
C -1.8350 -2.7940 1.5870
C -0.9490 -3.9030 2.1540
C 0.1660 -3.3120 3.0200
H -1.5460 -4.6090 2.7420
H 0.8400 -4.0920 3.3850
O -2.3440 4.3440 -2.2260
H -0.5950 2.3590 -1.5700
H 2.8850 4.6040 -2.6390
H 1.4420 6.5180 -3.2930
H -1.0290 6.3620 -3.0790
C -5.1420 -0.1770 0.1040
C -4.2700 -1.2200 0.8240
N -3.7860 -2.3670 -0.0400

C -2.8910 -1.8000 -1.1280
C -1.0240 -3.1130 -4.2420
C -1.5410 -2.1150 -3.2130
C -2.2310 -2.8210 -2.0430
H -0.4680 -2.6050 -5.0380
H -2.2440 -1.4210 -3.6950
H -1.4860 -3.4060 -1.4960
H -5.5770 -0.5960 -0.8130
H -6.0040 0.0430 0.7490
H -4.7870 -1.6800 1.6700
H -3.3620 -0.7440 1.2120
C -4.9390 -3.1130 -0.6800
H -3.3990 0.8700 -0.5880
H -4.2510 1.7050 0.6970
H -5.1510 1.4290 -2.2110
H -6.1430 2.1690 -0.9590
H -4.5550 3.9980 -0.6430
H -4.8560 3.8310 -2.3800
H -2.7330 2.3250 -2.4310
H -2.4520 2.9130 -0.7710
H -6.6990 -5.2030 -0.7940
H -6.6290 -2.4240 0.4870
H -8.9370 -3.5320 0.5010
H -9.1380 -5.1100 -0.2780
H -8.2030 -4.9730 1.2240
H -7.4260 -3.7570 -1.4920
H -5.8660 -3.8700 1.1350
H -2.6920 -4.1510 0.1450
H -3.7520 -3.7930 1.5090
H -2.1920 -2.1680 2.4160
H -0.5040 -4.4710 1.3250
H -0.2530 -2.7970 3.8920
H 0.7610 -2.5940 2.4480
H -2.1390 -1.1800 -0.6380
H -3.5370 -1.1420 -1.7220
H -1.8490 -3.6650 -4.7020

H -0.3460 -3.8380 -3.7720
H -0.7130 -1.5060 -2.8270
H -2.9730 -3.5230 -2.4490
H -4.5330 -4.0600 -1.0320
H -5.2350 -2.5410 -1.5620
H 1.8970 -2.9980 -3.9140
H 4.6490 1.4450 3.3240
H 3.4420 -4.6690 2.0330
C 0.3010 0.0910 0.9030
O -0.9420 0.1180 0.7420
O 1.0980 -0.7830 0.4740
Al 2.9830 -0.7800 -0.1820
Br 5.2890 -0.8940 -1.0890
C -1.5410 1.7830 1.7310
C -0.0690 2.2090 1.8510
H -2.0360 1.7910 0.7830
H 0.1600 2.9400 1.0710
C 0.2980 2.7390 3.2350
H -0.1400 3.7390 3.3540
H 1.3860 2.8390 3.2640
O 0.8070 1.0840 1.6610
Br -2.5300 3.8600 1.9720
C -0.1990 1.8010 4.3400
H 0.0800 2.2080 5.3180
H 0.3060 0.8310 4.2410
C -2.1580 1.0500 2.9160
H -1.8220 0.0090 2.8450
H -3.2440 1.0600 2.8320
C -1.7120 1.6100 4.2750
H -2.2150 2.5700 4.4470
H -2.0420 0.9180 5.0610

I4a_Al cat. 2' (1,2-diaxial conformation)

C 1.9010 1.1270 -2.0160
C 1.2070 1.3620 -3.2590
N 1.9600 -0.2140 -1.7590

C 1.2870 -0.8240 -2.7810
C 0.8420 0.1510 -3.7380
C 2.4310 2.1420 -1.2160
H 1.0340 2.3360 -3.6930
C 4.7860 -0.0810 2.3850
C 3.2400 1.9010 -0.1040
H 0.2980 -0.0800 -4.6450
N 3.5520 0.6650 0.3970
C 3.8210 2.9270 0.7230
C 4.3160 0.8880 1.5120
C 4.5080 2.2970 1.7090
C 4.5040 -1.4370 2.3120
N 3.7250 -2.0270 1.3570
C 3.6750 -3.3550 1.6750
C 4.9610 -2.4190 3.2590
C 4.4430 -3.6100 2.8650
C 1.0110 -2.1770 -2.8760
C 1.3790 -3.1370 -1.9450
N 2.1070 -2.8960 -0.8140
C 2.2750 -4.1080 -0.2050
C 1.0630 -4.5370 -2.0440
C 1.6150 -5.1390 -0.9600
C 2.9920 -4.3280 0.9610
H 3.7130 3.9900 0.5610
H 5.0800 2.7360 2.5160
H 5.5940 -2.2060 4.1110
H 4.5630 -4.5830 3.3250
H 0.5050 -4.9870 -2.8550
H 1.5970 -6.1870 -0.6890
C -4.3370 2.5270 0.2670
C -4.5790 3.6930 -0.6980
C -3.5300 4.8100 -0.6030
C -2.1170 4.2740 -0.8020
C 1.9490 3.5350 -1.4580
C 0.5820 3.7620 -1.2420
C 0.0520 5.0450 -1.3730

C 0.8890 6.1060 -1.7380
C 2.2380 5.8710 -1.9680
C 2.7790 4.5910 -1.8300
C -9.6390 -1.6020 2.0770
C -8.7510 -1.6440 0.8350
C -7.2700 -1.4560 1.1830
H -2.3290 -1.7750 0.3750
C -4.3590 -2.3410 0.9850
C -2.8470 -2.2460 1.2170
C -2.2500 -3.6330 1.4760
C -0.7350 -3.5830 1.6510
H -2.7210 -4.0800 2.3620
H -0.3230 -4.5860 1.8030
O -1.2570 5.3480 -1.1640
H -0.0380 2.9070 -0.9880
H 3.8340 4.4140 -2.0110
H 2.8790 6.6960 -2.2620
H 0.4650 7.1000 -1.8410
C -5.1650 1.2820 -0.0820
C -4.6370 0.0770 0.6930
N -4.9410 -1.2780 0.0790
C -4.3080 -1.3260 -1.3130
C -2.4810 -3.7420 -3.6900
C -3.0510 -2.4430 -3.1280
C -3.8750 -2.6810 -1.8540
H -1.8960 -3.5540 -4.5970
H -3.6700 -1.9450 -3.8850
H -3.2290 -3.2060 -1.1470
H -5.0440 1.1110 -1.1560
H -6.2340 1.4440 0.1040
H -5.0150 0.0540 1.7180
H -3.5460 0.1330 0.7180
C -6.4260 -1.5030 -0.0830
H -3.2890 2.2230 0.1860
H -4.5200 2.8400 1.3040
H -4.5610 3.2990 -1.7230

H -5.5790 4.1180 -0.5440
H -3.5990 5.3280 0.3620
H -3.7300 5.5550 -1.3810
H -2.1010 3.4960 -1.5770
H -1.7430 3.8080 0.1180
H -8.8840 -2.6040 0.3200
H -7.1450 -0.4940 1.6930
H -9.5480 -0.6380 2.5900
H -10.6910 -1.7450 1.8140
H -9.3590 -2.3880 2.7870
H -9.0630 -0.8640 0.1310
H -6.9740 -2.2410 1.8870
H -4.6340 -3.2990 0.5390
H -4.8890 -2.2600 1.9350
H -2.6420 -1.5980 2.0750
H -2.4940 -4.2950 0.6330
H -0.4550 -2.9640 2.5090
H -0.2520 -3.1480 0.7710
H -3.4390 -0.6640 -1.2750
H -5.0370 -0.8810 -1.9930
H -3.2750 -4.4530 -3.9460
H -1.8220 -4.2200 -2.9570
H -2.2320 -1.7550 -2.8800
H -4.7320 -3.3340 -2.0660
H -6.5300 -2.4720 -0.5790
H -6.7720 -0.7350 -0.7800
H 0.4440 -2.5100 -3.7390
H 5.3970 0.2560 3.2160
H 3.0440 -5.3470 1.3310
C 0.6670 -0.0550 1.5170
O -0.2860 -0.2760 2.4210
O 1.2530 -0.9630 0.9560
Al 2.9180 -1.1310 -0.2640
Br 4.9360 -1.5150 -1.5890
C -0.5450 0.9830 3.0960
C -0.1190 1.9790 2.0180

H -1.6170 1.0300 3.2930
H -0.8990 2.0640 1.2560
C 0.3820 3.3310 2.4760
H -0.5030 3.9470 2.6810
H 0.9060 3.8000 1.6360
O 0.9390 1.2260 1.3800
Br -1.4190 0.6010 -0.8750
C 1.2570 3.2600 3.7260
H 1.4940 4.2750 4.0630
H 2.2090 2.7710 3.4830
C 0.2880 1.0370 4.3780
H 1.2550 0.5590 4.1800
H -0.2060 0.4490 5.1580
C 0.5430 2.4780 4.8310
H -0.4060 2.9720 5.0810
H 1.1440 2.4650 5.7460

I3b_Al cat. 2' (1,2-diaxial conformation)
C -2.2200 0.3450 2.3500
C -1.6060 -0.1080 3.5730
N -2.8750 -0.6990 1.7450
C -2.6810 -1.7880 2.5520
C -1.8920 -1.4280 3.6940
C -2.1520 1.6570 1.8690
H -1.0350 0.5130 4.2470
C -4.9020 1.7850 -2.1260
C -2.8210 2.0970 0.7220
H -1.6040 -2.1100 4.4840
N -3.6190 1.3250 -0.0830
C -2.7580 3.4400 0.2030
C -4.0740 2.1520 -1.0740
C -3.5450 3.4740 -0.9000
C -5.3680 0.5060 -2.3780
N -5.0910 -0.5950 -1.6180
C -5.6950 -1.6480 -2.2430
C -6.1800 0.1400 -3.5110

C -6.3800 -1.1980 -3.4280
C -3.1510 -3.0710 2.3080
C -3.8860 -3.4630 1.2020
N -4.3000 -2.6310 0.1980
C -5.0030 -3.4160 -0.6760
C -4.3180 -4.8110 0.9440
C -5.0070 -4.7830 -0.2240
C -5.6500 -2.9670 -1.8170
H -2.1730 4.2420 0.6280
H -3.7440 4.3100 -1.5570
H -6.5350 0.8320 -4.2620
H -6.9390 -1.8390 -4.0970
H -4.1120 -5.6570 1.5870
H -5.4900 -5.6010 -0.7420
C 6.0520 -0.1690 2.4080
C 4.6410 0.0700 2.9530
C 4.2560 1.5360 3.1500
C 2.7610 1.6130 3.3950
C -1.2600 2.6150 2.5840
C 0.1050 2.3240 2.6350
C 0.9860 3.1890 3.2840
C 0.5010 4.3660 3.8580
C -0.8570 4.6560 3.7990
C -1.7460 3.7810 3.1780
C 8.8440 -5.6830 -0.4800
C 7.4770 -5.4470 0.1580
C 6.8040 -4.1780 -0.3760
H 2.6190 -1.4660 -1.5790
C 4.4300 -2.6650 -1.5430
C 3.6200 -1.4710 -2.0250
C 3.5090 -1.4950 -3.5520
C 2.8900 -0.2070 -4.0910
H 4.5050 -1.6280 -3.9950
H 2.7650 -0.2480 -5.1770
O 2.3290 2.9720 3.3630
H 0.4590 1.4370 2.1240

H -2.8100 3.9980 3.1540
H -1.2300 5.5660 4.2590
H 1.1990 5.0350 4.3520
C 6.1480 -1.5560 1.7520
C 5.5160 -1.5150 0.3520
N 4.6960 -2.7320 -0.0540
C 3.4000 -2.6850 0.7350
C 0.0610 -4.5820 1.1080
C 1.1220 -3.4990 1.2890
C 2.3550 -3.7420 0.4090
H -0.8350 -4.3540 1.6920
H 1.4270 -3.4670 2.3430
H 2.0510 -3.6800 -0.6430
H 5.6460 -2.2720 2.4110
H 7.1900 -1.8860 1.6800
H 6.2900 -1.3970 -0.4090
H 4.8340 -0.6620 0.2680
C 5.4200 -4.0230 0.2450
H 6.2990 0.6010 1.6670
H 6.7950 -0.0860 3.2090
H 3.9200 -0.3500 2.2440
H 4.5180 -0.4890 3.8920
H 4.4730 2.0830 2.2270
H 4.8170 2.0020 3.9690
H 2.4860 1.1760 4.3660
H 2.2660 1.0320 2.6150
H 6.8270 -6.3110 -0.0290
H 7.4380 -3.3160 -0.1430
H 9.5180 -4.8410 -0.2900
H 9.3120 -6.5860 -0.0780
H 8.7540 -5.8050 -1.5650
H 7.5870 -5.3660 1.2470
H 6.7350 -4.2460 -1.4660
H 3.9390 -3.6040 -1.8120
H 5.4100 -2.6570 -2.0230
H 4.0890 -0.5350 -1.7110

H 2.9100 -2.3590 -3.8690
H 3.5190 0.6580 -3.8530
H 1.9060 -0.0310 -3.6450
H 2.9640 -1.6890 0.5890
H 3.6910 -2.7720 1.7850
H 0.4380 -5.5600 1.4270
H -0.2430 -4.6730 0.0590
H 0.7140 -2.5090 1.0590
H 2.7290 -4.7570 0.5840
H 4.7710 -4.8310 -0.0990
H 5.4860 -4.0970 1.3320
H -2.9110 -3.8330 3.0440
H -5.1880 2.5650 -2.8240
H -6.1780 -3.7040 -2.4140
Al -4.0900 -0.6200 0.1380
Br -6.0790 -0.1840 1.4380
C 2.8520 3.2070 -1.8920
C 2.2310 3.2500 -0.4870
H 3.5390 2.3650 -1.9470
H 3.0220 3.3850 0.2550
C 1.1700 4.3400 -0.3580
H 1.6720 5.3140 -0.3940
H 0.6990 4.2480 0.6260
O 1.5770 2.0060 -0.2550
Br 4.0410 4.7820 -2.1000
C 0.1220 4.2500 -1.4710
H -0.6040 5.0640 -1.3670
H -0.4350 3.3140 -1.3540
C 1.8130 3.1830 -3.0040
H 1.3150 2.2080 -2.9350
H 2.3080 3.2240 -3.9790
C 0.7690 4.2910 -2.8580
H 1.2500 5.2650 -3.0150
H 0.0070 4.1790 -3.6370
O 1.6960 -0.0880 0.4160
C 2.3690 0.9120 0.0850

O 3.6090 1.0480 0.0280
C -1.3960 -1.9260 -0.9250
C -1.0960 -0.4870 -0.9030
H -1.4330 -2.4460 0.0290
H -0.8840 -0.0270 0.0550
C -0.5730 0.2160 -2.1220
H 0.5010 0.3490 -1.9600
H -1.0180 1.2170 -2.1640
O -2.4600 -0.9550 -1.0510
C -0.8530 -0.5700 -3.4050
H -0.3390 -0.0940 -4.2460
H -1.9270 -0.5410 -3.6270
C -1.1780 -2.7650 -2.1640
H -2.1650 -3.0690 -2.5320
H -0.6500 -3.6830 -1.8830
C -0.3950 -2.0230 -3.2550
H 0.6730 -2.0280 -2.9930
H -0.4910 -2.5590 -4.2050

TS3b_Al cat. 2' (1,2-diaxial conformation)
C 2.2940 0.6370 -2.1910
C 1.5220 0.3470 -3.3760
N 2.9200 -0.5000 -1.7610
C 2.5690 -1.4940 -2.6320
C 1.6890 -0.9740 -3.6430
C 2.3810 1.8970 -1.5840
H 0.9410 1.0680 -3.9340
C 5.3210 1.3860 2.2410
C 3.1430 2.1700 -0.4400
H 1.2710 -1.5510 -4.4570
N 3.8890 1.2560 0.2510
C 3.2290 3.4580 0.2100
C 4.4530 1.9240 1.2980
C 4.0420 3.3030 1.2840
C 5.7710 0.0750 2.2860
N 5.4060 -0.9100 1.4200

C 6.0670 -2.0350 1.8100
C 6.6990 -0.4430 3.2640
C 6.8840 -1.7530 2.9670
C 2.9610 -2.8250 -2.5520
C 3.8120 -3.3690 -1.6020
N 4.3950 -2.6790 -0.5800
C 5.1730 -3.5710 0.0940
C 4.2230 -4.7520 -1.5650
C 5.0710 -4.8770 -0.5130
C 5.9610 -3.2780 1.2010
H 2.7310 4.3590 -0.1180
H 4.3480 4.0480 2.0080
H 7.1430 0.1360 4.0640
H 7.5120 -2.4760 3.4710
H 3.9030 -5.5110 -2.2670
H 5.5930 -5.7600 -0.1690
C -6.1920 1.4170 -1.6850
C -4.8260 1.5480 -2.3700
C -4.0980 2.8670 -2.1200
C -2.6920 2.7820 -2.6880
C 1.5640 3.0080 -2.1560
C 0.1710 2.9210 -2.0890
C -0.6300 3.9760 -2.5240
C -0.0360 5.1210 -3.0540
C 1.3500 5.2000 -3.1420
C 2.1530 4.1510 -2.7010
C -10.3610 -3.5480 -0.0060
C -9.0300 -3.5520 -0.7540
C -7.9250 -2.8390 0.0330
H -3.1100 -1.7730 1.3050
C -5.1690 -2.4690 1.2180
C -4.0310 -1.7190 1.8940
C -3.7720 -2.3050 3.2860
C -2.8210 -1.4310 4.1000
H -4.7200 -2.4140 3.8280
H -2.6100 -1.8780 5.0760

O -1.9900 3.9840 -2.3870
H -0.2650 2.0340 -1.6450
H 3.2340 4.2180 -2.7690
H 1.8090 6.0890 -3.5640
H -0.6710 5.9360 -3.3870
C -6.5540 -0.0640 -1.4790
C -5.8630 -0.5840 -0.2130
N -5.4820 -2.0570 -0.2050
C -4.2670 -2.2180 -1.1070
C -1.6540 -4.8670 -2.1400
C -2.3930 -3.5320 -2.0720
C -3.5480 -3.5590 -1.0630
H -0.7990 -4.8040 -2.8210
H -2.7810 -3.2810 -3.0670
H -3.1320 -3.7430 -0.0660
H -6.2410 -0.6130 -2.3730
H -7.6370 -0.2000 -1.3930
H -6.5050 -0.4210 0.6550
H -4.9270 -0.0500 -0.0450
C -6.6050 -2.9260 -0.7250
H -6.1810 1.9290 -0.7140
H -6.9670 1.9090 -2.2820
H -4.1720 0.7460 -2.0100
H -4.9540 1.3850 -3.4480
H -4.0250 3.0530 -1.0400
H -4.6360 3.7140 -2.5630
H -2.7090 2.6420 -3.7780
H -2.1960 1.9160 -2.2410
H -8.7240 -4.5860 -0.9570
H -8.2210 -1.7960 0.1920
H -10.7040 -2.5250 0.1810
H -11.1350 -4.0620 -0.5830
H -10.2700 -4.0550 0.9620
H -9.1520 -3.0630 -1.7290
H -7.8370 -3.3050 1.0200
H -4.9650 -3.5430 1.1890

H -6.0900 -2.3230 1.7830
H -4.2850 -0.6590 1.9950
H -3.3530 -3.3140 3.1800
H -3.2530 -0.4380 4.2690
H -1.8670 -1.2950 3.5800
H -3.5750 -1.4200 -0.8330
H -4.6250 -2.0220 -2.1210
H -2.3140 -5.6650 -2.4980
H -1.2750 -5.1650 -1.1560
H -1.7030 -2.7290 -1.7870
H -4.2190 -4.3920 -1.3030
H -6.2340 -3.9520 -0.7110
H -6.7520 -2.6430 -1.7690
H 2.5790 -3.4960 -3.3160
H 5.6920 2.0630 3.0050
H 6.5400 -4.0920 1.6270
Al 4.1120 -0.7200 -0.1300
Br 6.0570 -0.1320 -1.5930
C -2.4130 2.3600 2.0910
C -1.3790 2.4070 0.9570
H -3.1610 1.6010 1.8720
H -1.8660 2.7200 0.0320
C -0.1960 3.3110 1.2730
H -0.5560 4.3450 1.2260
H 0.5470 3.1930 0.4820
O -0.8550 1.0760 0.7740
Br -3.4470 4.0400 2.0100
C 0.4220 3.0320 2.6430
H 1.2290 3.7470 2.8280
H 0.8800 2.0350 2.6410
C -1.7900 2.1560 3.4660
H -1.4130 1.1250 3.4830
H -2.5650 2.2240 4.2360
C -0.6330 3.1140 3.7490
H -1.0200 4.1390 3.8180
H -0.1910 2.8730 4.7210

O -1.2090 -1.0190 0.1220
C -1.6760 0.1750 0.2010
O -2.8030 0.4930 -0.1830
C 0.6960 -1.4830 0.1980
C 1.4830 -0.6440 1.1820
H 0.8620 -1.2500 -0.8470
H 1.4370 0.4170 0.9080
C 0.9780 -0.8460 2.6100
H -0.0140 -0.3860 2.6980
H 1.6530 -0.3100 3.2880
O 2.7290 -1.2060 0.9950
C 0.9120 -2.3300 2.9810
H 0.5070 -2.4480 3.9930
H 1.9300 -2.7350 2.9880
C 0.5200 -2.9240 0.5430
H 1.5130 -3.3620 0.3900
H -0.1580 -3.3980 -0.1700
C 0.0570 -3.1270 1.9880
H -0.9900 -2.8080 2.0620
H 0.0850 -4.1950 2.2320

I4b_Al cat. 2' (1,2-diaxial conformation)
C 2.1050 0.4620 -2.2220
C 1.2570 0.1010 -3.3350
N 2.7000 -0.6600 -1.7170
C 2.2560 -1.7120 -2.4670
C 1.3470 -1.2460 -3.4790
C 2.2780 1.7670 -1.7380
H 0.6820 0.7940 -3.9320
C 5.3920 1.4650 1.9710
C 3.1130 2.1070 -0.6650
H 0.8610 -1.8770 -4.2120
N 3.8650 1.2280 0.0620
C 3.2780 3.4420 -0.1320
C 4.5060 1.9580 1.0190
C 4.1430 3.3470 0.9070

C 5.7790 0.1410 2.1210
N 5.3290 -0.9000 1.3680
C 5.9510 -2.0170 1.8360
C 6.7250 -0.3320 3.1060
C 6.8340 -1.6720 2.9270
C 2.5950 -3.0470 -2.2820
C 3.4700 -3.5450 -1.3270
N 4.1310 -2.7960 -0.4010
C 4.9080 -3.6590 0.3120
C 3.8270 -4.9370 -1.1870
C 4.7220 -5.0070 -0.1710
C 5.7610 -3.3040 1.3500
H 2.7940 4.3320 -0.5090
H 4.5120 4.1370 1.5480
H 7.2330 0.2950 3.8270
H 7.4480 -2.3760 3.4720
H 3.4400 -5.7390 -1.8030
H 5.2240 -5.8800 0.2260
C -6.2210 1.1640 -1.6520
C -4.8460 1.3150 -2.3110
C -4.1810 2.6810 -2.1550
C -2.7910 2.6170 -2.7610
C 1.4600 2.8530 -2.3540
C 0.0710 2.7940 -2.2220
C -0.7400 3.8200 -2.7000
C -0.1610 4.9200 -3.3310
C 1.2210 4.9740 -3.4800
C 2.0340 3.9490 -3.0020
C -9.9210 -4.2650 -0.0390
C -8.5690 -4.1110 -0.7320
C -7.5990 -3.2430 0.0760
H -2.9380 -1.6820 1.5050
C -4.9110 -2.5600 1.3340
C -3.8990 -1.6590 2.0250
C -3.6940 -2.0870 3.4820
C -2.8490 -1.0680 4.2450

H -4.6660 -2.1990 3.9790
H -2.6680 -1.3930 5.2740
O -2.0960 3.8340 -2.5080
H -0.3560 1.9450 -1.7020
H 3.1110 3.9980 -3.1230
H 1.6710 5.8270 -3.9800
H -0.8020 5.7160 -3.6950
C -6.5270 -0.3200 -1.3880
C -5.8090 -0.7720 -0.1090
N -5.2510 -2.1870 -0.0970
C -4.0160 -2.1910 -0.9850
C -1.1820 -4.5140 -2.2080
C -2.0470 -3.2670 -2.0400
C -3.1650 -3.4520 -1.0030
H -0.3900 -4.3340 -2.9410
H -2.4950 -3.0080 -3.0080
H -2.7140 -3.6300 -0.0200
H -6.2030 -0.8890 -2.2660
H -7.6030 -0.4920 -1.2880
H -6.4810 -0.6920 0.7480
H -4.9490 -0.1300 0.0810
C -6.2500 -3.1870 -0.6330
H -6.2540 1.7190 -0.7050
H -6.9990 1.5950 -2.2900
H -4.1610 0.5760 -1.8800
H -4.9390 1.0630 -3.3770
H -4.0910 2.9350 -1.0910
H -4.7710 3.4730 -2.6320
H -2.8380 2.4520 -3.8470
H -2.2630 1.7680 -2.3150
H -8.1240 -5.1010 -0.8950
H -8.0290 -2.2430 0.1920
H -10.3970 -3.2900 0.1150
H -10.5980 -4.8800 -0.6380
H -9.8080 -4.7420 0.9410
H -8.7120 -3.6640 -1.7240

H -7.4920 -3.6700 1.0790
H -4.5610 -3.5950 1.3110
H -5.8550 -2.5400 1.8800
H -4.2440 -0.6200 2.0170
H -3.2100 -3.0700 3.5130
H -3.3510 -0.0940 4.2820
H -1.8760 -0.9230 3.7640
H -3.4090 -1.3430 -0.6660
H -4.3820 -1.9800 -1.9920
H -1.7780 -5.3650 -2.5550
H -0.7010 -4.8010 -1.2670
H -1.4220 -2.4150 -1.7470
H -3.7510 -4.3410 -1.2650
H -5.7660 -4.1640 -0.5830
H -6.3920 -2.9450 -1.6880
H 2.1490 -3.7650 -2.9640
H 5.8260 2.1870 2.6550
H 6.3250 -4.1020 1.8230
Al 3.9450 -0.7930 -0.1150
Br 5.8910 -0.4850 -1.7440
C -2.2910 2.7360 2.0490
C -1.2840 2.6980 0.8920
H -3.0360 1.9530 1.9190
H -1.7910 2.9030 -0.0530
C -0.1070 3.6390 1.0950
H -0.4850 4.6600 0.9720
H 0.6170 3.4640 0.2960
O -0.7300 1.3590 0.8310
Br -3.3430 4.3910 1.8400
C 0.5480 3.4770 2.4670
H 1.3550 4.2090 2.5700
H 1.0150 2.4860 2.5350
C -1.6370 2.6600 3.4220
H -1.2550 1.6360 3.5300
H -2.3960 2.7970 4.1980
C -0.4790 3.6460 3.5900

H -0.8730 4.6710 3.5800
H -0.0100 3.4920 4.5670
O -1.0460 -0.8230 0.4770
C -1.5360 0.3930 0.4040
O -2.6780 0.5880 0.0170
C 0.3770 -1.2430 0.4230
C 1.3970 -0.4660 1.2930
H 0.6450 -1.1480 -0.6280
H 1.4110 0.5880 0.9850
C 0.9850 -0.5600 2.7690
H 0.0090 -0.0740 2.9080
H 1.7120 -0.0030 3.3700
O 2.6180 -1.0730 1.1030
C 0.9200 -2.0200 3.2270
H 0.5800 -2.0790 4.2690
H 1.9310 -2.4380 3.1890
C 0.3390 -2.7030 0.8470
H 1.3320 -3.1100 0.6420
H -0.3810 -3.2470 0.2290
C -0.0020 -2.8580 2.3330
H -1.0450 -2.5540 2.4920
H 0.0590 -3.9160 2.6130

I3a_Al cat. 2' (1,2-diequatorial conformation)

C 2.0010 0.8290 -2.2930
C 1.4660 0.8370 -3.6340
N 2.0840 -0.4520 -1.8340
C 1.6110 -1.2540 -2.8310
C 1.2490 -0.4580 -3.9750
C 2.3940 1.9770 -1.5960
H 1.3060 1.7240 -4.2300
C 4.2030 0.4540 2.6290
C 3.0470 1.9520 -0.3590
H 0.8690 -0.8540 -4.9080
N 3.2610 0.8340 0.3980
C 3.5680 3.1130 0.3260

C 3.8870 1.2520 1.5360
C 4.1090 2.6720 1.4870
C 3.8990 -0.8920 2.7660
N 3.2690 -1.6590 1.8280
C 3.1750 -2.9120 2.3600
C 4.2000 -1.6820 3.9330
C 3.7450 -2.9350 3.6830
C 1.4210 -2.6270 -2.7420
C 1.6050 -3.4010 -1.6050
N 2.0720 -2.9410 -0.4080
C 2.1160 -4.0190 0.4290
C 1.3210 -4.8120 -1.5160
C 1.6260 -5.1920 -0.2480
C 2.6180 -4.0120 1.7230
H 3.5190 4.1270 -0.0450
H 4.5990 3.2480 2.2620
H 4.6950 -1.3090 4.8200
H 3.7890 -3.8090 4.3210
H 0.9510 -5.4240 -2.3280
H 1.5550 -6.1760 0.1960
C -3.9700 1.9160 -0.4440
C -4.4960 3.0110 -1.3800
C -3.6100 4.2690 -1.4130
C -2.1690 3.8740 -1.6910
C 1.8990 3.2950 -2.0950
C 0.5180 3.4880 -1.9720
C -0.0590 4.7220 -2.2650
C 0.7490 5.7630 -2.7340
C 2.1130 5.5550 -2.8910
C 2.7010 4.3280 -2.5710
C -8.5090 -2.9960 0.5600
C -7.4000 -2.8790 -0.4830
C -6.0590 -2.4860 0.1450
H -0.9420 -2.2450 0.3570
C -3.0410 -2.8140 0.5530
C -1.7080 -2.3600 1.1270

C -1.2060 -3.3310 2.2040
C -0.2440 -2.6190 3.1550
H -2.0550 -3.7330 2.7740
H 0.1820 -3.3120 3.8880
O -1.3880 4.9830 -2.1040
H -0.0650 2.6540 -1.5990
H 3.7710 4.1820 -2.6810
H 2.7330 6.3660 -3.2630
H 0.2950 6.7220 -2.9650
C -4.5270 0.5200 -0.7490
C -3.7590 -0.5010 0.0910
N -3.6330 -1.8930 -0.4980
C -2.7200 -1.8100 -1.7110
C -1.4610 -4.2500 -4.4440
C -1.9080 -2.9500 -3.7820
C -2.2830 -3.1440 -2.3100
H -1.1720 -4.0820 -5.4860
H -2.7760 -2.5480 -4.3220
H -1.4220 -3.5410 -1.7600
H -4.3810 0.3400 -1.8190
H -5.6050 0.4640 -0.5620
H -4.2070 -0.6140 1.0800
H -2.7360 -0.1510 0.2250
C -4.9820 -2.4180 -0.9310
H -2.8860 1.8250 -0.5550
H -4.1480 2.1750 0.6080
H -4.5420 2.6050 -2.4010
H -5.5220 3.2850 -1.1110
H -3.6680 4.8130 -0.4630
H -3.9640 4.9450 -2.1980
H -2.1310 3.0960 -2.4680
H -1.7270 3.4510 -0.7840
H -7.2890 -3.8340 -1.0120
H -6.1740 -1.5200 0.6490
H -8.6570 -2.0450 1.0830
H -9.4580 -3.2730 0.0910

H -8.2670 -3.7580 1.3080
H -7.6800 -2.1340 -1.2380
H -5.7990 -3.2240 0.9110
H -2.9670 -3.8030 0.0940
H -3.7800 -2.8710 1.3540
H -1.8320 -1.3830 1.6000
H -0.7110 -4.1870 1.7290
H -0.7660 -1.8190 3.6940
H 0.5730 -2.1550 2.5980
H -1.8550 -1.2100 -1.4140
H -3.2770 -1.2400 -2.4560
H -2.2650 -4.9930 -4.4330
H -0.6030 -4.6870 -3.9230
H -1.1180 -2.1940 -3.8550
H -3.0760 -3.8980 -2.2570
H -4.8160 -3.4130 -1.3480
H -5.3110 -1.7700 -1.7470
H 1.0650 -3.1320 -3.6340
H 4.7000 0.9370 3.4640
H 2.6030 -4.9500 2.2690
C 0.1270 0.3150 0.5930
O -0.6850 0.5510 -0.3090
O 0.9260 -0.6670 0.6720
Al 2.6850 -1.0580 -0.0100
Br 4.9550 -1.5720 -0.9070
C -0.5800 2.3050 1.7220
C -1.3490 2.3870 3.0310
C -2.1440 3.6850 3.1280
C -1.2110 4.8960 3.0000
C -0.4140 4.8350 1.6960
C 0.3470 3.5140 1.5890
O 0.2030 1.1220 1.6950
H -1.2930 2.2810 0.8950
Br -2.5840 0.8490 3.1820
H -0.6730 2.2630 3.8790
H -2.8860 3.7090 2.3180

H -2.6930 3.7130 4.0730
H -0.5180 4.9130 3.8510
H -1.8040 5.8150 3.0520
H -1.0960 4.9410 0.8420
H 0.2910 5.6710 1.6370
H 0.8650 3.4380 0.6300
H 1.1150 3.4500 2.3700

TS3a_Al cat. 2’ (1,2-diequatorial conformation)
C -1.4640 0.6010 2.3880
C -0.6570 0.4650 3.5750
N -1.6940 -0.6260 1.8410
C -1.0480 -1.5330 2.6300
C -0.4300 -0.8640 3.7440
C -1.9620 1.8190 1.9050
H -0.3440 1.2820 4.2100
C -4.8950 0.7220 -1.7750
C -2.9410 1.9190 0.9120
H 0.1070 -1.3550 4.5440
N -3.4090 0.8740 0.1660
C -3.5820 3.1430 0.4940
C -4.3120 1.3980 -0.7100
C -4.4630 2.8090 -0.4820
C -4.5780 -0.5640 -2.1820
N -3.6850 -1.3910 -1.5610
C -3.6750 -2.5520 -2.2810
C -5.1310 -1.2130 -3.3440
C -4.5630 -2.4420 -3.4120
C -0.8990 -2.8830 2.3350
C -1.3020 -3.5000 1.1610
N -1.9870 -2.8930 0.1450
C -2.1960 -3.8520 -0.8040
C -1.0410 -4.8770 0.8270
C -1.5820 -5.0910 -0.4000
C -2.9590 -3.6930 -1.9520
H -3.3870 4.1230 0.9060

H -5.1310 3.4570 -1.0340
H -5.8580 -0.7690 -4.0110
H -4.7270 -3.2210 -4.1450
H -0.5200 -5.5790 1.4650
H -1.5980 -6.0050 -0.9790
C 4.7170 1.6140 -0.0980
C 5.2060 2.7770 0.7830
C 4.1800 3.8930 1.0190
C 2.8640 3.3990 1.5910
C -1.2810 3.0640 2.3610
C 0.0600 3.1850 1.9760
C 0.7740 4.3450 2.2560
C 0.1490 5.3930 2.9380
C -1.1750 5.2610 3.3370
C -1.8980 4.1010 3.0570
C 8.3630 -2.3530 -1.4370
C 7.2970 -2.8240 -0.4500
C 5.9600 -2.1120 -0.6740
H 0.7730 -2.3840 -0.5930
C 2.8770 -2.8620 -0.9040
C 1.5290 -2.3560 -1.3850
C 1.0370 -3.1590 -2.5960
C 0.0410 -2.3440 -3.4190
H 1.8890 -3.4290 -3.2360
H -0.3590 -2.9300 -4.2540
O 2.0630 4.5430 1.8680
H 0.5050 2.3670 1.4210
H -2.9320 4.0030 3.3750
H -1.6500 6.0740 3.8780
H 0.7140 6.2950 3.1510
C 4.2510 0.3930 0.7080
C 3.5340 -0.5790 -0.2270
N 3.5340 -2.0340 0.1920
C 2.7820 -2.1470 1.4990
C 2.0780 -4.9020 4.1320
C 2.4430 -3.5360 3.5600

C	2.6020	-3.5630	2.0370
H	1.9770	-4.8600	5.2200
H	3.3810	-3.1840	4.0090
H	1.7220	-4.0220	1.5750
H	3.5700	0.7030	1.5080
H	5.1230	-0.0540	1.2000
H	3.9560	-0.5480	-1.2320
H	2.4930	-0.2730	-0.3260
C	4.9470	-2.5540	0.3770
H	3.9080	1.9340	-0.7680
H	5.5250	1.2890	-0.7650
H	5.5400	2.3800	1.7520
H	6.0890	3.2360	0.3270
H	3.9690	4.4080	0.0740
H	4.6050	4.6370	1.7020
H	3.0150	2.8380	2.5250
H	2.3710	2.7360	0.8700
H	7.1550	-3.9080	-0.5480
H	6.1220	-1.0310	-0.6210
H	8.5410	-1.2770	-1.3370
H	9.3130	-2.8680	-1.2650
H	8.0560	-2.5470	-2.4710
H	7.6420	-2.6440	0.5760
H	5.6030	-2.3320	-1.6860
H	2.8230	-3.8880	-0.5300
H	3.5810	-2.8460	-1.7380
H	1.6360	-1.3180	-1.6940
H	0.5850	-4.1010	-2.2600
H	0.5330	-1.4490	-3.8170
H	-0.7940	-2.0100	-2.7990
H	1.8110	-1.6690	1.3500
H	3.3440	-1.5390	2.2110
H	2.8470	-5.6460	3.8920
H	1.1290	-5.2650	3.7220
H	1.6800	-2.7980	3.8340
H	3.4590	-4.2030	1.7980

H 4.8780 -3.6430 0.3800
H 5.2770 -2.2430 1.3710
H -0.3860 -3.4980 3.0670
H -5.6070 1.2740 -2.3810
H -3.0450 -4.5450 -2.6180
C -0.6170 0.7210 -1.0470
O 0.5200 1.1690 -0.7440
O -1.0810 -0.4090 -0.7710
Al -2.7250 -1.0190 0.1620
Br -4.7000 -1.7660 1.4730
C 1.5080 3.8280 -1.5560
C 0.6780 2.7250 -2.0970
H 2.5590 3.7310 -1.8300
C -0.7610 2.8400 -1.6480
H -0.7910 3.1440 -0.5930
O -1.3900 1.5820 -1.7530
C -1.3820 3.9540 -2.4730
H -2.4450 4.0440 -2.2300
H -1.2930 3.7470 -3.5460
C 0.9080 5.1010 -2.2340
H 1.1760 5.0870 -3.2970
H 1.3970 5.9770 -1.7950
C -0.6180 5.2370 -2.0900
H -0.8630 5.4940 -1.0520
H -0.9570 6.0700 -2.7130
H 1.4190 3.9100 -0.4690
Br 2.3320 0.9540 -3.0170
H 0.7490 2.6170 -3.1620

I4a_Al cat. 2' (1,2-diequatorial conformation)

C 2.1480 1.7930 -1.9270
C 1.8950 2.1050 -3.3100
N 2.6420 0.5200 -1.8190
C 2.7180 0.0300 -3.0910
C 2.2790 1.0220 -4.0330
C 1.9760 2.6900 -0.8740

H 1.5020 3.0460 -3.6690
C 3.5240 0.4250 3.1100
C 2.3940 2.4390 0.4350
H 2.2530 0.8850 -5.1060
N 2.8680 1.2380 0.8970
C 2.3970 3.4080 1.4980
C 3.1750 1.4300 2.2180
C 2.9170 2.7900 2.5920
C 3.5390 -0.9250 2.8100
N 3.3310 -1.4610 1.5660
C 3.4000 -2.8170 1.7240
C 3.7240 -1.9730 3.7780
C 3.6190 -3.1470 3.1080
C 3.0670 -1.2720 -3.4300
C 3.2330 -2.3040 -2.5240
N 3.1530 -2.1730 -1.1620
C 3.2870 -3.4340 -0.6510
C 3.4190 -3.6880 -2.8770
C 3.4280 -4.3910 -1.7180
C 3.3510 -3.7480 0.6970
H 2.0600 4.4300 1.4060
H 3.0820 3.2020 3.5790
H 3.9010 -1.8130 4.8330
H 3.6970 -4.1540 3.4960
H 3.5140 -4.0580 -3.8900
H 3.5420 -5.4580 -1.5770
C -4.9630 1.6550 -0.6210
C -5.3410 2.8940 -1.4520
C -4.4340 4.1150 -1.2600
C -2.9620 3.8300 -1.4950
C 1.2450 3.9650 -1.1340
C -0.1490 3.8820 -1.2290
C -0.9090 5.0410 -1.3780
C -0.2680 6.2820 -1.4630
C 1.1150 6.3520 -1.3920
C 1.8820 5.1980 -1.2240

C -8.2340 -2.9830 -1.5280
C -6.8450 -3.0050 -2.1620
C -5.8020 -2.3130 -1.2800
H -0.8060 -2.6620 0.0060
C -2.9770 -2.8220 -0.0740
C -1.6700 -2.6370 0.6770
C -1.5230 -3.7310 1.7380
C -0.1670 -3.6590 2.4360
H -2.3280 -3.6010 2.4710
H -0.0690 -4.4510 3.1860
O -2.2650 5.0640 -1.4260
H -0.6090 2.9040 -1.1550
H 2.9640 5.2560 -1.1540
H 1.6040 7.3190 -1.4650
H -0.8720 7.1760 -1.5820
C -4.1010 0.6490 -1.3980
C -3.6550 -0.4780 -0.4710
N -3.2930 -1.7850 -1.1470
C -2.1050 -1.5320 -2.0460
C 0.2790 -3.4800 -4.3760
C -0.2810 -2.3390 -3.5320
C -1.5540 -2.7430 -2.7840
H 1.1750 -3.1590 -4.9150
H -0.4930 -1.4750 -4.1750
H -1.3150 -3.5550 -2.0880
H -3.2270 1.1450 -1.8340
H -4.6990 0.2780 -2.2370
H -4.4050 -0.7080 0.2860
H -2.7620 -0.1720 0.0700
C -4.4470 -2.3090 -1.9760
H -4.4530 1.9540 0.3040
H -5.8720 1.1360 -0.2970
H -5.3650 2.6220 -2.5160
H -6.3610 3.2010 -1.1970
H -4.5470 4.5030 -0.2400
H -4.7500 4.9120 -1.9420

H -2.7890 3.3670 -2.4790
H -2.5900 3.1400 -0.7290
H -6.5380 -4.0430 -2.3440
H -6.1320 -1.2890 -1.0760
H -8.5770 -1.9550 -1.3680
H -8.9640 -3.4870 -2.1680
H -8.2300 -3.4890 -0.5570
H -6.8800 -2.5120 -3.1420
H -5.7460 -2.8290 -0.3150
H -2.9930 -3.7930 -0.5740
H -3.7950 -2.7750 0.6460
H -1.6820 -1.6780 1.2010
H -1.6510 -4.7180 1.2730
H -0.0380 -2.6970 2.9400
H 0.6540 -3.7660 1.7180
H -1.3310 -1.0810 -1.4220
H -2.4270 -0.7780 -2.7670
H -0.4540 -3.8230 -5.1150
H 0.5570 -4.3330 -3.7480
H 0.4700 -2.0100 -2.8060
H -2.2900 -3.1300 -3.4980
H -4.1740 -3.3240 -2.2710
H -4.4880 -1.7080 -2.8870
H 3.1260 -1.5150 -4.4860
H 3.7180 0.7130 4.1380
H 3.4450 -4.7950 0.9650
C 0.3110 -0.0780 0.8720
O -0.6230 0.8440 0.6200
O 0.9250 -0.6560 -0.0060
Al 3.1840 -0.4480 -0.1530
Br 5.5470 -0.0990 -0.4260
C -1.8170 2.5080 2.1470
C -1.2810 1.1240 1.8920
H -2.6110 2.7740 1.4420
C -0.1750 0.7980 2.8600
H 0.5640 1.6080 2.8910

O 0.4790 -0.2960 2.1690
C -0.7400 0.5500 4.2340
H 0.0420 0.2720 4.9470
H -1.4970 -0.2420 4.1950
C -2.3940 2.4260 3.5820
H -3.2590 1.7520 3.5590
H -2.7510 3.4140 3.8860
C -1.3900 1.8970 4.6280
H -0.5970 2.6420 4.7810
H -1.9040 1.7800 5.5870
H -1.0210 3.2570 2.0650
Br -4.0240 -1.1350 2.9900
H -2.0940 0.3930 1.9940

I3b_Al cat. 2' (1,2-diequatorial conformation)
C 2.1010 0.3910 -2.4900
C 1.5120 0.1190 -3.7770
N 2.6600 -0.7560 -1.9840
C 2.4260 -1.7350 -2.9100
C 1.7040 -1.1990 -4.0290
C 2.0720 1.6340 -1.8510
H 1.0170 0.8500 -4.3990
C 4.4720 1.0840 2.3290
C 2.6430 1.8760 -0.5970
H 1.4000 -1.7690 -4.8980
N 3.3700 0.9780 0.1380
C 2.5120 3.1120 0.1330
C 3.7140 1.6200 1.2950
C 3.1790 2.9510 1.3040
C 4.9800 -0.2020 2.3740
N 4.7900 -1.1590 1.4170
C 5.4060 -2.2850 1.8800
C 5.7550 -0.7350 3.4650
C 6.0250 -2.0280 3.1560
C 2.8260 -3.0610 -2.8090
C 3.5670 -3.6020 -1.7720

N 4.0240 -2.9080 -0.6850
C 4.7400 -3.8050 0.0620
C 3.9860 -4.9770 -1.6990
C 4.7150 -5.1020 -0.5620
C 5.3960 -3.5210 1.2490
H 1.9750 3.9840 -0.2120
H 3.3020 3.6630 2.1100
H 6.0430 -0.1790 4.3480
H 6.5800 -2.7580 3.7300
H 3.7490 -5.7330 -2.4360
H 5.2030 -5.9840 -0.1680
C -6.2490 0.9340 -2.0020
C -4.8360 0.9930 -2.5760
C -4.2970 2.3930 -2.8750
C -2.7990 2.2620 -3.0560
C 1.3040 2.7390 -2.4950
C -0.0720 2.5680 -2.6570
C -0.8510 3.5910 -3.1980
C -0.2420 4.7870 -3.5920
C 1.1280 4.9470 -3.4380
C 1.9110 3.9300 -2.8920
C -9.6300 -4.5910 0.2400
C -8.2570 -4.4510 -0.4140
C -7.4340 -3.3220 0.2130
H -2.8440 -1.4340 1.5560
C -4.8220 -2.3220 1.4440
C -3.8180 -1.3540 2.0500
C -3.6730 -1.6510 3.5460
C -2.8390 -0.5900 4.2550
H -4.6670 -1.7010 4.0100
H -2.7190 -0.8220 5.3180
O -2.2010 3.5210 -3.3350
H -0.5120 1.6460 -2.2990
H 2.9820 4.0590 -2.7720
H 1.5950 5.8770 -3.7490
H -0.8600 5.5780 -4.0060

C -6.5630 -0.4780 -1.4860
C -5.8530 -0.7480 -0.1490
N -5.1730 -2.1050 -0.0130
C -3.9270 -2.0790 -0.8790
C -0.8340 -4.2080 -1.7660
C -1.7720 -3.0080 -1.6740
C -3.0140 -3.2950 -0.8180
H 0.0690 -3.9570 -2.3320
H -2.0860 -2.7170 -2.6840
H -2.6890 -3.4920 0.2110
H -6.2600 -1.1910 -2.2610
H -7.6420 -0.6120 -1.3590
H -6.5640 -0.6820 0.6760
H -5.0680 -0.0050 0.0300
C -6.0690 -3.2370 -0.4590
H -6.3470 1.6550 -1.1820
H -6.9860 1.2160 -2.7630
H -4.1480 0.5380 -1.8560
H -4.7930 0.3780 -3.4870
H -4.4890 3.0510 -2.0200
H -4.7720 2.8340 -3.7590
H -2.5550 1.5610 -3.8690
H -2.3940 1.8470 -2.1320
H -7.7090 -5.3970 -0.3240
H -7.9810 -2.3790 0.1040
H -10.2110 -3.6680 0.1360
H -10.2020 -5.4030 -0.2210
H -9.5350 -4.8090 1.3090
H -8.3790 -4.2600 -1.4880
H -7.3290 -3.5150 1.2860
H -4.4670 -3.3520 1.5290
H -5.7660 -2.2550 1.9890
H -4.1370 -0.3170 1.9120
H -3.2160 -2.6400 3.6840
H -3.3040 0.3970 4.1680
H -1.8430 -0.5130 3.8100

H -3.3580 -1.1840 -0.5980
H -4.2820 -1.9400 -1.9030
H -1.3210 -5.0550 -2.2630
H -0.5200 -4.5470 -0.7710
H -1.2520 -2.1390 -1.2540
H -3.5090 -4.2010 -1.1860
H -5.5110 -4.1580 -0.2800
H -6.1890 -3.1340 -1.5390
H 2.5490 -3.7250 -3.6220
H 4.6790 1.7320 3.1740
H 5.9270 -4.3350 1.7330
Al 3.8380 -0.9240 -0.3520
Br 5.8600 -0.3380 -1.5380
C 1.0710 -2.2690 0.5570
C 0.8640 -0.8190 0.7030
H 1.0360 -2.6850 -0.4470
H 0.6430 -0.2430 -0.1900
C 0.4650 -0.2190 2.0160
H -0.6050 -0.0000 1.9610
H 0.9690 0.7470 2.1280
O 2.1970 -1.3860 0.7340
C 0.7830 -1.1490 3.1870
H 0.3660 -0.7240 4.1060
H 1.8680 -1.2140 3.3270
C 0.8510 -3.2220 1.7100
H 1.8260 -3.6480 1.9720
H 0.2250 -4.0530 1.3670
C 0.2060 -2.5450 2.9300
H -0.8740 -2.4470 2.7530
H 0.3260 -3.1860 3.8090
C -2.3730 1.2460 0.2330
O -3.5440 1.6080 0.4590
O -1.9600 0.2070 -0.3300
C -0.7610 5.1050 2.7670
C -0.6470 3.6720 2.2610
H -0.0110 5.2780 3.5450

C -1.6340 3.3590 1.1430
H -2.6560 3.3620 1.5360
O -1.3280 2.0790 0.6250
C -1.4980 4.3930 0.0210
H -2.2490 4.1660 -0.7420
H -0.5170 4.2550 -0.4510
C -0.6010 6.1050 1.6170
H 0.4110 6.0230 1.1950
H -0.7040 7.1240 2.0060
C -1.6320 5.8290 0.5220
H -2.6410 5.9920 0.9250
H -1.5040 6.5270 -0.3120
H -1.7460 5.2410 3.2310
Br -0.9450 2.4400 3.7780
H 0.3680 3.4430 1.9280

TS3b_Al cat. 2' (1,2-diequatorial conformation)

C 2.1720 0.4640 -2.4160
C 1.3900 0.1980 -3.6010
N 2.6550 -0.7120 -1.9120
C 2.1990 -1.7060 -2.7300
C 1.4050 -1.1460 -3.7900
C 2.3810 1.7350 -1.8680
H 0.9070 0.9480 -4.2100
C 5.1900 1.1220 2.0410
C 3.1500 1.9840 -0.7250
H 0.9420 -1.7150 -4.5860
N 3.7990 1.0380 0.0190
C 3.3470 3.2870 -0.1320
C 4.4070 1.6990 1.0470
C 4.1260 3.1070 0.9630
C 5.4910 -0.2260 2.1630
N 5.0460 -1.2080 1.3290
C 5.5600 -2.3780 1.8010
C 6.3220 -0.7930 3.1990
C 6.3670 -2.1290 2.9730

C 2.4430 -3.0650 -2.5710
C 3.2200 -3.6440 -1.5790
N 3.8660 -2.9660 -0.5880
C 4.5360 -3.8990 0.1460
C 3.4790 -5.0590 -1.4620
C 4.2990 -5.2170 -0.3930
C 5.3320 -3.6330 1.2540
H 2.9350 4.2110 -0.5110
H 4.4880 3.8520 1.6600
H 6.8010 -0.2260 3.9870
H 6.8910 -2.8910 3.5360
H 3.0860 -5.8160 -2.1290
H 4.7190 -6.1310 0.0060
C -6.0620 1.9550 -1.5140
C -4.6590 1.8690 -2.1050
C -3.9790 3.2130 -2.3840
C -2.4820 2.9670 -2.4090
C 1.6760 2.8880 -2.5010
C 0.2800 2.9180 -2.4360
C -0.4320 3.9940 -2.9640
C 0.2570 5.0460 -3.5750
C 1.6430 5.0060 -3.6510
C 2.3600 3.9330 -3.1190
C -10.2510 -3.3650 -0.9000
C -8.7970 -3.3620 -1.3660
C -7.9280 -2.4100 -0.5380
H -3.2880 -1.3420 1.4750
C -5.2060 -2.2520 0.9960
C -4.2460 -1.5620 1.9560
C -4.0280 -2.4920 3.1580
C -3.2920 -1.8190 4.3120
H -4.9970 -2.8610 3.5200
H -3.1310 -2.5250 5.1330
O -1.7870 4.1000 -2.9030
H -0.2200 2.1000 -1.9330
H 3.4430 3.9060 -3.1830

H 2.1730 5.8210 -4.1330
H -0.3070 5.8790 -3.9820
C -6.6670 0.5700 -1.2440
C -6.0210 -0.1620 -0.0490
N -5.4960 -1.5660 -0.3240
C -4.2370 -1.4280 -1.1590
C -1.4960 -3.5820 -2.8270
C -2.3270 -2.3590 -2.4440
C -3.4790 -2.7050 -1.4910
H -0.6800 -3.2970 -3.4980
H -2.7390 -1.9010 -3.3520
H -3.0670 -3.1530 -0.5790
H -6.5940 -0.0170 -2.1660
H -7.7380 0.6790 -1.0470
H -6.7380 -0.2690 0.7680
H -5.1580 0.3910 0.3290
C -6.5000 -2.4220 -1.0680
H -6.0330 2.5310 -0.5800
H -6.7280 2.4980 -2.1950
H -4.0250 1.3210 -1.4020
H -4.6900 1.2850 -3.0360
H -4.2150 3.9380 -1.5960
H -4.3150 3.6400 -3.3350
H -2.2510 2.0970 -3.0430
H -2.1540 2.7330 -1.3890
H -8.3870 -4.3780 -1.3020
H -8.3550 -1.4040 -0.5930
H -10.6950 -2.3670 -0.9880
H -10.8530 -4.0530 -1.5010
H -10.3290 -3.6760 0.1470
H -8.7500 -3.0720 -2.4230
H -7.9670 -2.7210 0.5120
H -4.8290 -3.2440 0.7400
H -6.1740 -2.3850 1.4820
H -4.6550 -0.6060 2.3000
H -3.4650 -3.3760 2.8280

H -3.8680 -0.9720 4.7020
H -2.3160 -1.4380 3.9970
H -3.5780 -0.7480 -0.6170
H -4.5540 -0.9350 -2.0800
H -2.1100 -4.3330 -3.3380
H -1.0490 -4.0540 -1.9460
H -1.6900 -1.6020 -1.9720
H -4.1230 -3.4540 -1.9650
H -6.1050 -3.4390 -1.0420
H -6.4850 -2.0960 -2.1100
H 1.9980 -3.7330 -3.3030
H 5.6090 1.7930 2.7850
H 5.8080 -4.4810 1.7360
Al 3.8240 -0.9650 -0.2730
Br 5.8580 -0.7220 -1.7330
C 0.3790 -1.1250 0.2720
C 1.2930 -0.4680 1.2530
H 0.5150 -0.8340 -0.7610
H 1.4250 0.6000 1.0530
C 0.9260 -0.7210 2.7100
H 0.0340 -0.1380 2.9650
H 1.7520 -0.3600 3.3330
O 2.3680 -1.2500 0.8520
C 0.6690 -2.2080 2.9690
H 0.3530 -2.3570 4.0080
H 1.6040 -2.7610 2.8270
C -0.0420 -2.5330 0.5500
H 0.8060 -3.1620 0.2540
H -0.8760 -2.7900 -0.1050
C -0.4010 -2.7550 2.0200
H -1.3500 -2.2450 2.2170
H -0.5650 -3.8240 2.1980
C -1.8300 0.8050 0.6010
O -2.9840 1.2410 0.5950
O -1.4940 -0.3870 0.2840
C -0.9020 4.1110 3.7340

C -0.7840 2.7620 3.0380
H -0.7180 3.9870 4.8050
C -1.0300 2.8650 1.5360
H -2.0690 3.1510 1.3450
O -0.7750 1.6020 0.9250
C -0.0620 3.8760 0.9250
H -0.2770 3.9660 -0.1430
H 0.9560 3.4760 1.0110
C 0.0830 5.1100 3.1180
H 1.1120 4.7710 3.3010
H -0.0260 6.0810 3.6120
C -0.1500 5.2390 1.6120
H -1.1420 5.6780 1.4340
H 0.5820 5.9200 1.1670
H -1.9280 4.4860 3.6210
Br -2.0510 1.4800 3.8440
H 0.1960 2.3100 3.2120

I4b_Al cat. 2' (1,2-diequatorial conformation)
C 2.1610 0.5120 -2.3740
C 1.3900 0.2610 -3.5690
N 2.6550 -0.6680 -1.8900
C 2.2250 -1.6480 -2.7370
C 1.4260 -1.0780 -3.7880
C 2.3580 1.7760 -1.8020
H 0.9030 1.0180 -4.1680
C 5.1630 1.1120 2.1010
C 3.1230 2.0120 -0.6530
H 0.9800 -1.6360 -4.6010
N 3.7620 1.0560 0.0840
C 3.3310 3.3100 -0.0500
C 4.3750 1.7020 1.1180
C 4.1060 3.1140 1.0460
C 5.4810 -0.2350 2.1960
N 5.0490 -1.2050 1.3450
C 5.5840 -2.3760 1.7870

C 6.3260 -0.8110 3.2180
C 6.3910 -2.1400 2.9630
C 2.5090 -3.0050 -2.6250
C 3.3010 -3.5960 -1.6510
N 3.9090 -2.9350 -0.6260
C 4.5990 -3.8720 0.0830
C 3.6040 -5.0060 -1.5820
C 4.4120 -5.1770 -0.5070
C 5.3810 -3.6200 1.2040
H 2.9310 4.2420 -0.4240
H 4.4760 3.8520 1.7470
H 6.8000 -0.2540 4.0160
H 6.9290 -2.9060 3.5060
H 3.2440 -5.7500 -2.2810
H 4.8550 -6.0910 -0.1340
C -6.0730 2.0700 -1.2980
C -4.6960 1.9780 -1.9460
C -3.9970 3.3150 -2.2160
C -2.5080 3.0370 -2.3130
C 1.6550 2.9370 -2.4230
C 0.2570 2.9620 -2.3760
C -0.4530 4.0570 -2.8680
C 0.2390 5.1280 -3.4420
C 1.6250 5.0880 -3.5120
C 2.3400 4.0010 -3.0060
C -10.3150 -3.2770 -0.6940
C -8.9160 -3.1730 -1.2970
C -7.9730 -2.3410 -0.4190
H -3.2140 -1.4770 1.3830
C -5.1940 -2.2700 0.9710
C -4.1590 -1.6570 1.9030
C -3.9300 -2.6270 3.0690
C -3.0080 -2.0580 4.1440
H -4.8940 -2.8930 3.5220
H -2.8350 -2.7960 4.9340
O -1.8080 4.1680 -2.8000

H -0.2460 2.1230 -1.9130
H 3.4240 3.9790 -3.0600
H 2.1580 5.9180 -3.9670
H -0.3220 5.9740 -3.8230
C -6.6990 0.6870 -1.0630
C -6.0210 -0.1170 0.0670
N -5.5300 -1.5120 -0.2990
C -4.3070 -1.3510 -1.1820
C -1.7440 -3.4600 -3.1630
C -2.5040 -2.2430 -2.6400
C -3.5740 -2.6160 -1.6040
H -0.9650 -3.1540 -3.8680
H -2.9830 -1.7280 -3.4830
H -3.0900 -3.0880 -0.7410
H -6.6800 0.1440 -2.0140
H -7.7570 0.8070 -0.8160
H -6.7070 -0.2540 0.9050
H -5.1380 0.4050 0.4410
C -6.5830 -2.3110 -1.0410
H -5.9980 2.6070 -0.3430
H -6.7500 2.6530 -1.9320
H -4.0440 1.3930 -1.2910
H -4.7750 1.4240 -2.8920
H -4.1830 4.0240 -1.4010
H -4.3630 3.7730 -3.1410
H -2.3230 2.1800 -2.9790
H -2.1420 2.7650 -1.3150
H -8.4970 -4.1780 -1.4310
H -8.3830 -1.3310 -0.3190
H -10.7680 -2.2860 -0.5740
H -10.9730 -3.8720 -1.3350
H -10.2840 -3.7550 0.2910
H -8.9760 -2.7210 -2.2950
H -7.9470 -2.7820 0.5830
H -4.8660 -3.2610 0.6480
H -6.1380 -2.3920 1.5040

H -4.4960 -0.6900 2.2910
H -3.5020 -3.5600 2.6790
H -3.4470 -1.1680 4.6070
H -2.0380 -1.7760 3.7260
H -3.6270 -0.6920 -0.6400
H -4.6590 -0.8180 -2.0670
H -2.4170 -4.1530 -3.6800
H -1.2560 -4.0090 -2.3500
H -1.8020 -1.5270 -2.1960
H -4.2520 -3.3530 -2.0480
H -6.1920 -3.3270 -1.1170
H -6.6320 -1.9080 -2.0540
H 2.0860 -3.6590 -3.3820
H 5.5820 1.7740 2.8530
H 5.8740 -4.4710 1.6650
Al 3.7730 -0.9490 -0.2170
Br 5.8500 -0.6210 -1.6800
C 0.1440 -0.9840 0.1610
C 1.2080 -0.6120 1.2310
H 0.4430 -0.5870 -0.8100
H 1.3470 0.4770 1.2470
C 0.7360 -1.0970 2.6090
H -0.1890 -0.5810 2.8990
H 1.5000 -0.8230 3.3460
O 2.3660 -1.2690 0.8850
C 0.5350 -2.6160 2.6010
H 0.1590 -2.9600 3.5730
H 1.5110 -3.0870 2.4400
C -0.0140 -2.4970 0.1200
H 0.9520 -2.9050 -0.1850
H -0.7490 -2.7720 -0.6400
C -0.4210 -3.0580 1.4870
H -1.4370 -2.7180 1.7220
H -0.4610 -4.1530 1.4340
C -1.6240 0.7310 0.6240
O -2.8000 1.0460 0.5800

O -1.2420 -0.5010 0.3720
C -0.9020 3.9970 3.7820
C -0.7560 2.6660 3.0520
H -0.7470 3.8390 4.8530
C -0.9450 2.8210 1.5460
H -1.9810 3.0870 1.3160
O -0.6290 1.5720 0.9050
C 0.0310 3.8560 0.9980
H -0.1410 3.9700 -0.0750
H 1.0480 3.4640 1.1170
C 0.0920 5.0230 3.2260
H 1.1180 4.6880 3.4290
H -0.0430 5.9770 3.7470
C -0.1000 5.1970 1.7200
H -1.0900 5.6290 1.5240
H 0.6380 5.8970 1.3160
H -1.9260 4.3670 3.6510
Br -2.0530 1.3690 3.7790
H 0.2170 2.2080 3.2450

R_Mg cat. 3'

C 1.6020 1.6460 -1.6620
C 0.4820 1.7420 -2.5770
N 2.2020 0.4290 -1.8140
C 1.5150 -0.2470 -2.7780
C 0.4280 0.5690 -3.2610
C 2.0250 2.6590 -0.7780
H -0.1670 2.5990 -2.6850
C 5.9940 1.0130 1.5120
C 3.1550 2.5920 0.0640
H -0.2730 0.2800 -4.0350
N 4.0250 1.5420 0.1380
C 3.5410 3.6000 1.0320
C 4.9400 1.8390 1.1030
C 4.6490 3.1360 1.6660
C 6.2990 -0.2670 1.0520

N 5.5750 -0.9560 0.1240
C 6.1860 -2.1590 -0.0560
C 7.4240 -1.0710 1.4820
C 7.3560 -2.2410 0.7950
C 1.8190 -1.5300 -3.2460
C 2.8660 -2.3580 -2.8390
N 3.7750 -2.0500 -1.8720
C 4.6460 -3.0950 -1.7870
C 3.1640 -3.6640 -3.3870
C 4.2640 -4.1220 -2.7330
C 5.7520 -3.1540 -0.9350
H 3.0230 4.5330 1.2070
H 5.2140 3.6160 2.4550
H 8.1650 -0.7650 2.2100
H 8.0310 -3.0860 0.8470
H 2.6060 -4.1520 -4.1770
H 4.7840 -5.0600 -2.8780
C -5.4960 2.1070 0.3820
C -5.4880 3.4170 -0.4240
C -4.4310 4.4370 0.0050
C -2.9940 3.9590 -0.1280
C 1.2160 3.9130 -0.7370
C -0.1260 3.8720 -0.3370
C -0.8720 5.0510 -0.3100
C -0.2770 6.2710 -0.6500
C 1.0540 6.3050 -1.0360
C 1.8010 5.1300 -1.0940
C -9.2940 -1.9230 -1.7900
C -7.8080 -2.1770 -2.0310
C -6.9470 -1.6880 -0.8620
H -2.7420 -2.0640 2.0010
C -4.5880 -2.6700 0.9990
C -3.7320 -2.4640 2.2440
C -3.5940 -3.7910 2.9980
C -3.0100 -3.6050 4.3960
H -4.5780 -4.2730 3.0780

H -2.8740 -4.5690 4.8960
O -2.1790 5.1160 0.0480
H -0.5580 2.9270 -0.0130
H 2.8380 5.1530 -1.4150
H 1.5120 7.2510 -1.3100
H -0.8800 7.1720 -0.6140
C -4.7740 0.9500 -0.3170
C -4.8140 -0.2670 0.5950
N -4.4910 -1.5910 -0.0580
C -3.0910 -1.5250 -0.6560
C -0.5000 -4.0460 -2.0390
C -1.2020 -2.7070 -1.8300
C -2.4910 -2.8760 -1.0230
H 0.4330 -3.9190 -2.5940
H -1.4310 -2.2430 -2.7980
H -2.2590 -3.4420 -0.1140
H -3.7270 1.2150 -0.5020
H -5.2570 0.7650 -1.2840
H -5.7970 -0.3910 1.0560
H -4.0680 -0.1150 1.3790
C -5.4720 -1.9220 -1.1670
H -5.0390 2.2690 1.3670
H -6.5330 1.7990 0.5680
H -5.3640 3.1920 -1.4920
H -6.4660 3.9020 -0.3300
H -4.6080 4.7350 1.0460
H -4.5390 5.3400 -0.6070
H -2.8120 3.5360 -1.1280
H -2.7450 3.1890 0.6140
H -7.6370 -3.2490 -2.1880
H -7.1390 -0.6220 -0.7020
H -9.4930 -0.8540 -1.6560
H -9.8940 -2.2730 -2.6360
H -9.6420 -2.4440 -0.8910
H -7.4920 -1.6710 -2.9520
H -7.2550 -2.2120 0.0500

H -4.3360 -3.6100 0.5040
H -5.6410 -2.7280 1.2820
H -4.2010 -1.7230 2.9000
H -2.9610 -4.4710 2.4130
H -3.6710 -2.9910 5.0160
H -2.0380 -3.1050 4.3520
H -2.4590 -0.9820 0.0560
H -3.1780 -0.8950 -1.5440
H -1.1380 -4.7450 -2.5920
H -0.2510 -4.5060 -1.0760
H -0.5270 -2.0150 -1.3170
H -3.1910 -3.4840 -1.6090
H -5.3040 -2.9710 -1.4190
H -5.1800 -1.3260 -2.0330
H 1.1710 -1.9190 -4.0270
H 6.6500 1.4190 2.2780
H 6.3490 -4.0620 -0.9760
C 1.7020 -0.1100 1.7570
C 1.0260 -1.0630 0.8860
C 0.4030 -2.3280 1.4290
C 0.2960 -2.3250 2.9580
C 1.5680 -1.7960 3.6230
C 1.7940 -0.3310 3.2400
O 2.4820 -1.0290 0.9400
H 1.7590 0.9200 1.4190
Br -1.6560 0.8130 1.7800
H 0.6400 -0.6750 -0.0530
H -0.5960 -2.4320 0.9940
H 0.9970 -3.1800 1.0760
H 0.0650 -3.3360 3.3130
H -0.5400 -1.6690 3.2350
H 1.4860 -1.8790 4.7120
H 2.4320 -2.3990 3.3170
H 1.0140 0.2960 3.6880
H 2.7630 0.0340 3.6010
Mg 3.7230 -0.3730 -0.6330

TS1_Mg cat. 3'

C 1.7810 1.6290 -1.4540
C 0.6280 1.8930 -2.2940
N 2.1690 0.3320 -1.6190
C 1.3230 -0.2330 -2.5270
C 0.3420 0.7370 -2.9490
C 2.4210 2.5760 -0.6250
H 0.1210 2.8430 -2.3850
C 6.3070 0.3890 1.3080
C 3.5870 2.3410 0.1290
H -0.4420 0.5580 -3.6740
N 4.2760 1.1650 0.1690
C 4.2320 3.3060 1.0030
C 5.3360 1.3460 1.0050
C 5.3180 2.6900 1.5350
C 6.3880 -0.9170 0.8270
N 5.4760 -1.5040 0.0020
C 5.9290 -2.7610 -0.2590
C 7.4610 -1.8460 1.1140
C 7.1780 -2.9890 0.4380
C 1.4060 -1.5410 -3.0090
C 2.3710 -2.4990 -2.7010
N 3.3790 -2.3340 -1.7990
C 4.1330 -3.4690 -1.8330
C 2.4810 -3.8010 -3.3260
C 3.5700 -4.4040 -2.7830
C 5.3000 -3.6790 -1.0980
H 3.8950 4.3150 1.1880
H 6.0410 3.0970 2.2300
H 8.3170 -1.6350 1.7430
H 7.7540 -3.9050 0.4010
H 1.8190 -4.1840 -4.0940
H 3.9780 -5.3810 -3.0110
C -4.6000 2.5370 0.3580
C -4.5880 3.7960 -0.5130

C -3.7000 4.9110 0.0480
C -2.2520 4.4480 0.1560
C 1.8220 3.9420 -0.5750
C 0.4990 4.1000 -0.1470
C -0.0960 5.3620 -0.1710
C 0.6490 6.4820 -0.5530
C 1.9690 6.3240 -0.9500
C 2.5540 5.0600 -0.9830
C -9.7050 -1.2250 -1.7310
C -8.2230 -1.3900 -2.0580
C -7.3420 -1.3110 -0.8060
H -3.1100 -2.0310 1.9100
C -5.0680 -2.3100 0.9780
C -4.1560 -2.1910 2.1950
C -4.2810 -3.4580 3.0480
C -3.6030 -3.3170 4.4080
H -5.3440 -3.6910 3.1960
H -3.6960 -4.2420 4.9870
O -1.4010 5.5860 0.1350
H -0.0440 3.2200 0.1880
H 3.5740 4.9350 -1.3330
H 2.5410 7.1920 -1.2630
H 0.1690 7.4550 -0.5540
C -4.9650 1.2740 -0.4270
C -4.9680 0.0930 0.5310
N -4.8530 -1.2770 -0.1050
C -3.4680 -1.4080 -0.7320
C -0.9940 -4.1840 -1.7550
C -1.6380 -2.8010 -1.7140
C -2.9740 -2.8290 -0.9610
H -0.0230 -4.1500 -2.2540
H -1.7940 -2.4210 -2.7310
H -2.8170 -3.3350 -0.0010
H -4.2080 1.1390 -1.2080
H -5.9350 1.3880 -0.9250
H -5.8760 0.0860 1.1390

H -4.1090 0.1750 1.2000
C -5.8800 -1.4720 -1.1990
H -3.6060 2.3600 0.7830
H -5.2860 2.6740 1.2040
H -4.2140 3.5380 -1.5140
H -5.6100 4.1660 -0.6530
H -4.0680 5.2530 1.0230
H -3.7290 5.7710 -0.6290
H -2.0090 3.8020 -0.7000
H -2.0670 3.8620 1.0650
H -8.0590 -2.3540 -2.5560
H -7.5110 -0.3450 -0.3160
H -9.8970 -0.2530 -1.2640
H -10.3150 -1.2890 -2.6370
H -10.0450 -2.0040 -1.0400
H -7.9140 -0.6130 -2.7690
H -7.6550 -2.0910 -0.1050
H -4.9640 -3.2870 0.5020
H -6.1060 -2.2090 1.2970
H -4.4480 -1.3250 2.7980
H -3.8500 -4.3070 2.5010
H -4.0560 -2.5070 4.9900
H -2.5380 -3.0930 4.2960
H -2.7710 -0.8600 -0.0920
H -3.5130 -0.8740 -1.6840
H -1.6320 -4.9050 -2.2780
H -0.8240 -4.5580 -0.7390
H -0.9520 -2.0960 -1.2290
H -3.6960 -3.4290 -1.5270
H -5.7050 -2.4700 -1.6090
H -5.6280 -0.7470 -1.9750
H 0.6570 -1.8300 -3.7430
H 7.1000 0.7070 1.9800
H 5.7880 -4.6420 -1.2230
C 1.6680 -0.2940 1.7880
C 0.5610 -0.8580 0.9870

C -0.0520 -2.1640 1.4170
C -0.1940 -2.2740 2.9360
C 1.1110 -1.9150 3.6530
C 1.5590 -0.4970 3.2910
O 2.4710 -1.2240 1.1320
H 1.8950 0.7540 1.5480
Br -1.3100 0.7160 1.3810
H 0.5380 -0.5880 -0.0610
H -1.0200 -2.2920 0.9250
H 0.6010 -2.9580 1.0370
H -0.5120 -3.2900 3.1970
H -0.9810 -1.5810 3.2600
H 0.9740 -1.9970 4.7380
H 1.8940 -2.6290 3.3700
H 0.8360 0.2330 3.6750
H 2.5310 -0.2740 3.7450
Mg 3.5740 -0.7200 -0.4580

I1_Mg cat. 3'

C 1.8550 1.5830 -1.4990
C 0.6980 1.8290 -2.3410
N 2.2410 0.2830 -1.6310
C 1.3870 -0.3060 -2.5150
C 0.4050 0.6550 -2.9600
C 2.5010 2.5490 -0.6960
H 0.1940 2.7780 -2.4600
C 6.3560 0.3830 1.3240
C 3.6660 2.3260 0.0650
H -0.3820 0.4570 -3.6780
N 4.3550 1.1520 0.1230
C 4.2990 3.3030 0.9350
C 5.3980 1.3410 0.9780
C 5.3750 2.6920 1.4910
C 6.4280 -0.9390 0.8850
N 5.5200 -1.5390 0.0680
C 5.9550 -2.8100 -0.1460

C 7.4860 -1.8730 1.2160
C 7.1940 -3.0340 0.5730
C 1.4580 -1.6290 -2.9610
C 2.4140 -2.5880 -2.6230
N 3.4220 -2.4020 -1.7280
C 4.1590 -3.5470 -1.7140
C 2.5060 -3.9150 -3.1990
C 3.5880 -4.5110 -2.6310
C 5.3190 -3.7480 -0.9610
H 3.9580 4.3150 1.1010
H 6.0890 3.1060 2.1930
H 8.3390 -1.6520 1.8460
H 7.7580 -3.9590 0.5720
H 1.8410 -4.3170 -3.9530
H 3.9830 -5.5010 -2.8210
C -4.5250 2.5570 0.4840
C -4.5260 3.8430 -0.3490
C -3.5950 4.9280 0.2010
C -2.1480 4.4480 0.2220
C 1.9030 3.9150 -0.6540
C 0.5910 4.0800 -0.1910
C 0.0030 5.3450 -0.1890
C 0.7390 6.4620 -0.5930
C 2.0450 6.2980 -1.0320
C 2.6250 5.0320 -1.0810
C -9.7740 -0.9360 -1.6540
C -8.3060 -1.1430 -2.0190
C -7.4000 -1.1380 -0.7820
H -3.1670 -2.2050 1.8310
C -5.1430 -2.3140 0.9100
C -4.2180 -2.3000 2.1220
C -4.4190 -3.5900 2.9250
C -3.7280 -3.5460 4.2850
H -5.4940 -3.7620 3.0710
H -3.8680 -4.4880 4.8230
O -1.2880 5.5760 0.1770

H 0.0570 3.2030 0.1590
H 3.6360 4.9040 -1.4550
H 2.6110 7.1640 -1.3610
H 0.2640 7.4380 -0.5750
C -4.9340 1.3290 -0.3330
C -4.9600 0.1090 0.5770
N -4.9010 -1.2340 -0.1210
C -3.5310 -1.3790 -0.7760
C -1.1640 -4.1350 -2.0700
C -1.7760 -2.7480 -1.9060
C -3.0890 -2.7950 -1.1130
H -0.2160 -4.0790 -2.6100
H -1.9600 -2.2950 -2.8880
H -2.9250 -3.3740 -0.1970
H -4.1970 1.2040 -1.1330
H -5.9090 1.4880 -0.8090
H -5.8580 0.1060 1.2000
H -4.0930 0.1310 1.2390
C -5.9510 -1.3400 -1.2080
H -3.5190 2.3600 0.8710
H -5.1780 2.6740 1.3590
H -4.2040 3.6070 -1.3730
H -5.5470 4.2320 -0.4290
H -3.9090 5.2440 1.2030
H -3.6480 5.8080 -0.4480
H -1.9560 3.8110 -0.6540
H -1.9270 3.8500 1.1160
H -8.1870 -2.0950 -2.5520
H -7.5240 -0.1840 -0.2580
H -9.9220 0.0260 -1.1530
H -10.4040 -0.9500 -2.5490
H -10.1280 -1.7240 -0.9810
H -7.9830 -0.3540 -2.7100
H -7.7290 -1.9300 -0.1030
H -5.0850 -3.2670 0.3810
H -6.1730 -2.1870 1.2480

H -4.4480 -1.4420 2.7610
H -4.0440 -4.4400 2.3410
H -4.1330 -2.7390 4.9050
H -2.6530 -3.3760 4.1760
H -2.8080 -0.9000 -0.1140
H -3.5690 -0.7820 -1.6890
H -1.8360 -4.8050 -2.6190
H -0.9580 -4.5850 -1.0930
H -1.0560 -2.0950 -1.3980
H -3.8450 -3.3280 -1.7020
H -5.8230 -2.3270 -1.6600
H -5.6820 -0.5950 -1.9590
H 0.7060 -1.9310 -3.6860
H 7.1400 0.7120 2.0010
H 5.7930 -4.7220 -1.0470
C 1.5490 -0.3010 1.6960
C 0.2330 -0.6760 0.9810
C -0.2620 -2.0530 1.3900
C -0.3800 -2.2100 2.9060
C 0.9280 -1.8340 3.6120
C 1.3840 -0.4270 3.2210
O 2.4920 -1.1700 1.2120
H 1.7660 0.7600 1.4600
Br -1.2070 0.7030 1.3730
H 0.3480 -0.5720 -0.0960
H -1.2070 -2.2970 0.8940
H 0.4910 -2.7500 1.0040
H -0.6560 -3.2450 3.1410
H -1.1930 -1.5670 3.2710
H 0.8000 -1.9120 4.6990
H 1.7090 -2.5440 3.3220
H 0.6630 0.3190 3.5840
H 2.3520 -0.1990 3.6820
Mg 3.5790 -0.7770 -0.3520

I2_Mg cat. 3'

C	1.5640	1.9500	-1.4680
C	0.3910	2.1520	-2.3000
N	2.0390	0.6860	-1.6570
C	1.2250	0.0800	-2.5650
C	0.1750	0.9870	-2.9660
C	2.1460	2.9210	-0.6200
H	-0.1740	3.0690	-2.3810
C	6.1480	0.9300	1.2990
C	3.3160	2.7360	0.1460
H	-0.5990	0.7650	-3.6900
N	4.0750	1.6030	0.1620
C	3.8840	3.7140	1.0570
C	5.1090	1.8260	1.0190
C	4.9970	3.1490	1.5920
C	6.3350	-0.3440	0.7610
N	5.4780	-0.9630	-0.0960
C	6.0410	-2.1560	-0.4290
C	7.4880	-1.1890	1.0010
C	7.3070	-2.3120	0.2590
C	1.3950	-1.2100	-3.0850
C	2.4360	-2.1010	-2.8220
N	3.4480	-1.8820	-1.9390
C	4.2930	-2.9450	-2.0280
C	2.6340	-3.3710	-3.4910
C	3.7860	-3.8960	-2.9960
C	5.4870	-3.0860	-1.3130
H	3.4800	4.6950	1.2610
H	5.6850	3.5780	2.3100
H	8.3240	-0.9350	1.6420
H	7.9640	-3.1690	0.1700
H	1.9820	-3.7840	-4.2510
H	4.2670	-4.8280	-3.2640
C	-4.7550	2.4150	0.4830
C	-4.8870	3.7250	-0.2980
C	-4.0590	4.8720	0.2930

C -2.5780 4.5160 0.3040
C 1.4780 4.2530 -0.5360
C 0.1590 4.3350 -0.0760
C -0.4990 5.5650 -0.0460
C 0.1780 6.7320 -0.4100
C 1.4960 6.6500 -0.8390
C 2.1440 5.4190 -0.9210
C -9.8590 -1.3560 -1.6540
C -8.3830 -1.4250 -2.0380
C -7.4680 -1.4330 -0.8080
H -3.1810 -2.2830 1.7860
C -5.1430 -2.4820 0.8420
C -4.2300 -2.4360 2.0620
C -4.3720 -3.7470 2.8430
C -3.6800 -3.6970 4.2020
H -5.4390 -3.9660 2.9880
H -3.7930 -4.6490 4.7300
O -1.8060 5.7050 0.3080
H -0.3300 3.4230 0.2480
H 3.1630 5.3570 -1.2900
H 2.0180 7.5550 -1.1360
H -0.3470 7.6800 -0.3690
C -5.1580 1.1890 -0.3400
C -5.0990 -0.0460 0.5500
N -4.9640 -1.3720 -0.1710
C -3.5920 -1.4280 -0.8350
C -1.0650 -4.0140 -2.1850
C -1.7600 -2.6700 -1.9950
C -3.0730 -2.8090 -1.2110
H -0.1150 -3.8870 -2.7110
H -1.9650 -2.2070 -2.9690
H -2.8790 -3.4040 -0.3120
H -4.4590 1.1080 -1.1800
H -6.1600 1.3160 -0.7650
H -5.9940 -0.1140 1.1720
H -4.2350 0.0170 1.2130

C -6.0130 -1.5160 -1.2530
H -3.7140 2.2600 0.7860
H -5.3440 2.4710 1.4080
H -4.5520 3.5610 -1.3320
H -5.9410 4.0170 -0.3570
H -4.4010 5.1240 1.3040
H -4.1910 5.7660 -0.3250
H -2.3350 3.9330 -0.5980
H -2.3130 3.9000 1.1730
H -8.1980 -2.3270 -2.6340
H -7.6480 -0.5210 -0.2270
H -10.0750 -0.4450 -1.0840
H -10.4940 -1.3540 -2.5440
H -10.1460 -2.2150 -1.0370
H -8.1270 -0.5690 -2.6760
H -7.7380 -2.2830 -0.1740
H -5.0240 -3.4210 0.2980
H -6.1810 -2.4250 1.1750
H -4.5100 -1.6010 2.7120
H -3.9630 -4.5700 2.2450
H -4.1060 -2.9080 4.8310
H -2.6100 -3.4960 4.0930
H -2.8920 -0.9320 -0.1590
H -3.6630 -0.8070 -1.7300
H -1.6890 -4.7100 -2.7560
H -0.8400 -4.4740 -1.2160
H -1.0820 -1.9890 -1.4690
H -3.7970 -3.3660 -1.8180
H -5.8210 -2.4750 -1.7400
H -5.8040 -0.7270 -1.9780
H 0.6560 -1.5330 -3.8150
H 6.9080 1.2800 1.9930
H 6.0520 -3.9990 -1.4820
C 1.4390 -0.1700 1.5780
C 0.1070 -0.5680 0.9120
C -0.2950 -1.9830 1.2820

C -0.3580 -2.1980 2.7960
C 0.9500 -1.7810 3.4800
C 1.3530 -0.3530 3.1040
O 2.3870 -0.9840 1.0080
H 1.6070 0.9030 1.3690
Br -1.3650 0.7230 1.4320
H 0.1690 -0.4130 -0.1640
H -1.2370 -2.2690 0.8050
H 0.4940 -2.6040 0.8430
H -0.5780 -3.2530 3.0020
H -1.1900 -1.6100 3.2090
H 0.8450 -1.8760 4.5680
H 1.7500 -2.4620 3.1760
H 0.6280 0.3600 3.5200
H 2.3330 -0.1090 3.5280
C 3.0650 -3.8230 0.9450
O 2.2070 -4.1530 0.2260
O 3.9360 -3.6090 1.6880
Mg 3.4820 -0.3390 -0.4730

TS2_Mg cat. 3'
C 1.7060 1.7830 -1.6480
C 0.5450 2.0540 -2.4730
N 2.0610 0.4730 -1.7840
C 1.1790 -0.0970 -2.6550
C 0.2180 0.8880 -3.0890
C 2.3780 2.7350 -0.8520
H 0.0590 3.0140 -2.5770
C 6.2770 0.5170 1.0240
C 3.5670 2.4980 -0.1320
H -0.5850 0.7080 -3.7940
N 4.2420 1.3140 -0.0990
C 4.2490 3.4660 0.7090
C 5.3240 1.4890 0.7100
C 5.3430 2.8420 1.2160
C 6.3000 -0.8140 0.6080

N 5.3480 -1.4040 -0.1660
C 5.7350 -2.6940 -0.3640
C 7.3360 -1.7740 0.9260
C 6.9880 -2.9390 0.3200
C 1.1960 -1.4300 -3.0780
C 2.1240 -2.4150 -2.7370
N 3.1640 -2.2410 -1.8760
C 3.8650 -3.4100 -1.8530
C 2.1540 -3.7590 -3.2760
C 3.2320 -4.3760 -2.7250
C 5.0430 -3.6280 -1.1360
H 3.9300 4.4830 0.8860
H 6.0920 3.2490 1.8850
H 8.2140 -1.5670 1.5250
H 7.5200 -3.8820 0.3260
H 1.4560 -4.1600 -4.0010
H 3.5870 -5.3850 -2.8980
C -4.5900 2.4600 0.9500
C -4.6580 3.8060 0.2100
C -3.6740 4.8630 0.7170
C -2.2270 4.4350 0.4960
C 1.7560 4.0870 -0.7300
C 0.4710 4.1880 -0.1830
C -0.1490 5.4300 -0.0590
C 0.5290 6.5900 -0.4450
C 1.8060 6.4890 -0.9790
C 2.4190 5.2460 -1.1360
C -10.0340 -0.6150 -0.9430
C -8.6230 -0.7590 -1.5100
C -7.5860 -0.9990 -0.4070
H -3.1720 -2.8810 1.3320
C -5.2500 -2.4610 0.8590
C -4.1290 -2.7530 1.8470
C -4.4540 -4.0370 2.6180
C -3.3580 -4.4130 3.6120
H -5.4070 -3.9110 3.1480

H -3.6270 -5.3180 4.1640
O -1.4130 5.5950 0.4210
H -0.0200 3.2760 0.1350
H 3.4090 5.1730 -1.5760
H 2.3260 7.3890 -1.2920
H 0.0360 7.5510 -0.3340
C -4.9640 1.2960 0.0270
C -4.9470 -0.0180 0.7940
N -5.0450 -1.2740 -0.0560
C -3.7620 -1.4050 -0.8620
C -1.7970 -3.9700 -2.9700
C -2.1700 -2.6480 -2.3070
C -3.4910 -2.7440 -1.5320
H -0.8420 -3.8800 -3.4960
H -2.2480 -1.8590 -3.0650
H -3.4070 -3.5470 -0.7920
H -4.2330 1.2750 -0.7890
H -5.9480 1.4810 -0.4180
H -5.7650 -0.0580 1.5160
H -4.0070 -0.1020 1.3410
C -6.2080 -1.1970 -1.0250
H -3.5790 2.2790 1.3320
H -5.2480 2.4800 1.8280
H -4.4520 3.6400 -0.8560
H -5.6800 4.1990 0.2640
H -3.8480 5.0870 1.7760
H -3.8350 5.7930 0.1610
H -2.1420 3.8720 -0.4460
H -1.8700 3.7800 1.3020
H -8.5950 -1.5890 -2.2260
H -7.5920 -0.1420 0.2750
H -10.0890 0.2190 -0.2350
H -10.7580 -0.4270 -1.7410
H -10.3410 -1.5250 -0.4160
H -8.3550 0.1470 -2.0680
H -7.8840 -1.8790 0.1720

H -5.4220 -3.3220 0.2080
H -6.1750 -2.2680 1.4040
H -4.0040 -1.9290 2.5560
H -4.5990 -4.8590 1.9050
H -3.1910 -3.6110 4.3380
H -2.4100 -4.6030 3.0960
H -2.9460 -1.1470 -0.1890
H -3.8010 -0.6200 -1.6190
H -2.5570 -4.2790 -3.6960
H -1.6910 -4.7660 -2.2260
H -1.3640 -2.3410 -1.6280
H -4.2950 -3.0210 -2.2240
H -6.1860 -2.1250 -1.6010
H -5.9780 -0.3790 -1.7100
H 0.4200 -1.7180 -3.7830
H 7.0920 0.8360 1.6690
H 5.4830 -4.6190 -1.2120
C 1.3770 -0.0710 1.4320
C 0.1370 -0.6170 0.7010
C -0.3980 -1.8840 1.3430
C -0.7200 -1.6930 2.8250
C 0.5150 -1.1900 3.5780
C 1.0990 0.0730 2.9350
O 2.3970 -0.9630 1.0950
H 1.5980 0.9330 1.0390
Br -1.2870 0.8000 0.6560
H 0.3550 -0.7520 -0.3560
H -1.2570 -2.2690 0.7830
H 0.4080 -2.6200 1.2350
H -1.0690 -2.6380 3.2540
H -1.5400 -0.9700 2.9280
H 0.2620 -0.9850 4.6250
H 1.2640 -1.9890 3.5930
H 0.3830 0.8960 3.0550
H 2.0250 0.3680 3.4350
C 3.4000 -1.9970 2.3330

O 3.2200 -3.1120 1.9540

O 3.9040 -1.2300 3.0930

Mg 3.4490 -0.5930 -0.5800

I3a_Mg cat. 3' (1,2-diaxial conformation)

C -2.4640 0.6620 2.6110

C -1.9820 0.6630 3.9780

N -2.7410 -0.6150 2.2280

C -2.4460 -1.4270 3.2780

C -2.0000 -0.6300 4.4000

C -2.6570 1.8080 1.8190

H -1.6950 1.5430 4.5380

C -4.4230 0.3350 -2.4500

C -3.2710 1.8250 0.5520

H -1.7220 -1.0180 5.3720

N -3.5970 0.7190 -0.1740

C -3.6360 3.0160 -0.1880

C -4.1150 1.1500 -1.3550

C -4.1930 2.5940 -1.3540

C -4.2600 -1.0480 -2.5440

N -3.8000 -1.8530 -1.5470

C -3.8260 -3.1320 -2.0130

C -4.5770 -1.8500 -3.7080

C -4.3030 -3.1410 -3.3810

C -2.4840 -2.8250 3.2490

C -2.7210 -3.6420 2.1420

N -2.9880 -3.1990 0.8810

C -3.1460 -4.2960 0.0900

C -2.6980 -5.0900 2.1520

C -2.9520 -5.4950 0.8780

C -3.4970 -4.2650 -1.2630

H -3.4950 4.0330 0.1500

H -4.5910 3.1990 -2.1600

H -4.9690 -1.4660 -4.6420

H -4.4240 -4.0260 -3.9930

H -2.5170 -5.7050 3.0250

H -3.0240 -6.5070 0.5000
C 3.9310 1.5240 0.3930
C 4.4530 2.4980 1.4480
C 3.5660 3.7440 1.5920
C 2.1060 3.3680 1.7900
C -2.0220 3.0810 2.2850
C -0.6360 3.1680 2.1050
C 0.0470 4.3370 2.4350
C -0.6590 5.4220 2.9690
C -2.0300 5.3220 3.1600
C -2.7230 4.1570 2.8210
C 8.3590 -3.9470 -0.3770
C 7.0750 -3.8120 0.4390
C 6.0520 -2.8990 -0.2450
H 1.0000 -1.9640 -0.8210
C 2.9460 -2.9170 -0.9440
C 1.6810 -2.3570 -1.5780
C 0.9240 -3.4370 -2.3570
C -0.2910 -2.8470 -3.0740
H 1.5930 -3.9210 -3.0820
H -0.8740 -3.6280 -3.5710
O 1.3860 4.4990 2.2630
H -0.1250 2.3110 1.6790
H -3.7970 4.0890 2.9650
H -2.5700 6.1670 3.5790
H -0.1190 6.3280 3.2240
C 4.8240 0.3030 0.1530
C 4.1080 -0.7580 -0.6980
N 3.6470 -1.9960 0.0430
C 2.7070 -1.5820 1.1650
C 0.7520 -3.2910 4.0150
C 1.2420 -2.1710 3.1020
C 2.0410 -2.7230 1.9160
H 0.1610 -2.8880 4.8420
H 1.8710 -1.4810 3.6800
H 1.3560 -3.2740 1.2620

H 5.1620 -0.1120 1.1090
H 5.7370 0.6060 -0.3710
H 4.7300 -1.1150 -1.5190
H 3.2060 -0.3270 -1.1340
C 4.8230 -2.7450 0.6420
H 2.9310 1.1810 0.6810
H 3.8050 2.0580 -0.5560
H 4.5090 1.9810 2.4160
H 5.4760 2.8090 1.2010
H 3.6500 4.3720 0.6970
H 3.9040 4.3410 2.4460
H 2.0120 2.5470 2.5170
H 1.6740 3.0220 0.8450
H 6.6300 -4.8020 0.5970
H 6.5170 -1.9240 -0.4280
H 8.8370 -2.9720 -0.5220
H 9.0750 -4.6020 0.1280
H 8.1540 -4.3730 -1.3660
H 7.3110 -3.4110 1.4320
H 5.7910 -3.3260 -1.2200
H 2.7200 -3.8330 -0.3950
H 3.6840 -3.1650 -1.7100
H 1.9270 -1.5390 -2.2640
H 0.5950 -4.2160 -1.6580
H 0.0210 -2.1220 -3.8360
H -0.9460 -2.3290 -2.3670
H 1.9550 -0.9090 0.7450
H 3.3180 -0.9940 1.8550
H 1.5960 -3.8480 4.4400
H 0.1190 -3.9950 3.4640
H 0.3940 -1.5880 2.7270
H 2.7850 -3.4360 2.2910
H 4.4420 -3.7280 0.9250
H 5.0950 -2.2250 1.5630
H -2.2600 -3.3330 4.1830
H -4.8100 0.8380 -3.3320

H -3.5810 -5.2240 -1.7670
C -0.3120 0.1540 -0.3710
O 0.5840 0.6410 0.3360
O -0.9030 -0.9490 -0.2010
C 1.3010 1.9120 -2.1950
C -0.1590 2.1010 -1.7610
H 1.8300 1.3700 -1.4170
H -0.1990 2.6930 -0.8420
C -0.9950 2.7480 -2.8580
H -0.6540 3.7850 -2.9690
H -2.0330 2.7780 -2.5240
O -0.7170 0.8100 -1.5060
Br 2.1860 3.6810 -2.1860
C -0.8700 2.0140 -4.1960
H -1.4580 2.5370 -4.9580
H -1.2990 1.0090 -4.0940
C 1.4370 1.2390 -3.5530
H 1.0820 0.2080 -3.4170
H 2.4930 1.1850 -3.8400
C 0.5930 1.9100 -4.6380
H 0.9920 2.9130 -4.8350
H 0.6760 1.3420 -5.5710
Mg -2.8600 -1.2120 0.2170

TS3a_Mg cat. 3' (1,2-diaxial conformation)
C -2.1650 0.8250 2.6120
C -1.5760 0.7550 3.9340
N -2.5830 -0.4150 2.2360
C -2.2770 -1.2730 3.2490
C -1.6710 -0.5400 4.3380
C -2.3130 2.0020 1.8500
H -1.1730 1.5960 4.4830
C -4.7470 0.8200 -2.1760
C -3.0450 2.1110 0.6550
H -1.3550 -0.9670 5.2810
N -3.6390 1.0720 -0.0000

C -3.2480 3.3360 -0.0950
C -4.1770 1.5730 -1.1440
C -3.9750 3.0040 -1.1940
C -4.8130 -0.5710 -2.2710
N -4.3230 -1.4420 -1.3460
C -4.5770 -2.7010 -1.8000
C -5.3990 -1.3090 -3.3710
C -5.2490 -2.6290 -3.0810
C -2.4510 -2.6600 3.2080
C -2.9180 -3.4230 2.1370
N -3.3220 -2.9230 0.9340
C -3.7190 -3.9780 0.1700
C -3.0490 -4.8650 2.1310
C -3.5370 -5.2090 0.9090
C -4.2730 -3.8780 -1.1110
H -2.8840 4.3140 0.1880
H -4.3210 3.6580 -1.9850
H -5.8660 -0.8660 -4.2410
H -5.5700 -3.4820 -3.6660
H -2.8040 -5.5170 2.9600
H -3.7730 -6.1990 0.5380
C 4.0760 1.1250 0.0570
C 4.7960 1.9700 1.1110
C 4.0730 3.2880 1.4280
C 2.6030 3.0510 1.7250
C -1.5230 3.1920 2.2910
C -0.1340 3.1200 2.1240
C 0.6800 4.2000 2.4640
C 0.1000 5.3580 2.9950
C -1.2750 5.4210 3.1680
C -2.0950 4.3460 2.8180
C 8.1180 -4.5050 -0.8240
C 6.9630 -4.1910 0.1240
C 5.8500 -3.3970 -0.5690
H 0.7500 -2.4880 -0.6830
C 2.7190 -3.3720 -0.9630

C 1.3730 -2.8930 -1.4840
C 0.6160 -4.0490 -2.1460
C -0.7460 -3.5990 -2.6740
H 1.2150 -4.4700 -2.9640
H -1.2830 -4.4340 -3.1350
O 2.0300 4.2070 2.3130
H 0.2790 2.2060 1.7140
H -3.1710 4.4050 2.9530
H -1.7170 6.3220 3.5830
H 0.7420 6.1930 3.2570
C 4.8220 -0.1590 -0.3280
C 3.9180 -1.2050 -1.0050
N 3.5170 -2.3810 -0.1290
C 2.6880 -1.8540 1.0290
C 0.8390 -3.2550 4.1140
C 1.3310 -2.2330 3.0920
C 2.0990 -2.9090 1.9530
H 0.2840 -2.7660 4.9190
H 1.9770 -1.4990 3.5890
H 1.4090 -3.5640 1.4090
H 5.3130 -0.5760 0.5580
H 5.6360 0.0840 -1.0190
H 4.3910 -1.6390 -1.8860
H 2.9790 -0.7470 -1.3170
C 4.7300 -3.1070 0.4220
H 3.0860 0.8500 0.4370
H 3.9090 1.7360 -0.8390
H 4.8910 1.3790 2.0330
H 5.8170 2.1910 0.7760
H 4.1440 3.9760 0.5780
H 4.5470 3.7690 2.2910
H 2.4710 2.1910 2.4010
H 2.0750 2.8410 0.7900
H 6.5500 -5.1250 0.5250
H 6.2740 -2.4670 -0.9610
H 8.5630 -3.5860 -1.2200

H 8.9050 -5.0640 -0.3090
H 7.7770 -5.1070 -1.6730
H 7.3350 -3.6180 0.9820
H 5.4800 -3.9740 -1.4240
H 2.5840 -4.2520 -0.3320
H 3.3680 -3.6610 -1.7940
H 1.5050 -2.0880 -2.2150
H 0.4750 -4.8540 -1.4130
H -0.6340 -2.8120 -3.4290
H -1.3670 -3.1970 -1.8680
H 1.9020 -1.2330 0.5920
H 3.3550 -1.2010 1.5970
H 1.6790 -3.7970 4.5640
H 0.1730 -3.9860 3.6440
H 0.4790 -1.6800 2.6800
H 2.8860 -3.5410 2.3800
H 4.3580 -4.0410 0.8440
H 5.1100 -2.5080 1.2520
H -2.1700 -3.2060 4.1040
H -5.1500 1.3810 -3.0150
H -4.5400 -4.8110 -1.5990
C -0.4790 0.0070 -0.8470
O 0.7710 0.1240 -0.6990
O -1.1820 -0.9420 -0.4520
C 1.1920 1.7860 -1.7620
C -0.2840 2.1800 -1.7230
H 1.8160 1.9410 -0.9120
H -0.4660 2.8460 -0.8740
C -0.7770 2.7910 -3.0310
H -0.3730 3.8020 -3.1100
H -1.8670 2.8600 -2.9660
O -1.0810 0.9960 -1.5310
Br 2.1640 4.1210 -2.0000
C -0.3520 1.9500 -4.2380
H -0.7160 2.4230 -5.1560
H -0.8280 0.9630 -4.1790

C 1.7320 1.1630 -3.0220
H 1.4350 0.1070 -3.0010
H 2.8250 1.1990 -3.0120
C 1.1700 1.7930 -4.3050
H 1.6360 2.7730 -4.4440
H 1.4520 1.1640 -5.1570
Mg -3.1050 -0.9400 0.2790

I4a_Mg cat. 3' (1,2-diaxial conformation)
C 2.2110 0.7170 -2.3370
C 1.4530 1.0570 -3.5250
N 2.1140 -0.6210 -2.1020
C 1.2860 -1.1350 -3.0540
C 0.8910 -0.0930 -3.9740
C 2.9150 1.6400 -1.5410
H 1.3700 2.0470 -3.9520
C 5.2800 -0.9380 1.8310
C 3.7720 1.3030 -0.4750
H 0.2520 -0.2320 -4.8370
N 4.0030 0.0350 -0.0300
C 4.5100 2.2430 0.3450
C 4.8480 0.1280 1.0370
C 5.1910 1.5120 1.2660
C 4.8890 -2.2770 1.7410
N 3.9770 -2.7660 0.8550
C 3.8260 -4.0930 1.1230
C 5.3530 -3.3440 2.6010
C 4.6940 -4.4700 2.2180
C 0.8340 -2.4550 -3.1110
C 1.1660 -3.4990 -2.2440
N 2.0160 -3.3930 -1.1850
C 2.1320 -4.6340 -0.6320
C 0.7010 -4.8640 -2.3580
C 1.2990 -5.5670 -1.3580
C 2.9590 -4.9550 0.4460
H 4.5110 3.3170 0.2250

H 5.8580 1.8710 2.0410
H 6.0890 -3.2360 3.3880
H 4.7800 -5.4670 2.6320
H 0.0230 -5.2300 -3.1190
H 1.2020 -6.6220 -1.1340
C -3.5400 2.8420 0.4900
C -3.7680 4.0660 -0.4040
C -2.5820 5.0420 -0.4440
C -1.2850 4.3330 -0.8080
C 2.5960 3.0880 -1.7400
C 1.2800 3.4850 -1.4560
C 0.9170 4.8290 -1.5330
C 1.8650 5.7840 -1.9210
C 3.1590 5.3820 -2.2220
C 3.5350 4.0400 -2.1320
C -9.2210 -0.6640 2.5870
C -8.4180 -0.6240 1.2890
C -6.9190 -0.8340 1.5300
H -2.1410 -1.7130 0.3100
C -4.1810 -2.0150 1.0560
C -2.6600 -2.1540 1.1680
C -2.2610 -3.6270 1.3060
C -0.7470 -3.8140 1.3410
H -2.7180 -4.0520 2.2100
H -0.4840 -4.8730 1.4230
O -0.3300 5.2930 -1.2420
H 0.5660 2.7140 -1.1830
H 4.5510 3.7360 -2.3610
H 3.8880 6.1250 -2.5310
H 1.5700 6.8270 -1.9810
C -4.5940 1.7460 0.2760
C -4.1370 0.4360 0.9210
N -4.6690 -0.8250 0.2590
C -4.1500 -0.8620 -1.1800
C -2.8500 -3.3420 -3.8250
C -3.2070 -2.0170 -3.1560

C -3.9520 -2.2240 -1.8290
H -2.3300 -3.1740 -4.7730
H -3.8180 -1.4060 -3.8340
H -3.3300 -2.8730 -1.2070
H -4.6960 1.6120 -0.8050
H -5.5760 2.0530 0.6540
H -4.4150 0.3840 1.9760
H -3.0510 0.3560 0.8380
C -6.1780 -0.8400 0.2000
H -2.5780 2.3920 0.2260
H -3.4930 3.1390 1.5470
H -3.9480 3.7120 -1.4280
H -4.6740 4.6040 -0.0960
H -2.4650 5.5520 0.5200
H -2.7810 5.8160 -1.1940
H -1.4540 3.5820 -1.5930
H -0.8860 3.7950 0.0600
H -8.7890 -1.3950 0.6020
H -6.5500 -0.0330 2.1800
H -8.8820 0.1100 3.2840
H -10.2860 -0.5010 2.3940
H -9.1140 -1.6340 3.0860
H -8.5710 0.3410 0.7900
H -6.7740 -1.7800 2.0620
H -4.6260 -2.8930 0.5830
H -4.6250 -1.9190 2.0480
H -2.2970 -1.5950 2.0370
H -2.6730 -4.1930 0.4590
H -0.3000 -3.2830 2.1870
H -0.2820 -3.4180 0.4330
H -3.1960 -0.3290 -1.1740
H -4.8560 -0.2770 -1.7710
H -3.7450 -3.9390 -4.0340
H -2.1900 -3.9330 -3.1790
H -2.2920 -1.4480 -2.9490
H -4.9040 -2.7430 -2.0000

H -6.4480 -1.7250 -0.3830
H -6.4640 0.0380 -0.3830
H 0.1490 -2.6960 -3.9200
H 5.9820 -0.6920 2.6230
H 2.9450 -5.9910 0.7770
C 0.9600 -0.2230 1.6820
O -0.0140 -0.1390 2.5880
O 1.3400 -1.2750 1.2080
C -0.0170 1.2180 3.1050
C 0.6120 1.9710 1.9320
H -1.0590 1.5020 3.2580
H -0.1300 2.1130 1.1410
C 1.3630 3.2460 2.2440
H 0.6120 4.0420 2.3490
H 1.9740 3.5020 1.3720
O 1.5050 0.9530 1.4250
Br -0.9730 0.5620 -0.8440
C 2.1970 3.1560 3.5210
H 2.6310 4.1360 3.7430
H 3.0320 2.4610 3.3640
C 0.7960 1.2630 4.3990
H 1.6480 0.5810 4.2940
H 0.1860 0.8870 5.2260
C 1.3320 2.6700 4.6860
H 0.5000 3.3690 4.8450
H 1.9100 2.6490 5.6160
Mg 2.7250 -1.6010 -0.3640

I3b_Mg cat. 3' (1,2-diaxial conformation)
C -2.4760 0.2390 2.4950
C -1.6650 -0.2440 3.5950
N -3.1950 -0.8040 1.9780
C -2.8590 -1.9200 2.6880
C -1.8970 -1.5780 3.7050
C -2.5160 1.5710 2.0260
H -1.0140 0.3620 4.2090

C -5.8500 1.7360 -1.5240
C -3.3450 2.0400 0.9840
H -1.4730 -2.2710 4.4200
N -4.2730 1.2960 0.3100
C -3.3320 3.3860 0.4450
C -4.8510 2.1120 -0.6180
C -4.2690 3.4290 -0.5380
C -6.4120 0.4690 -1.6890
N -6.0520 -0.6440 -0.9880
C -6.8000 -1.6790 -1.4640
C -7.4490 0.1310 -2.6400
C -7.6910 -1.2000 -2.4980
C -3.3790 -3.2040 2.4860
C -4.3400 -3.5930 1.5500
N -4.9510 -2.7550 0.6650
C -5.8530 -3.4990 -0.0380
C -4.8640 -4.9320 1.3950
C -5.8000 -4.8740 0.4110
C -6.7090 -3.0040 -1.0260
H -2.6810 4.1840 0.7700
H -4.5400 4.2710 -1.1620
H -7.9220 0.8280 -3.3200
H -8.4000 -1.8120 -3.0410
H -4.5560 -5.7920 1.9760
H -6.4160 -5.6770 0.0250
C 5.8110 -0.0870 2.3240
C 4.3890 0.1330 2.8410
C 3.9840 1.5930 3.0340
C 2.4880 1.6500 3.2790
C -1.5820 2.5510 2.6560
C -0.2070 2.3050 2.6110
C 0.6880 3.1900 3.2140
C 0.2120 4.3540 3.8210
C -1.1540 4.6070 3.8470
C -2.0550 3.7060 3.2860
C 8.9030 -5.3150 -0.5860

C 7.4960 -5.2000 -0.0020
C 6.7630 -3.9530 -0.5060
H 2.3970 -1.5410 -1.7250
C 4.3120 -2.5580 -1.7010
C 3.3990 -1.4290 -2.1540
C 3.3030 -1.4020 -3.6810
C 2.5520 -0.1640 -4.1660
H 4.3090 -1.4150 -4.1210
H 2.4110 -0.1780 -5.2510
O 2.0380 3.0010 3.2210
H 0.1450 1.4370 2.0670
H -3.1230 3.8930 3.3380
H -1.5230 5.5070 4.3310
H 0.9220 5.0380 4.2740
C 5.9340 -1.4630 1.6490
C 5.3050 -1.4130 0.2470
N 4.5570 -2.6590 -0.2090
C 3.2490 -2.7110 0.5620
C 0.0060 -4.7920 0.7920
C 0.9930 -3.6490 1.0190
C 2.2710 -3.8150 0.1860
H -0.9330 -4.6100 1.3230
H 1.2530 -3.6020 2.0850
H 2.0020 -3.7540 -0.8760
H 5.4460 -2.1990 2.2960
H 6.9820 -1.7720 1.5730
H 6.0780 -1.2300 -0.5030
H 4.5830 -0.5940 0.1820
C 5.3480 -3.9160 0.0600
H 6.0680 0.6950 1.5990
H 6.5360 -0.0090 3.1420
H 3.6840 -0.2920 2.1190
H 4.2550 -0.4280 3.7770
H 4.1950 2.1410 2.1100
H 4.5380 2.0660 3.8540
H 2.2250 1.2300 4.2620

H 1.9970 1.0450 2.5150
H 6.9160 -6.0940 -0.2610
H 7.3290 -3.0640 -0.2080
H 9.5110 -4.4420 -0.3220
H 9.4120 -6.2060 -0.2060
H 8.8700 -5.3850 -1.6780
H 7.5530 -5.1680 1.0930
H 6.7410 -3.9740 -1.6010
H 3.9180 -3.5280 -2.0150
H 5.2960 -2.4400 -2.1600
H 3.7670 -0.4640 -1.7970
H 2.7960 -2.3080 -4.0390
H 3.0970 0.7490 -3.9040
H 1.5650 -0.1040 -3.6970
H 2.7580 -1.7360 0.4480
H 3.5320 -2.8200 1.6120
H 0.4190 -5.7450 1.1430
H -0.2330 -4.9090 -0.2710
H 0.5360 -2.6830 0.7770
H 2.6910 -4.8130 0.3600
H 4.7640 -4.7430 -0.3490
H 5.3740 -4.0410 1.1440
H -3.0010 -3.9820 3.1430
H -6.2210 2.5190 -2.1810
H -7.3730 -3.7210 -1.5000
C 2.4030 3.2750 -1.8550
C 1.7670 3.2160 -0.4570
H 3.1410 2.4810 -1.9410
H 2.5420 3.3690 0.2980
C 0.6410 4.2340 -0.2960
H 1.0860 5.2360 -0.2940
H 0.1700 4.0800 0.6790
O 1.1950 1.9240 -0.2800
Br 3.4940 4.9280 -1.9830
C -0.3940 4.1280 -1.4200
H -1.1620 4.8980 -1.2900

H -0.9030 3.1600 -1.3450
C 1.3780 3.2370 -2.9790
H 0.9450 2.2310 -2.9620
H 1.8790 3.3570 -3.9460
C 0.2590 4.2640 -2.7980
H 0.6740 5.2740 -2.9120
H -0.4870 4.1340 -3.5900
O 1.4490 -0.1890 0.2920
C 2.0560 0.8660 0.0010
O 3.2830 1.0810 -0.0690
C -1.7760 -2.0070 -0.9470
C -1.5320 -0.5590 -0.9360
H -1.8190 -2.5210 0.0100
H -1.3630 -0.0740 0.0200
C -0.9970 0.1470 -2.1480
H 0.0660 0.3230 -1.9540
H -1.4790 1.1290 -2.2220
O -2.8740 -1.0770 -1.1100
C -1.1960 -0.6680 -3.4270
H -0.6840 -0.1770 -4.2620
H -2.2610 -0.7050 -3.6830
C -1.4620 -2.8490 -2.1650
H -2.4130 -3.2010 -2.5830
H -0.9110 -3.7400 -1.8470
C -0.6620 -2.0870 -3.2300
H 0.3880 -2.0230 -2.9150
H -0.6780 -2.6470 -4.1720
Mg -4.4190 -0.7740 0.2920

TS3b_Mg cat. 3' (1,2-diaxial conformation)
C 2.5450 0.5960 -2.4040
C 1.6780 0.2880 -3.5300
N 3.2200 -0.5360 -2.0360
C 2.8150 -1.5380 -2.8660
C 1.8390 -1.0360 -3.8000
C 2.6730 1.8590 -1.7950

H 1.0460 0.9940 -4.0440
C 6.0360 1.4210 1.6980
C 3.5390 2.1660 -0.7210
H 1.3620 -1.6130 -4.5840
N 4.4050 1.2820 -0.1430
C 3.6340 3.4460 -0.0530
C 5.0550 1.9520 0.8590
C 4.5740 3.3110 0.9230
C 6.5470 0.1190 1.6960
N 6.1180 -0.8760 0.8760
C 6.8490 -1.9890 1.1770
C 7.5960 -0.3750 2.5600
C 7.7900 -1.6770 2.2350
C 3.2690 -2.8640 -2.8260
C 4.2490 -3.4030 -1.9900
N 4.9210 -2.7080 -1.0320
C 5.8100 -3.5650 -0.4610
C 4.7230 -4.7680 -2.0290
C 5.6970 -4.8710 -1.0800
C 6.7030 -3.2340 0.5620
H 3.0650 4.3290 -0.2990
H 4.9130 4.0640 1.6260
H 8.1180 0.2140 3.3100
H 8.4920 -2.3810 2.6640
H 4.3640 -5.5370 -2.7020
H 6.2890 -5.7370 -0.8240
C -5.8860 1.2980 -1.6620
C -4.5550 1.4290 -2.4070
C -3.8320 2.7590 -2.2020
C -2.4290 2.6470 -2.7700
C 1.8200 2.9630 -2.3220
C 0.4270 2.8670 -2.2420
C -0.3910 3.9050 -2.6890
C 0.1870 5.0570 -3.2230
C 1.5700 5.1570 -3.3120
C 2.3890 4.1200 -2.8730

C -9.9170 -3.6530 0.2180
C -8.6110 -3.6100 -0.5690
C -7.4810 -2.9540 0.2300
H -2.7000 -1.7150 1.4300
C -4.7510 -2.4460 1.3630
C -3.6260 -1.6510 2.0080
C -3.3810 -2.1680 3.4290
C -2.5020 -1.2180 4.2380
H -4.3340 -2.3080 3.9520
H -2.3040 -1.6060 5.2370
O -1.7510 3.8870 -2.5860
H 0.0070 1.9710 -1.7940
H 3.4690 4.1980 -2.9550
H 2.0150 6.0500 -3.7360
H -0.4570 5.8580 -3.5630
C -6.2130 -0.1870 -1.4030
C -5.4750 -0.6420 -0.1420
N -5.0660 -2.1070 -0.0790
C -3.8480 -2.2820 -0.9780
C -1.1880 -4.9090 -1.9280
C -1.9880 -3.6140 -1.9420
C -3.1180 -3.6140 -0.9000
H -0.3660 -4.8710 -2.6520
H -2.4160 -3.4600 -2.9410
H -2.6750 -3.7560 0.0920
H -5.9060 -0.7570 -2.2830
H -7.2910 -0.3480 -1.2880
H -6.0840 -0.4400 0.7390
H -4.5380 -0.0900 -0.0320
C -6.1730 -3.0180 -0.5550
H -5.8420 1.8290 -0.7060
H -6.6960 1.7580 -2.2390
H -3.8780 0.6390 -2.0610
H -4.7250 1.2510 -3.4750
H -3.7640 2.9900 -1.1310
H -4.3660 3.5870 -2.6830

H -2.4430 2.4070 -3.8400
H -1.9200 1.8370 -2.2460
H -8.3120 -4.6290 -0.8490
H -7.7540 -1.9110 0.4470
H -10.2460 -2.6430 0.4840
H -10.7140 -4.1240 -0.3680
H -9.8030 -4.2240 1.1490
H -8.7580 -3.0580 -1.5040
H -7.3740 -3.4630 1.1890
H -4.5380 -3.5210 1.3910
H -5.6780 -2.2770 1.9180
H -3.8970 -0.5890 2.0570
H -2.9070 -3.1550 3.3760
H -2.9830 -0.2350 4.3430
H -1.5340 -1.0600 3.7420
H -3.1670 -1.4640 -0.7240
H -4.2140 -2.1110 -1.9910
H -1.8170 -5.7730 -2.1820
H -0.7520 -5.1020 -0.9410
H -1.3300 -2.7540 -1.7390
H -3.7850 -4.4620 -1.0900
H -5.7720 -4.0310 -0.5300
H -6.3510 -2.7660 -1.6020
H 2.8220 -3.5400 -3.5500
H 6.4620 2.1030 2.4300
H 7.3540 -4.0260 0.9140
C -2.0240 2.4090 2.0530
C -0.9850 2.4100 0.9220
H -2.7650 1.6300 1.8640
H -1.4760 2.6950 -0.0100
C 0.1900 3.3370 1.2040
H -0.1660 4.3670 1.0980
H 0.9420 3.1750 0.4260
O -0.4630 1.0860 0.7930
Br -3.0850 4.0760 1.8890
C 0.7970 3.1300 2.5930

H 1.6020 3.8570 2.7470
H 1.2570 2.1360 2.6480
C -1.4170 2.2800 3.4410
H -1.0260 1.2570 3.5090
H -2.1920 2.3790 4.2030
C -0.2690 3.2680 3.6830
H -0.6700 4.2900 3.6880
H 0.1660 3.0880 4.6720
O -0.7690 -1.0100 0.1420
C -1.2710 0.1470 0.2140
O -2.4070 0.4780 -0.1710
C 1.1520 -1.4980 0.3920
C 1.8280 -0.6250 1.3680
H 1.3320 -1.2710 -0.6470
H 1.8580 0.4320 1.0790
C 1.3710 -0.7940 2.8090
H 0.4040 -0.2860 2.9070
H 2.0790 -0.2810 3.4750
O 2.9790 -1.3420 1.0540
C 1.2350 -2.2670 3.1970
H 0.8310 -2.3490 4.2140
H 2.2310 -2.7240 3.2080
C 0.8280 -2.9120 0.7760
H 1.7360 -3.5020 0.6240
H 0.0770 -3.2880 0.0770
C 0.3410 -3.0280 2.2210
H -0.6800 -2.6300 2.2740
H 0.2870 -4.0890 2.4980
Mg 4.3580 -0.8210 -0.2760

I4b_Mg cat. 3' (1,2-diaxial conformation)
C 2.3260 0.2820 -2.4650
C 1.3680 -0.0260 -3.5090
N 2.8690 -0.8750 -1.9880
C 2.3020 -1.9000 -2.6860
C 1.3540 -1.3790 -3.6410

C 2.6570 1.5830 -2.0320
H 0.8070 0.6980 -4.0830
C 6.2500 1.1260 1.2070
C 3.6530 1.8970 -1.0860
H 0.7800 -1.9720 -4.3430
N 4.4460 0.9860 -0.4550
C 3.9840 3.2330 -0.6190
C 5.2710 1.6800 0.3770
C 4.9920 3.0950 0.2800
C 6.5650 -0.2240 1.3580
N 5.9240 -1.2480 0.7330
C 6.5280 -2.3990 1.1300
C 7.6290 -0.7460 2.1940
C 7.6080 -2.0960 2.0510
C 2.6020 -3.2570 -2.5300
C 3.5530 -3.8150 -1.6770
N 4.3360 -3.1090 -0.8150
C 5.1630 -4.0030 -0.2080
C 3.8790 -5.2250 -1.5990
C 4.8790 -5.3410 -0.6870
C 6.1680 -3.6790 0.7070
H 3.5080 4.1510 -0.9350
H 5.5020 3.8740 0.8330
H 8.2990 -0.1460 2.7980
H 8.2580 -2.8290 2.5130
H 3.4100 -6.0080 -2.1820
H 5.3940 -6.2400 -0.3700
C -5.7730 1.6810 -0.8100
C -4.4820 1.6680 -1.6230
C -3.7280 2.9940 -1.6900
C -2.4060 2.7500 -2.3940
C 1.8530 2.7140 -2.5840
C 0.4800 2.7400 -2.3240
C -0.3040 3.8220 -2.7160
C 0.2800 4.8850 -3.4050
C 1.6400 4.8490 -3.6920

C 2.4280 3.7720 -3.2910
C -9.9020 -3.7350 -0.2620
C -8.5190 -3.6120 -0.8970
C -7.5560 -2.7970 -0.0260
H -2.7790 -1.8560 1.6540
C -4.7480 -2.7080 1.2810
C -3.7060 -2.0790 2.1930
C -3.4150 -3.0500 3.3440
C -2.4920 -2.4450 4.3980
H -4.3590 -3.3520 3.8160
H -2.2950 -3.1620 5.2010
O -1.6290 3.9390 -2.3940
H 0.0610 1.9160 -1.7580
H 3.4910 3.7550 -3.5120
H 2.0920 5.6730 -4.2360
H -0.3400 5.7240 -3.7030
C -6.3420 0.2640 -0.6490
C -5.6030 -0.5510 0.4300
N -5.1200 -1.9390 0.0300
C -3.9150 -1.7710 -0.8810
C -1.3580 -3.9730 -2.7750
C -2.1450 -2.7310 -2.3610
C -3.1500 -3.0370 -1.2440
H -0.6350 -3.7330 -3.5590
H -2.6800 -2.3310 -3.2320
H -2.6050 -3.4150 -0.3700
H -6.3030 -0.2270 -1.6270
H -7.4020 0.3160 -0.3850
H -6.2430 -0.6980 1.3020
H -4.7050 -0.0250 0.7600
C -6.1890 -2.7290 -0.6960
H -5.5920 2.1240 0.1780
H -6.5210 2.3120 -1.3030
H -3.7990 0.9350 -1.1850
H -4.7090 1.3220 -2.6420
H -3.5280 3.3680 -0.6770

H -4.3080 3.7610 -2.2150
H -2.5610 2.4210 -3.4310
H -1.8890 1.9420 -1.8650
H -8.1000 -4.6120 -1.0640
H -7.9730 -1.7960 0.1220
H -10.3580 -2.7490 -0.1170
H -10.5710 -4.3250 -0.8950
H -9.8430 -4.2260 0.7150
H -8.6070 -3.1400 -1.8830
H -7.4900 -3.2700 0.9590
H -4.4140 -3.6920 0.9440
H -5.6770 -2.8480 1.8350
H -4.0730 -1.1330 2.6040
H -2.9600 -3.9630 2.9390
H -2.9370 -1.5490 4.8450
H -1.5320 -2.1610 3.9590
H -3.2470 -1.0670 -0.3810
H -4.2970 -1.2900 -1.7840
H -2.0280 -4.7500 -3.1590
H -0.8040 -4.3940 -1.9300
H -1.4540 -1.9450 -2.0310
H -3.8190 -3.8340 -1.5860
H -5.7900 -3.7380 -0.8180
H -6.2820 -2.2940 -1.6930
H 2.0500 -3.9480 -3.1630
H 6.8380 1.8290 1.7930
H 6.7460 -4.5080 1.1090
C -1.4490 3.0940 2.2110
C -0.6300 2.8200 0.9420
H -2.3050 2.4250 2.2520
H -1.2340 3.0340 0.0580
C 0.6760 3.6040 0.9040
H 0.4170 4.6510 0.7120
H 1.2660 3.2570 0.0540
O -0.2620 1.4190 0.9070
Br -2.2780 4.8690 1.9760

C 1.4880 3.4880 2.1960
H 2.3730 4.1270 2.1180
H 1.8590 2.4610 2.3020
C -0.6210 3.0250 3.4870
H -0.3490 1.9680 3.6200
H -1.2430 3.3050 4.3420
C 0.6530 3.8680 3.4190
H 0.3810 4.9300 3.3700
H 1.2300 3.7260 4.3390
O -0.8040 -0.7310 0.7640
C -1.2270 0.5120 0.7800
O -2.4170 0.7750 0.6930
C 0.6110 -1.1130 0.5470
C 1.5690 -0.7850 1.7190
H 0.9400 -0.5790 -0.3480
H 1.5030 0.2980 1.9170
C 1.0890 -1.5170 2.9860
H 0.1090 -1.1150 3.2830
H 1.7900 -1.2920 3.7980
O 2.8270 -1.1670 1.3510
C 0.9990 -3.0290 2.7670
H 0.6190 -3.5270 3.6690
H 2.0100 -3.4110 2.5860
C 0.5520 -2.6130 0.3110
H 1.5580 -2.9270 0.0250
H -0.1080 -2.8300 -0.5330
C 0.1130 -3.3730 1.5650
H -0.9320 -3.1250 1.7960
H 0.1420 -4.4520 1.3680
Mg 4.0030 -1.0890 -0.1760

I3a_Mg cat. 3' (1,2-diequatorial conformation)
C 2.4640 -0.4040 2.4370
C 1.8990 -0.5310 3.7660
N 2.4520 0.9040 2.0600
C 1.8950 1.6130 3.0790

C	1.5640	0.7230	4.1700
C	2.9730	-1.4720	1.6720
H	1.7970	-1.4560	4.3160
C	4.7090	0.4300	-2.4430
C	3.6440	-1.3430	0.4410
H	1.1260	1.0270	5.1130
N	3.7930	-0.1760	-0.2480
C	4.2510	-2.4270	-0.3100
C	4.4410	-0.4710	-1.4080
C	4.7600	-1.8810	-1.4440
C	4.3500	1.7770	-2.5080
N	3.6520	2.4490	-1.5510
C	3.5310	3.7380	-1.9750
C	4.6760	2.6740	-3.5970
C	4.1650	3.8890	-3.2680
C	1.6320	2.9860	3.0600
C	1.8300	3.8720	2.0000
N	2.3200	3.5310	0.7750
C	2.3940	4.6750	0.0390
C	1.5630	5.2940	2.0390
C	1.9050	5.7910	0.8200
C	2.9270	4.7670	-1.2500
H	4.2790	-3.4640	-0.0070
H	5.2870	-2.3820	-2.2470
H	5.2300	2.4000	-4.4860
H	4.2180	4.8130	-3.8310
H	1.1860	5.8350	2.8990
H	1.8570	6.8170	0.4790
C	-3.4420	-2.3480	0.3300
C	-3.7880	-3.4860	1.2980
C	-2.7050	-4.5720	1.3880
C	-1.3590	-3.9490	1.7200
C	2.6240	-2.8550	2.1210
C	1.2720	-3.2080	2.0140
C	0.8570	-4.5120	2.2820
C	1.7920	-5.4600	2.7100

C 3.1240 -5.0950 2.8510
C 3.5510 -3.7990 2.5530
C -8.7650 1.7530 -0.6380
C -7.6310 1.8400 0.3820
C -6.2560 1.6530 -0.2690
H -1.1920 2.1760 -0.4670
C -3.3400 2.4670 -0.7180
C -1.9290 2.2990 -1.2640
C -1.5390 3.5140 -2.1100
C -0.1680 3.3310 -2.7580
H -2.2990 3.6870 -2.8850
H 0.1130 4.2150 -3.3400
O -0.4290 -4.9390 2.1290
H 0.5820 -2.4460 1.6710
H 4.5980 -3.5280 2.6490
H 3.8440 -5.8340 3.1890
H 1.4590 -6.4720 2.9210
C -4.2250 -1.0590 0.6010
C -3.6610 0.0690 -0.2640
N -3.7560 1.4590 0.3330
C -2.8230 1.5230 1.5350
C -1.5800 4.1610 4.0710
C -1.8760 2.7940 3.4620
C -2.5450 2.9140 2.0890
H -1.0750 4.0600 5.0370
H -2.5280 2.2220 4.1360
H -1.8810 3.4710 1.4190
H -4.1070 -0.8320 1.6650
H -5.2990 -1.1950 0.4260
H -4.1530 0.1070 -1.2370
H -2.5970 -0.1020 -0.4300
C -5.1650 1.7620 0.7890
H -2.3890 -2.0750 0.4340
H -3.5750 -2.6640 -0.7130
H -3.9230 -3.0610 2.3030
H -4.7470 -3.9420 1.0250

H -2.6280 -5.1250 0.4430
H -2.9750 -5.2950 2.1660
H -1.4680 -3.1960 2.5160
H -0.9650 -3.4360 0.8400
H -7.6660 2.8130 0.8890
H -6.2280 0.6750 -0.7610
H -8.7700 0.7770 -1.1370
H -9.7370 1.8880 -0.1550
H -8.6620 2.5240 -1.4090
H -7.7730 1.0770 1.1570
H -6.1270 2.4130 -1.0460
H -3.4700 3.4520 -0.2620
H -4.0650 2.3810 -1.5300
H -1.8670 1.4000 -1.8860
H -1.5300 4.4100 -1.4740
H -0.1660 2.4640 -3.4280
H 0.6010 3.1590 -2.0010
H -1.8950 1.0220 1.2430
H -3.2950 0.9140 2.3080
H -2.5040 4.7290 4.2320
H -0.9340 4.7480 3.4110
H -0.9460 2.2240 3.3600
H -3.4660 3.4990 2.1990
H -5.1500 2.7700 1.2060
H -5.3740 1.0690 1.6070
H 1.2170 3.4090 3.9710
H 5.2450 0.0310 -3.3000
H 2.9120 5.7490 -1.7150
C 0.2870 -0.1940 -0.5670
O -0.5220 -0.5730 0.2950
O 0.8750 0.9180 -0.6360
C 0.0310 -2.3120 -1.6640
C -0.6830 -2.5300 -2.9900
C -1.2610 -3.9370 -3.0910
C -0.1590 -4.9890 -2.9100
C 0.5830 -4.7800 -1.5880

C 1.1340 -3.3580 -1.4980
O 0.6040 -1.0180 -1.6240
H -0.6970 -2.4000 -0.8560
Br -2.1440 -1.2110 -3.1880
H -0.0150 -2.3060 -3.8240
H -2.0190 -4.0660 -2.3060
H -1.7660 -4.0630 -4.0530
H 0.5540 -4.9180 -3.7420
H -0.6050 -5.9880 -2.9550
H -0.1000 -4.9680 -0.7480
H 1.4010 -5.5020 -1.4890
H 1.6200 -3.1860 -0.5350
H 1.8960 -3.1920 -2.2700
Mg 2.6360 1.5620 0.0700

TS3a_Mg cat. 3' (1,2-diequatorial conformation)

C -1.6220 -0.5330 -2.5130
C -0.7150 -0.3070 -3.6220
N -2.1360 0.6580 -2.0970
C -1.6120 1.6250 -2.8970
C -0.7240 1.0290 -3.8690
C -1.9790 -1.7960 -2.0050
H -0.1760 -1.0760 -4.1590
C -5.3270 -1.0600 1.4400
C -2.9940 -2.0340 -1.0520
H -0.1930 1.5680 -4.6450
N -3.6670 -1.0640 -0.3720
C -3.4590 -3.3370 -0.6170
C -4.5200 -1.6880 0.4850
C -4.4240 -3.1170 0.3160
C -5.4230 0.3060 1.6960
N -4.7210 1.2750 1.0420
C -5.1530 2.4720 1.5240
C -6.3170 0.9130 2.6600
C -6.1470 2.2570 2.5560
C -1.8920 2.9920 -2.7970

C -2.6720 3.6220 -1.8280
N -3.2640 2.9990 -0.7680
C -3.9400 3.9550 -0.0710
C -2.9740 5.0390 -1.7920
C -3.7470 5.2470 -0.6960
C -4.7680 3.7190 1.0280
H -3.1040 -4.2920 -0.9790
H -5.0070 -3.8530 0.8570
H -6.9920 0.3710 3.3100
H -6.6550 3.0400 3.1040
H -2.6490 5.7640 -2.5280
H -4.1790 6.1770 -0.3480
C 5.0600 -1.0100 -0.4750
C 5.3790 -2.0100 -1.5970
C 4.4740 -3.2470 -1.6140
C 2.9980 -2.9190 -1.7500
C -1.1560 -2.9660 -2.4320
C 0.1960 -2.9650 -2.0620
C 0.9980 -4.0720 -2.3320
C 0.4590 -5.1870 -2.9780
C -0.8740 -5.1720 -3.3680
C -1.6840 -4.0670 -3.1060
C 7.6540 4.3670 0.3100
C 6.2630 4.3060 -0.3180
C 5.3970 3.2080 0.3080
H 0.5270 2.1890 1.6570
C 2.6420 2.6660 1.6050
C 1.4420 1.9590 2.2100
C 1.2600 2.3450 3.6790
C 0.1340 1.5280 4.3110
H 2.1940 2.1540 4.2220
H -0.0360 1.8190 5.3530
O 2.3080 -4.1470 -1.9700
H 0.5860 -2.1010 -1.5350
H -2.7240 -4.0620 -3.4160
H -1.2870 -6.0310 -3.8880

H 1.0980 -6.0400 -3.1790
C 4.1480 0.1500 -0.9120
C 3.6150 0.8150 0.3480
N 3.0290 2.2020 0.2080
C 1.8210 2.1270 -0.7090
C 0.7330 5.5420 -2.2840
C 1.3640 4.1550 -2.2180
C 1.0670 3.4470 -0.8920
H 0.8760 6.0010 -3.2670
H 2.4470 4.2430 -2.3740
H -0.0040 3.2230 -0.8430
H 3.3160 -0.2190 -1.5200
H 4.7260 0.8340 -1.5440
H 4.4030 0.8940 1.0990
H 2.8400 0.1860 0.7810
C 4.0340 3.1700 -0.3700
H 4.6000 -1.5280 0.3780
H 5.9890 -0.5740 -0.0890
H 5.3290 -1.5050 -2.5710
H 6.4110 -2.3610 -1.4890
H 4.6230 -3.8220 -0.6920
H 4.7580 -3.8960 -2.4490
H 2.8170 -2.2490 -2.6020
H 2.6210 -2.4250 -0.8430
H 5.7640 5.2760 -0.2000
H 5.9080 2.2460 0.1960
H 8.1860 3.4180 0.1770
H 8.2560 5.1580 -0.1450
H 7.5900 4.5670 1.3850
H 6.3540 4.1290 -1.3970
H 5.2990 3.4000 1.3820
H 2.4800 3.7450 1.5510
H 3.5220 2.4950 2.2280
H 1.5860 0.8760 2.1740
H 1.0490 3.4190 3.7700
H 0.3910 0.4630 4.2930

H -0.8030 1.6560 3.7590
H 1.1850 1.3370 -0.3050
H 2.2030 1.7750 -1.6700
H 1.1740 6.2080 -1.5330
H -0.3420 5.4870 -2.0840
H 0.9880 3.5280 -3.0350
H 1.2540 4.1340 -0.0590
H 3.5650 4.1560 -0.3260
H 4.1500 2.9110 -1.4240
H -1.4490 3.6350 -3.5530
H -5.9500 -1.7120 2.0470
H -5.2220 4.5910 1.4920
C -0.6780 -0.3300 0.9210
O 0.4190 -0.5440 0.3930
O -1.3900 0.7060 0.9090
C 1.4300 -4.0060 1.6590
C 0.6640 -2.8220 2.0460
H 2.4200 -3.9900 2.1120
C -0.6190 -2.5950 1.4090
H -0.6240 -2.8380 0.3440
O -1.2370 -1.3730 1.6630
C -1.4170 -3.7380 2.1550
H -2.4480 -3.5760 1.8300
H -1.3790 -3.5880 3.2400
C 0.5910 -5.2300 2.1810
H 0.6670 -5.2680 3.2720
H 1.0600 -6.1340 1.7830
C -0.8700 -5.1030 1.7570
H -0.9660 -5.2360 0.6730
H -1.4640 -5.8870 2.2360
H 1.5080 -4.0870 0.5690
Br 3.1630 -1.3560 2.9890
H 0.8760 -2.3210 2.9860
Mg -3.0710 0.9610 -0.2330

I4a_Mg cat. 3' (1,2-diequatorial conformation)

C 2.7330 1.7500 -2.0450
C 2.4860 2.0400 -3.4430
N 3.1680 0.4620 -1.9230
C 3.1900 -0.0830 -3.1680
C 2.7900 0.9120 -4.1390
C 2.5620 2.6570 -0.9860
H 2.1420 2.9880 -3.8330
C 3.7240 0.3630 3.1340
C 2.8900 2.4250 0.3660
H 2.7360 0.7540 -5.2090
N 3.2940 1.2270 0.8800
C 2.8190 3.4020 1.4300
C 3.4640 1.3940 2.2210
C 3.2040 2.7690 2.5730
C 3.8280 -0.9990 2.8580
N 3.7320 -1.5610 1.6180
C 3.9100 -2.9020 1.7660
C 4.0580 -2.0360 3.8410
C 4.1030 -3.2150 3.1670
C 3.4800 -1.4230 -3.4590
C 3.6910 -2.4550 -2.5460
N 3.6410 -2.3220 -1.1880
C 3.8680 -3.5530 -0.6480
C 3.9560 -3.8390 -2.8830
C 4.0550 -4.5190 -1.7110
C 3.9530 -3.8280 0.7190
H 2.5290 4.4380 1.3130
H 3.2820 3.1860 3.5690
H 4.1760 -1.8710 4.9050
H 4.2630 -4.2070 3.5680
H 4.0530 -4.2280 -3.8890
H 4.2520 -5.5730 -1.5650
C -4.4290 1.6440 -0.7620
C -4.7640 2.8630 -1.6420
C -3.8420 4.0730 -1.4620

C -2.3680 3.7710 -1.6700
C 1.8390 3.9320 -1.2820
C 0.4470 3.8440 -1.3980
C -0.3170 4.9960 -1.5720
C 0.3180 6.2400 -1.6690
C 1.7000 6.3160 -1.5780
C 2.4700 5.1680 -1.3790
C -7.8500 -2.9530 -1.4330
C -6.4650 -3.0460 -2.0710
C -5.3980 -2.3470 -1.2230
H -0.4110 -2.6080 0.1280
C -2.5720 -2.8480 0.0050
C -1.2910 -2.5940 0.7790
C -1.1230 -3.6400 1.8830
C 0.2280 -3.5030 2.5830
H -1.9360 -3.5000 2.6060
H 0.3360 -4.2480 3.3780
O -1.6740 5.0090 -1.6360
H -0.0120 2.8670 -1.3160
H 3.5500 5.2340 -1.2900
H 2.1860 7.2840 -1.6570
H -0.2880 7.1290 -1.8090
C -3.6230 0.5680 -1.5020
C -3.2090 -0.5230 -0.5220
N -2.8760 -1.8710 -1.1250
C -1.6880 -1.6920 -2.0430
C 0.7120 -3.8150 -4.1990
C 0.1120 -2.5990 -3.5010
C -1.1260 -2.9580 -2.6710
H 1.5760 -3.5260 -4.8050
H -0.1570 -1.8390 -4.2470
H -0.8370 -3.6840 -1.9040
H -2.7380 1.0110 -1.9720
H -4.2480 0.1790 -2.3140
H -3.9650 -0.6940 0.2450
H -2.3110 -0.2100 0.0040

C -4.0440 -2.4190 -1.9170
H -3.8900 1.9590 0.1410
H -5.3540 1.1810 -0.4000
H -4.7610 2.5580 -2.6980
H -5.7850 3.1950 -1.4270
H -3.9670 4.4870 -0.4530
H -4.1370 4.8590 -2.1660
H -2.1890 3.2750 -2.6360
H -2.0040 3.1040 -0.8780
H -6.1920 -4.1000 -2.2100
H -5.6970 -1.3050 -1.0690
H -8.1550 -1.9090 -1.3070
H -8.6010 -3.4520 -2.0530
H -7.8590 -3.4260 -0.4450
H -6.4900 -2.5940 -3.0710
H -5.3580 -2.8160 -0.2340
H -2.5560 -3.8420 -0.4480
H -3.4110 -2.7830 0.7010
H -1.3520 -1.6200 1.2720
H -1.2220 -4.6490 1.4600
H 0.3380 -2.5100 3.0320
H 1.0570 -3.6380 1.8780
H -0.9160 -1.1850 -1.4600
H -2.0140 -1.0040 -2.8260
H -0.0200 -4.2940 -4.8600
H 1.0530 -4.5560 -3.4690
H 0.8640 -2.1430 -2.8470
H -1.8690 -3.4400 -3.3160
H -3.7970 -3.4570 -2.1490
H -4.0740 -1.8740 -2.8630
H 3.5000 -1.6940 -4.5120
H 3.8230 0.6550 4.1760
H 4.1220 -4.8650 0.9940
C 0.4630 0.1480 0.7940
O -0.4340 1.1090 0.5670
O 1.0160 -0.4680 -0.1000

C -1.5880 2.7650 2.1390
C -1.0700 1.3800 1.8540
H -2.3850 3.0560 1.4490
C 0.0480 1.0250 2.7980
H 0.8040 1.8190 2.8180
O 0.6650 -0.0780 2.0830
C -0.4900 0.7680 4.1810
H 0.3070 0.4820 4.8740
H -1.2480 -0.0220 4.1500
C -2.1480 2.6570 3.5800
H -3.0110 1.9810 3.5580
H -2.5040 3.6390 3.9050
C -1.1270 2.1140 4.6020
H -0.3300 2.8550 4.7480
H -1.6240 1.9880 5.5680
H -0.7840 3.5070 2.0660
Br -3.7000 -1.0030 2.9470
H -1.8870 0.6530 1.9530
Mg 3.1830 -0.5950 -0.1360

I3b_Mg cat. 3' (1,2-diequatorial conformation)

C 2.3190 0.1530 -2.7210
C 1.5790 -0.1920 -3.9200
N 2.9470 -0.9640 -2.2480
C 2.6280 -1.9970 -3.0790
C 1.7590 -1.5220 -4.1290
C 2.3720 1.4320 -2.1270
H 1.0010 0.4960 -4.5200
C 5.3100 1.1040 1.7420
C 3.0950 1.7640 -0.9620
H 1.3600 -2.1300 -4.9320
N 3.9370 0.9280 -0.2900
C 3.0240 3.0320 -0.2620
C 4.4080 1.6050 0.7960
C 3.8370 2.9310 0.8230
C 5.8700 -0.1740 1.7920

N 5.5870 -1.1840 0.9230
C 6.2910 -2.2780 1.3250
C 6.8140 -0.6410 2.7850
C 7.0790 -1.9420 2.4930
C 3.0920 -3.3140 -2.9610
C 4.0060 -3.8140 -2.0320
N 4.5950 -3.0820 -1.0460
C 5.4390 -3.9110 -0.3690
C 4.4950 -5.1760 -1.9810
C 5.3840 -5.2340 -0.9540
C 6.2270 -3.5390 0.7230
H 2.4250 3.8800 -0.5620
H 4.0330 3.6810 1.5790
H 7.2140 -0.0440 3.5950
H 7.7380 -2.6230 3.0180
H 4.1970 -5.9710 -2.6520
H 5.9580 -6.0890 -0.6160
C -6.0280 0.8970 -1.8540
C -4.6270 0.8830 -2.4570
C -4.0720 2.2430 -2.8790
C -2.5800 2.0750 -3.0800
C 1.5580 2.5160 -2.7510
C 0.1710 2.3580 -2.8300
C -0.6220 3.3660 -3.3780
C -0.0270 4.5380 -3.8540
C 1.3510 4.6890 -3.7770
C 2.1500 3.6850 -3.2310
C -9.4120 -4.4340 0.7600
C -8.0560 -4.3510 0.0620
C -7.1920 -3.2130 0.6170
H -2.5610 -1.2320 1.6900
C -4.5130 -2.1810 1.7030
C -3.5170 -1.1550 2.2200
C -3.3020 -1.3530 3.7230
C -2.4500 -0.2340 4.3130
H -4.2730 -1.3830 4.2350

H -2.2540 -0.4010 5.3770
O -1.9780 3.3080 -3.4490
H -0.2610 1.4610 -2.4050
H 3.2270 3.8080 -3.1750
H 1.8100 5.6000 -4.1510
H -0.6590 5.3150 -4.2710
C -6.3690 -0.4670 -1.2370
C -5.6100 -0.6850 0.0840
N -4.9280 -2.0370 0.2540
C -3.7220 -2.0560 -0.6670
C -0.7100 -4.2460 -1.6750
C -1.6290 -3.0330 -1.5520
C -2.8100 -3.2730 -0.6010
H 0.1600 -4.0120 -2.2990
H -2.0120 -2.7710 -2.5470
H -2.4190 -3.4170 0.4130
H -6.1290 -1.2370 -1.9790
H -7.4450 -0.5490 -1.0560
H -6.2860 -0.5780 0.9330
H -4.8170 0.0610 0.1970
C -5.8450 -3.1850 -0.0940
H -6.0900 1.6740 -1.0810
H -6.7740 1.1480 -2.6170
H -3.9310 0.4790 -1.7150
H -4.6120 0.1930 -3.3140
H -4.2340 2.9710 -2.0760
H -4.5580 2.6210 -3.7850
H -2.3630 1.3220 -3.8540
H -2.1590 1.7130 -2.1410
H -7.5230 -5.3040 0.1760
H -7.7250 -2.2670 0.4800
H -9.9730 -3.5010 0.6380
H -10.0160 -5.2480 0.3470
H -9.2900 -4.6160 1.8340
H -8.2040 -4.2010 -1.0140
H -7.0620 -3.3610 1.6940

H -4.1190 -3.1940 1.8150
H -5.4350 -2.1210 2.2840
H -3.8720 -0.1370 2.0420
H -2.8240 -2.3250 3.9060
H -2.9440 0.7370 4.2020
H -1.4890 -0.1600 3.7970
H -3.1340 -1.1570 -0.4480
H -4.1250 -1.9570 -1.6780
H -1.2330 -5.0970 -2.1270
H -0.3380 -4.5690 -0.6960
H -1.0710 -2.1580 -1.2010
H -3.3310 -4.1950 -0.8880
H -5.2910 -4.0990 0.1260
H -5.9940 -3.1480 -1.1750
H 2.7220 -4.0180 -3.7020
H 5.6070 1.7920 2.5290
H 6.8480 -4.3160 1.1600
C 1.2950 -2.2850 0.6060
C 1.2670 -0.8230 0.7440
H 1.2140 -2.7020 -0.3970
H 1.1270 -0.2280 -0.1550
C 0.9110 -0.1690 2.0440
H -0.1190 0.1840 1.9530
H 1.5330 0.7250 2.1680
O 2.5220 -1.5480 0.7840
C 1.0670 -1.1210 3.2300
H 0.6710 -0.6410 4.1310
H 2.1300 -1.3190 3.4150
C 0.9330 -3.1930 1.7610
H 1.8420 -3.7280 2.0610
H 0.2250 -3.9510 1.4070
C 0.3340 -2.4360 2.9560
H -0.7190 -2.2100 2.7400
H 0.3440 -3.0820 3.8410
C -2.0470 1.2660 0.2650
O -3.1970 1.7020 0.4730

O -1.6900 0.1810 -0.2470
C -0.1620 5.2300 2.4500
C -0.1190 3.7560 2.0620
H 0.6400 5.4440 3.1640
C -1.1890 3.3870 1.0420
H -2.1820 3.4660 1.4960
O -0.9570 2.0570 0.6240
C -1.0890 4.3160 -0.1720
H -1.8890 4.0500 -0.8700
H -0.1410 4.1050 -0.6820
C -0.0480 6.1270 1.2120
H 0.9330 5.9810 0.7400
H -0.1020 7.1770 1.5190
C -1.1500 5.7940 0.2060
H -2.1290 6.0260 0.6480
H -1.0510 6.4100 -0.6940
H -1.1120 5.4350 2.9600
Br -0.3500 2.6660 3.6960
H 0.8650 3.4670 1.6830
Mg 4.0910 -1.1360 -0.5190

TS3b_Mg cat. 3' (1,2-diequatorial conformation)
C 2.4120 0.3700 -2.6110
C 1.5100 0.1160 -3.7180
N 2.9350 -0.8130 -2.1750
C 2.3970 -1.8030 -2.9430
C 1.4960 -1.2290 -3.9150
C 2.7000 1.6390 -2.0680
H 0.9730 0.8680 -4.2790
C 6.0240 0.9890 1.4230
C 3.6000 1.8920 -1.0130
H 0.9490 -1.7850 -4.6670
N 4.3570 0.9500 -0.3830
C 3.8560 3.1910 -0.4190
C 5.0930 1.5900 0.5680
C 4.7830 3.0010 0.5560

C 6.3710 -0.3610 1.4830
N 5.8050 -1.3450 0.7310
C 6.4070 -2.5140 1.0800
C 7.3840 -0.9290 2.3500
C 7.4090 -2.2640 2.0980
C 2.6800 -3.1680 -2.8290
C 3.5990 -3.7740 -1.9710
N 4.3610 -3.1160 -1.0540
C 5.1550 -4.0420 -0.4520
C 3.9150 -5.1880 -1.9450
C 4.8830 -5.3530 -1.0050
C 6.1010 -3.7660 0.5400
H 3.3850 4.1200 -0.7100
H 5.2210 3.7440 1.2120
H 7.9940 -0.3680 3.0470
H 8.0420 -3.0180 2.5480
H 3.4620 -5.9410 -2.5770
H 5.3800 -6.2690 -0.7120
C -5.7560 2.0230 -1.3930
C -4.3750 1.9180 -2.0300
C -3.6700 3.2500 -2.3040
C -2.1830 2.9650 -2.3950
C 1.9720 2.8110 -2.6390
C 0.5800 2.8660 -2.5160
C -0.1320 3.9670 -2.9940
C 0.5500 5.0200 -3.6110
C 1.9300 4.9560 -3.7460
C 2.6460 3.8590 -3.2670
C -9.9740 -3.2740 -0.6180
C -8.5690 -3.1750 -1.2060
C -7.6290 -2.3530 -0.3170
H -2.9280 -1.3310 1.5260
C -4.8880 -2.1830 1.1130
C -3.8790 -1.5140 2.0360
C -3.6650 -2.4380 3.2440
C -2.8520 -1.7950 4.3630

H -4.6390 -2.7500 3.6440
H -2.6990 -2.5040 5.1840
O -1.4800 4.0990 -2.8780
H 0.0840 2.0480 -2.0090
H 3.7250 3.8150 -3.3770
H 2.4550 5.7720 -4.2330
H -0.0160 5.8710 -3.9760
C -6.3590 0.6400 -1.1080
C -5.6780 -0.0870 0.0700
N -5.1910 -1.5040 -0.2060
C -3.9470 -1.4020 -1.0710
C -1.3100 -3.6580 -2.7710
C -2.0900 -2.4040 -2.3870
C -3.2110 -2.6970 -1.3800
H -0.5070 -3.4130 -3.4720
H -2.5260 -1.9570 -3.2900
H -2.7700 -3.1120 -0.4660
H -6.3050 0.0550 -2.0320
H -7.4260 0.7450 -0.8870
H -6.3630 -0.1670 0.9160
H -4.7890 0.4530 0.4040
C -6.2300 -2.3410 -0.9210
H -5.6900 2.5960 -0.4590
H -6.4390 2.5750 -2.0510
H -3.7300 1.3420 -1.3600
H -4.4500 1.3540 -2.9710
H -3.8550 3.9610 -1.4900
H -4.0320 3.7100 -3.2300
H -2.0000 2.1130 -3.0670
H -1.8230 2.6870 -1.3970
H -8.1550 -4.1830 -1.3420
H -8.0280 -1.3390 -0.2230
H -10.4220 -2.2820 -0.4970
H -10.6290 -3.8620 -1.2680
H -9.9550 -3.7560 0.3660
H -8.6170 -2.7180 -2.2020

H -7.6190 -2.7930 0.6850
H -4.5540 -3.1920 0.8610
H -5.8460 -2.2730 1.6280
H -4.2450 -0.5400 2.3780
H -3.1630 -3.3540 2.9060
H -3.3680 -0.9170 4.7680
H -1.8700 -1.4690 4.0080
H -3.2700 -0.7140 -0.5610
H -4.2790 -0.9300 -1.9980
H -1.9620 -4.4010 -3.2460
H -0.8480 -4.1270 -1.8950
H -1.4150 -1.6540 -1.9580
H -3.8770 -3.4580 -1.8030
H -5.8330 -3.3580 -0.9460
H -6.2680 -1.9840 -1.9520
H 2.1490 -3.8260 -3.5120
H 6.5460 1.6540 2.1060
H 6.6640 -4.6130 0.9240
C 0.8020 -1.2100 0.3720
C 1.6030 -0.5910 1.4450
H 0.9850 -0.8470 -0.6300
H 1.7790 0.4800 1.3080
C 1.1670 -0.9200 2.8640
H 0.2780 -0.3230 3.1030
H 1.9630 -0.6150 3.5540
O 2.6340 -1.3990 0.9720
C 0.8630 -2.4120 3.0260
H 0.4780 -2.6060 4.0350
H 1.7930 -2.9790 2.9150
C 0.3010 -2.6150 0.5510
H 1.1110 -3.2910 0.2610
H -0.5180 -2.7770 -0.1500
C -0.1550 -2.8880 1.9860
H -1.1000 -2.3590 2.1460
H -0.3570 -3.9590 2.1090
C -1.4170 0.7330 0.5700

O -2.5640 1.1960 0.5370
O -1.0770 -0.4560 0.2880
C -0.5210 4.1060 3.6550
C -0.4060 2.7390 2.9930
H -0.3680 4.0040 4.7340
C -0.6030 2.8090 1.4810
H -1.6270 3.1180 1.2530
O -0.3560 1.5340 0.9040
C 0.4070 3.7890 0.8830
H 0.2330 3.8540 -0.1940
H 1.4150 3.3740 1.0140
C 0.4970 5.0780 3.0460
H 1.5140 4.7310 3.2720
H 0.3840 6.0620 3.5130
C 0.3160 5.1700 1.5310
H -0.6640 5.6160 1.3090
H 1.0710 5.8320 1.0930
H -1.5360 4.4930 3.5040
Br -1.7200 1.5030 3.7960
H 0.5590 2.2730 3.2080
Mg 4.0340 -1.1370 -0.3970

I4b_Mg cat. 3' (1,2-diequatorial conformation)
C 2.3200 0.4180 -2.5490
C 1.3740 0.2080 -3.6290
N 2.8050 -0.7870 -2.1290
C 2.2070 -1.7470 -2.8900
C 1.2990 -1.1340 -3.8300
C 2.6840 1.6740 -2.0200
H 0.8580 0.9860 -4.1740
C 6.1440 0.8710 1.2970
C 3.6390 1.8840 -1.0060
H 0.7140 -1.6630 -4.5720
N 4.3760 0.9050 -0.4080
C 3.9930 3.1720 -0.4340
C 5.1930 1.5120 0.4960

C 4.9580 2.9380 0.4920
C 6.4360 -0.4930 1.3330
N 5.7880 -1.4490 0.6140
C 6.3690 -2.6400 0.9200
C 7.4800 -1.1020 2.1350
C 7.4400 -2.4340 1.8770
C 2.4480 -3.1230 -2.8090
C 3.3780 -3.7690 -1.9970
N 4.1900 -3.1480 -1.0980
C 4.9860 -4.1060 -0.5520
C 3.6570 -5.1910 -2.0130
C 4.6580 -5.4000 -1.1180
C 5.9910 -3.8750 0.3900
H 3.5580 4.1240 -0.7060
H 5.4720 3.6590 1.1170
H 8.1510 -0.5670 2.7960
H 8.0720 -3.2140 2.2830
H 3.1580 -5.9190 -2.6410
H 5.1440 -6.3340 -0.8640
C -5.7240 2.2620 -1.1300
C -4.3520 2.1400 -1.7830
C -3.6280 3.4610 -2.0560
C -2.1510 3.1450 -2.2000
C 1.9840 2.8750 -2.5650
C 0.5970 2.9700 -2.4130
C -0.0960 4.0970 -2.8540
C 0.6010 5.1400 -3.4730
C 1.9750 5.0360 -3.6420
C 2.6710 3.9130 -3.1960
C -10.1200 -2.9180 -0.5550
C -8.7180 -2.8630 -1.1570
C -7.7420 -2.0780 -0.2740
H -2.9370 -1.4010 1.5170
C -4.9480 -2.1180 1.1000
C -3.8920 -1.5440 2.0320
C -3.7110 -2.5220 3.2010

C -2.7380 -2.0130 4.2580
H -4.6860 -2.7190 3.6660
H -2.6370 -2.7370 5.0720
O -1.4380 4.2640 -2.6970
H 0.0900 2.1570 -1.9110
H 3.7450 3.8400 -3.3340
H 2.5120 5.8430 -4.1320
H 0.0520 6.0130 -3.8110
C -6.3780 0.8920 -0.9020
C -5.7070 0.0660 0.2150
N -5.2670 -1.3420 -0.1620
C -4.0430 -1.2250 -1.0530
C -1.6860 -3.5060 -3.1030
C -2.3580 -2.2340 -2.5910
C -3.3650 -2.5230 -1.4700
H -0.9640 -3.2740 -3.8910
H -2.8780 -1.7410 -3.4230
H -2.8380 -2.9690 -0.6190
H -6.3760 0.3570 -1.8570
H -7.4320 1.0330 -0.6450
H -6.3820 -0.0500 1.0650
H -4.8020 0.5590 0.5750
C -6.3530 -2.1000 -0.9000
H -5.6330 2.7920 -0.1730
H -6.3900 2.8640 -1.7600
H -3.7080 1.5390 -1.1340
H -4.4490 1.5900 -2.7300
H -3.7730 4.1650 -1.2280
H -4.0080 3.9390 -2.9650
H -2.0110 2.2930 -2.8830
H -1.7610 2.8490 -1.2180
H -8.3400 -3.8830 -1.3000
H -8.1100 -1.0530 -0.1640
H -10.5350 -1.9120 -0.4280
H -10.7990 -3.4830 -1.2000
H -10.1080 -3.4030 0.4270

H -8.7600 -2.4010 -2.1510
H -7.7310 -2.5290 0.7240
H -4.6520 -3.1160 0.7690
H -5.8940 -2.2160 1.6360
H -4.1920 -0.5650 2.4190
H -3.3520 -3.4840 2.8100
H -3.0830 -1.0670 4.6900
H -1.7460 -1.8480 3.8280
H -3.3360 -0.5880 -0.5190
H -4.3840 -0.6830 -1.9380
H -2.4260 -4.2020 -3.5150
H -1.1470 -4.0250 -2.3030
H -1.6010 -1.5260 -2.2330
H -4.0880 -3.2600 -1.8350
H -6.0050 -3.1310 -0.9750
H -6.3900 -1.6960 -1.9130
H 1.8690 -3.7510 -3.4820
H 6.7350 1.5110 1.9470
H 6.5470 -4.7440 0.7330
C 0.4670 -1.0420 0.3070
C 1.4480 -0.8360 1.4960
H 0.8660 -0.5460 -0.5790
H 1.5410 0.2450 1.6870
C 0.8730 -1.4980 2.7590
H -0.0470 -0.9770 3.0560
H 1.5950 -1.3600 3.5730
O 2.6450 -1.3930 1.1340
C 0.6150 -2.9900 2.5320
H 0.1730 -3.4470 3.4260
H 1.5810 -3.4760 2.3570
C 0.2590 -2.5290 0.0680
H 1.2340 -2.9440 -0.1940
H -0.4040 -2.6790 -0.7870
C -0.2870 -3.2300 1.3170
H -1.2980 -2.8570 1.5310
H -0.3840 -4.3050 1.1210

C -1.2230 0.7370 0.6830
O -2.3790 1.1200 0.6720
O -0.9150 -0.5230 0.4760
C -0.1240 3.9150 3.7920
C -0.1170 2.5880 3.0410
H 0.0510 3.7280 4.8550
C -0.3460 2.7840 1.5430
H -1.3600 3.1500 1.3570
O -0.1650 1.5300 0.8660
C 0.7020 3.7380 0.9770
H 0.5010 3.8870 -0.0870
H 1.6850 3.2560 1.0490
C 0.9360 4.8610 3.2190
H 1.9350 4.4370 3.3840
H 0.8990 5.8150 3.7550
C 0.7140 5.0730 1.7210
H -0.2410 5.5920 1.5630
H 1.4960 5.7130 1.3020
H -1.1170 4.3730 3.7000
Br -1.4840 1.3930 3.8160
H 0.8220 2.0500 3.1930
Mg 3.8930 -1.1770 -0.3200