

Electronic Supplementary Information for:

Stereospecific Insertion of Cyclopropenes into Mg–Mg Bonds

Feriel Rekhroukh,[‡] Linxing Zhang,[‡] Richard Y. Kong, Andrew J. P. White, Mark R. Crimmin*

Department of Chemistry, Molecular Sciences Research Hub, Imperial College London, 82 Wood Lane, Shepherds Bush, London, W12 0BZ, UK.

*Corresponding author. E-mail: m.crimmin@imperial.ac.uk

[‡]joint 1st authors

Table of contents

1- Materials and methods	S3
2- Experimental procedures and analytical data	S4
3- NMR spectra	S16
4- X-ray Crystallographic Data	S26
5- Computational details	S30
6- Cartesian coordinates of the stationary points	S40

1- Materials and methods

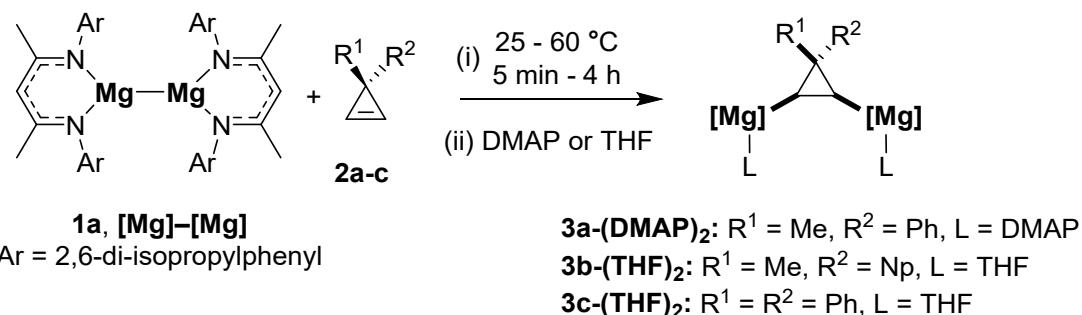
All reactions and manipulations were carried out under an atmosphere of dry argon or dinitrogen using standard Schlenk techniques or in a glovebox under inert atmosphere.

Solvents for air sensitive procedures (toluene, n-hexane) were dried using a solvent purification system (SPS) and stored over activated 3 Å molecular sieves under an inert atmosphere of N₂ or argon before use. C₆H₆ (Sigma-Aldrich anhydrous grade), C₆D₆ was degassed by the freeze-pump-thaw method (x 3) and stored under inert atmosphere over activated 3 Å molecular sieves. Complexes **1a**, **1b**,¹ **S1**² and cyclopropenes **2a-c**³ were synthesized according to the literature procedure.

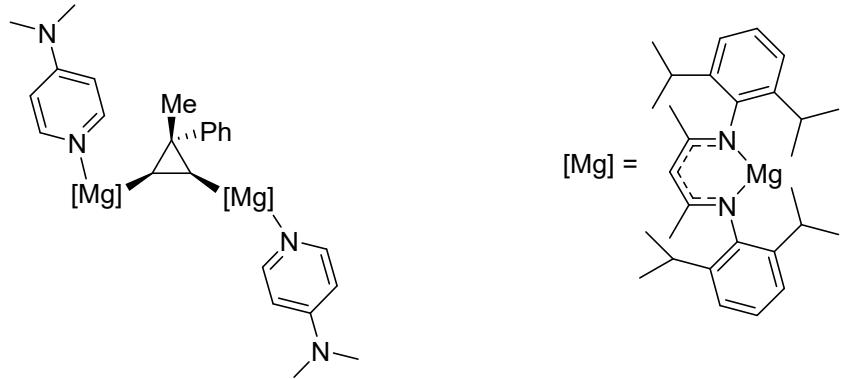
Solution ¹H, ¹³C NMR spectra were recorded on Bruker Avance 400 or 500 spectrometers at 298 K. Chemical shifts (δ) are expressed with a positive sign, in parts per million. ¹H and ¹³C chemical shifts reported are referenced internally to residual protio- (¹H) or deutero- (¹³C) solvent. The following abbreviations and their combinations are used: br, broad; s, singlet; d, doublet; t, triplet; q, quartet, m, multiplet.

2- Experimental procedures and analytical data

2-1- General procedure for the preparation of 3a-c



In a glovebox, in a J-Young NMR tube, to a solution of **1a** (15 mg, 0.017 mmol, 1 equiv.) in C₆D₆ (0.600 mL), cyclopropene (**2a-c**) was added by micropipette (0.033 mmol, 2 equiv.). An instant colour change from the characteristic light yellow to deep yellow is observed. The reaction mixture was monitored by ¹H NMR spectroscopy. The reaction was complete within the acquisition of the first time point (5min) by ¹H NMR spectroscopy for **3a** and **3b**. The reaction required 4h at 60 °C for **3c** to be formed with completion. The J-Young NMR tube was returned to the glovebox and a solution of 4-dimethylaminopyridine (3.2 mg, 0.025 mmol, 1.5 equiv.) or THF (2 μL, 0.025 mmol, 1.5 equiv.) in C₆D₆ was added to the reaction mixture. The reaction mixture was then decanted into a scintillation vial and the solvent was removed in vacuo to yield a yellow oil. The oil was washed three times with cold *n*-hexane until a solid was obtained. Crystals could be obtained by recrystallisation of the solid from toluene (~0.2 mL) / *n*-hexane (~0.1 mL)

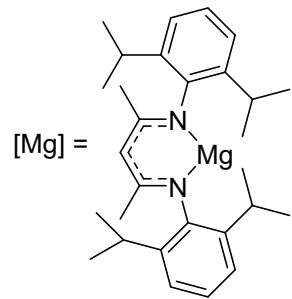
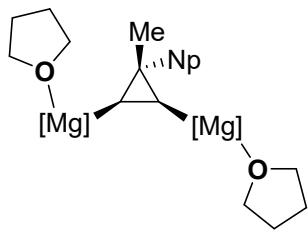
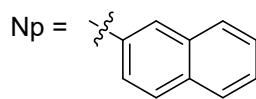


COMPLEX 3a.(DMAP)₂:

Yield: 13 mg, 0.010 mmol (**61 %**).

¹H NMR (400 MHz, C₆D₆): δ -0.47 (s, 2H, MgCH), 0.56 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 0.64 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 0.94 (bs, 3H, CH₃^{cyclopropane}), 1.03 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.15 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.21 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.30 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.70 (s, 6H, CHC(CH₃)), 1.73 (s, 6H, CHC(CH₃)), 2.27 (s, 12H, CH₃^{DMAP}), 2.83-2.97 (m, 4H, CH(CH₃)₂), 3.47-3.53 (m, 2H, CH(CH₃)₂), 3.53-3.69 (m, 2H, CH(CH₃)₂), 4.95 (s, 2H, C(CH₃)CHC(CH₃)) , 5.82 (d, ³J_{HH} = 7.1 Hz, 4H, ArH^{DMAP}), 6.43 (d, ³J_{HH} = 7.6 Hz, 2H, ArH^{Ph ortho}), 6.91-6.97 (m, 1H, ArH^{Ph para}), 6.97-7.03 (m, 2H, ArH^{Ph meta}), 7.06-7.19 (m, 12H, ArH^{Dipp}), 8.46 (bs, 4H, ArH^{DMAP}).

¹³C{¹H} NMR (100 MHz, C₆D₆): δ 23.19 (CH(CH₃)₂), 23.95 (CH(CH₃)₂), 24.06 (CH(CH₃)₂), 24.15 (CH(CH₃)₂), 24.72 (CH(CH₃)₂), 24.82 (CH(CH₃)₂), 25.02 (CHC(CH₃)), 25.36 (CHC(CH₃)), 25.98 (C^{IV-cyclopropane}), 26.38 (CH(CH₃)₂), 28.05 (CH(CH₃)₂), 28.91 (CH(CH₃)₂), 29.22 (CH(CH₃)₂), 33.30 (CH₃^{cyclopropane}), 35.09 (MgCH), 38.89 (CH₃^{DMAP}), 94.01 (C(CH₃)CHC(CH₃)), 106.63 (CH_{meta}^{DMAP}), 119.02 (CH^{Ph para}), 122.70 (CH^{Dipp}), 123.03 (CH^{Dipp}), 124.00 (CH^{Dipp}), 124.44 (CH^{Dipp}), 124.60 (CH^{Dipp}), 124.73 (CH^{Dipp}), 125.60 (CH^{Ph ortho}), 127.10 (CH^{Ph meta}), 142.24 (CH^{Dipp}), 142.48 (C^{IV-Dipp}), 143.09 (C^{IV-Dipp}), 147.83 (C^{IV-Dipp}), 148.37 (C^{IV-Dipp}), 149.88 (CH_{ortho}^{DMAP}), 155.10 (C^{IV-DMAP}), 160.03 (C^{IV-Ph}), 167.77 (C(CH₃)CHC(CH₃)), 167.83 (C(CH₃)CHC(CH₃)).

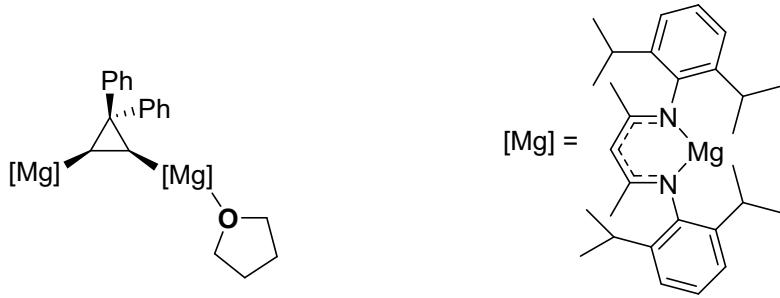


COMPLEX 3b.(THF)₂:

Yield: 15 mg, 0.012 mmol (**73 %**).

¹H NMR (400 MHz, C₆D₆): δ -0.70 (s, 2H, MgCH), 0.76 (s, 3H, CH₃cyclopropane), 0.93 (d, ³J_{HH} = 6.8 Hz, 12H, CH(CH₃)₂), 1.07-1.15 (m, 36H, CH(CH₃)₂), 1.37 (m, 8H, CH₂THF), 1.58 (s, 12H, CHC(CH₃)), 3.02-3.18 (m, 8H, CH(CH₃)₂), 3.52 (m, 8H, CH₂THF), 4.73 (s, 2H, C(CH₃)CHC(CH₃)), 6.32 (d, ³J_{HH} = 6.8 Hz, 1H, ArH^{naphthyl}), 6.81 (s, 1H, ArH^{naphthyl}), 6.91-7.10 (m, 12H, ArH^{Dipp}), 7.24-7.33 (m, 2H, ArH^{naphthyl}), 7.43 (t, ³J_{HH} = 7.4 Hz, 1H, ArH^{naphthyl}), 7.75 (d, ³J_{HH} = 7.4 Hz, 1H, ArH^{naphthyl}), 7.78 (d, ³J_{HH} = 7.4 Hz, 1H, ArH^{naphthyl}).

¹³C{¹H} NMR (100 MHz, C₆D₆): δ 24.40 (CH(CH₃)₂), 24.51 (CH(CH₃)₂), 24.64 (CHC(CH₃)), 25.87 (CH₂THF), 26.78 (C^{IV}-cyclopropane), 28.24 (CH(CH₃)₂), 28.33 (CH(CH₃)₂), 32.77 (CH₃cyclopropane), 33.99 (MgCH), 69.94 (CH₂THF), 94.49 (C(CH₃)CHC(CH₃)), 121.37 (CH^{naphthyl}), 121.98 (CH^{naphthyl}), 123.60 (CH^{Dipp}), 123.79 (CH^{Dipp}), 124.32 (CH^{naphthyl}), 124.99 (CH^{Dipp}), 125.65 (CH^{naphthyl}), 126.44 (CH^{naphthyl}), 126.86 (CH^{naphthyl}), 127.06 (CH^{naphthyl}), 130.56 (C^{IV}-naphthyl), 134.64 (C^{IV}-naphthyl), 142.10 (C^{IV}-Dipp), 142.24 (C^{IV}-Dipp), 146.90 (C^{IV}-Dipp), 157.27 (C^{IV}-naphthyl), 167.81 (C(CH₃)CHC(CH₃)).



COMPLEX 3c.(THF):

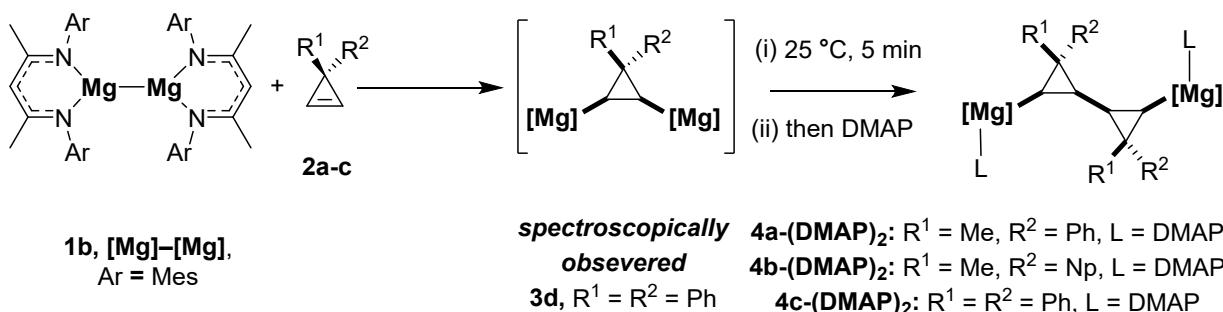
Yield: 15 mg, 0.013 mmol (77%).

¹H NMR (400 MHz, C₆D₆): δ -0.19 (s, 2H, MgCH), 0.95 (d, ³J_{HH} = 6.8 Hz, 12H, CH(CH₃)₂), 1.07 (d, ³J_{HH} = 6.8 Hz, 12H, CH(CH₃)₂), 1.15 (d, ³J_{HH} = 6.8 Hz, 12H, CH(CH₃)₂), 1.18 (d, ³J_{HH} = 6.8 Hz, 12H, CH(CH₃)₂), 1.33 (m, 4H, CH₂^{THF}), 1.58 (s, 12H, CHC(CH₃)), 2.98-3.04 (m, 4H, CH(CH₃)₂), 3.08-3.17 (m, 4H, CH(CH₃)₂), 3.51 (m, 4H, CH₂^{THF}), 4.83 (s, 2H, C(CH₃)CHC(CH₃)), 6.15 (d, ³J_{HH} = 6.3 Hz, 2H, ArH^{Ph}), 6.54 (t, ³J_{HH} = 7.5 Hz, 2H, ArH^{Ph}), 6.70 (t, ³J_{HH} = 6.3 Hz, 1H, ArH^{Ph}), 6.81-6.90 (m, 5H, ArH^{Ph}), 7.00-7.14 (m, 12H, ArH^{Dipp}).

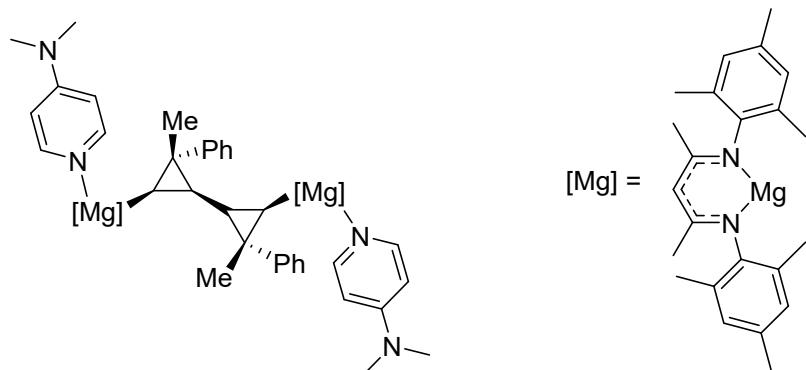
¹³C{¹H} NMR (100 MHz, C₆D₆): δ 24.29 (CH(CH₃)₂), 24.49 (CH(CH₃)₂), 24.71 (CHC(CH₃)), 24.78 (CH(CH₃)₂), 25.45 (CH(CH₃)₂), 25.88 (CH₂^{THF}), 28.25 (CH(CH₃)₂), 28.92 (CH(CH₃)₂), 33.69 (MgCH), 38.84 (C^{IV}-cyclopropane), 70.15 (CH₂^{THF}), 95.48 (C(CH₃)CHC(CH₃)), 123.76 (CH^{Ph}), 123.87 (CH^{Dipp}), 124.11 (CH^{Dipp}), 125.31 (CH^{Dipp}), 127.32 (CH^{Ph}), 127.34 (CH^{Ph}), 128.32 (CH^{Ph}), 128.33 (CH^{Ph}), 142.05 (C^{IV}-Dipp), 142.37 (C^{IV}-Dipp), 146.37 (C^{IV}-Dipp), 155.05 (C^{IV}-Ph), 157.58 (C^{IV}-Ph), 168.86 (C(CH₃)CHC(CH₃)).

Note: NMR data are consistent with facile exchange of THF between the two Mg centres resulting in a time-averaged symmetric structure in solution.

2-2- General procedure for the preparation of 4a-c



In a glovebox, in a J-Young NMR tube, to a solution of **1b** (15 mg, 0.021 mmol, 1 equiv.) in C₆D₆ (0.600 mL), cyclopropene was added by micropipette (0.042 mmol, 2 equiv.). An instant colour change from the characteristic light yellow to orange is observed. The reaction mixture was monitored by ¹H NMR spectroscopy. The reaction was complete within the acquisition of the first time point (5min) by ¹H NMR spectroscopy for **4a-c**. The J-Young NMR tube was returned to the glovebox and a solution of 4-dimethylaminopyridine (3.8 mg, 0.031 mmol, 1.5 equiv.) in C₆D₆ was added to the reaction mixture. The reaction mixture was then decanted into a scintillation vial and the solvent was removed in vacuo to yield a yellow oil. The oil was washed three times with cold *n*-hexane until a solid was obtained. Crystals could be obtained by recrystallisation of the solid from toluene (~0.2 mL) / *n*-hexane (~0.1 mL)



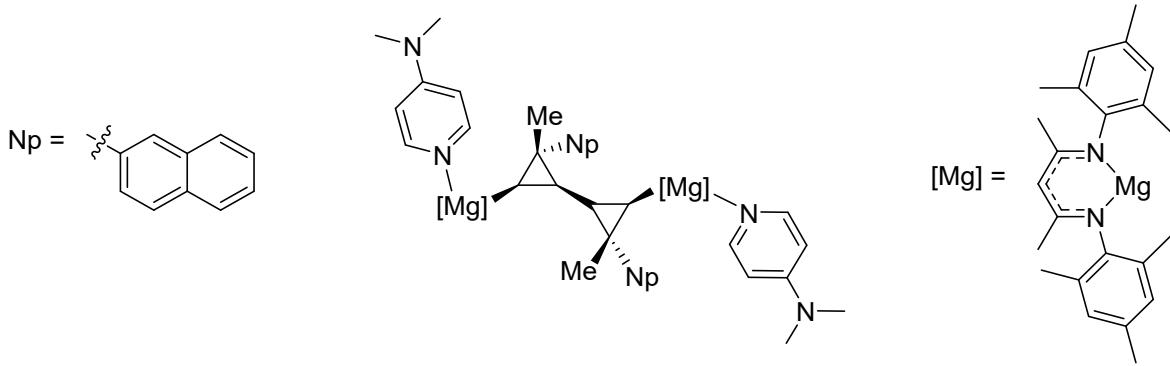
COMPLEX 4a.(DMAP)₂:

Yield: 12.5 mg, 0.010 mmol (49%).

¹H NMR (400 MHz, C₆D₆): δ 0.14 (d, ³J_{HH} = 10.6 Hz, 2H, MgCH), 0.79 (s, 6H, CH₃^{cyclopropane}), 0.96 (d, ³J_{HH} = 10.6 Hz, 2H, MgCHCH), 1.76 (s, 6H, CHC(CH₃)), 1.85 (s, 6H, CHC(CH₃)), 1.96 (s, 12H, CH₃^{DMAP}), 2.01 (s, 6H, CH₃^{Mes}), 2.03 (s, 6H, CH₃^{Mes}), 2.14 (s, 6H, CH₃^{Mes}), 2.29 (s, 6H, CH₃^{Mes}), 2.44 (s, 6H, CH₃^{Mes}), 2.57 (s, 6H, CH₃^{Mes}), 5.07 (s, 2H, C(CH₃)CHC(CH₃)), 5.75 (d, ³J_{HH} = 7.1 Hz, 4H, ArH^{DMAP}), 6.70-6.73 (m, 4H, ArH^{Mes}), 6.89-6.91 (m, 2H, ArH^{Mes}), 6.96-7.01 (m, 2H, ArH^{Ph}), 7.01-7.03 (m, 2H, ArH^{Mes}), 7.10-7.15 (m, 4H, ArH^{Ph}), 7.17-7.24 (m, 4H, ArH^{Ph}), 7.95 (d, ³J_{HH} = 7.1 Hz, 4H, ArH^{DMAP}).

¹³C{¹H} NMR (100 MHz, C₆D₆): δ 18.98 (CH₃^{Mes}), 19.00 (CH₃^{Mes}), 19.31 (CH₃^{Mes}), 19.81 (CH₃^{Mes}), 20.97 (CH₃^{Mes}), 21.36 (CH₃^{Mes}), 22.57 (CH₃^{cyclopropane}), 23.36 (CHC(CH₃)), 23.84 (CHC(CH₃)), 28.10 (C^{IV}-cyclopropane), 34.57 (MgCH), 38.01 (CH₃^{DMAP}), 48.37 (MgCHCH), 94.09 (C(CH₃)CHC(CH₃)), 106.50 (CH_{meta}^{DMAP}), 121.21 (CH^{Ph}), 125.00 (CH^{Ph}), 127.26 (CH^{Ph}), 128.95 (CH^{Mes}), 129.97 (CH^{Mes}), 130.12 (CH^{Mes}), 131.18 (C^{IV}-Mes), 131.38 (C^{IV}-Mes), 132.36 (C^{IV}-Mes), 132.55 (C^{IV}-Mes), 133.49 (C^{IV}-Mes), 147.14 (C^{IV}-Mes), 147.31 (C^{IV}-Mes), 149.21 (CH_{ortho}^{DMAP}), 154.82 (C^{IV}-DMAP), 156.88 (C^{IV}-Ph), 166.75 (C(CH₃)CHC(CH₃)), 167.08 (C(CH₃)CHC(CH₃)).

Anal. Calc. (C₈₀H₉₈Mg₂N₈): C, 78.74, H, 8.09; N, 9.18. Found: C, 78.40; H, 8.18; N, 8.13.

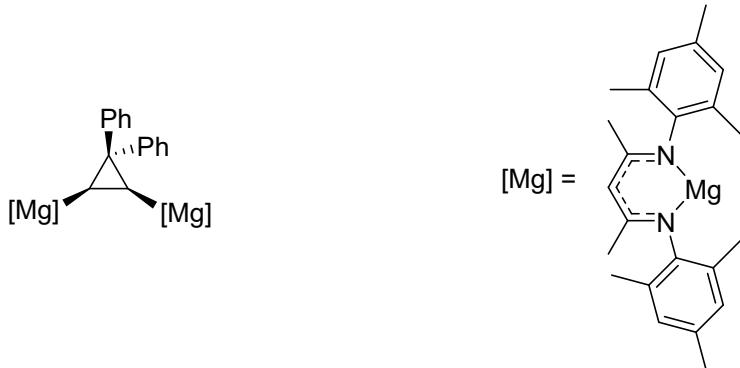


COMPLEX 4b.(DMAP)₂:

Yield: 18 mg, 0.013 mmol (70%).

¹H NMR (400 MHz, C₆D₆): δ 0.43 (d, ³J_{HH} = 10.5 Hz, 2H, MgCH), 0.92 (s, 6H, CH₃cyclopropane), 1.19 (d, ³J_{HH} = 10.5 Hz, 2H, MgCHCH), 1.70 (s, 6H, CHC(CH₃)), 1.73 (s, 12H, CH₃DMAP), 1.87 (s, 6H, CHC(CH₃)), 1.95 (s, 6H, CH₃Mes), 2.04 (s, 6H, CH₃Mes), 2.07 (s, 6H, CH₃Mes), 2.15 (s, 6H, CH₃Mes), 2.51 (s, 6H, CH₃Mes), 2.60 (s, 6H, CH₃Mes), 5.07 (s, 2H, C(CH₃)CHC(CH₃)), 5.47 (d, ³J_{HH} = 6.8 Hz, 4H, ArH^{DMAP}), 6.49 (s, 2H, ArH^{Mes}), 6.60 (s, 2H, ArH^{Mes}), 6.97 (s, 2H, ArH^{Mes}), 7.12 (s, 2H, ArH^{Mes}), 7.16-7.20 (m, 1H, ArH^{naphthyl}), 7.20-7.30 (m, 4H, ArH^{naphthyl}), 7.59 (bs, 2H, ArH^{naphthyl}), 7.65-7.71 (m, 7H, ArH^{naphthyl}), 7.82 (d, ³J_{HH} = 6.8 Hz, 4H, ArH^{DMAP}).

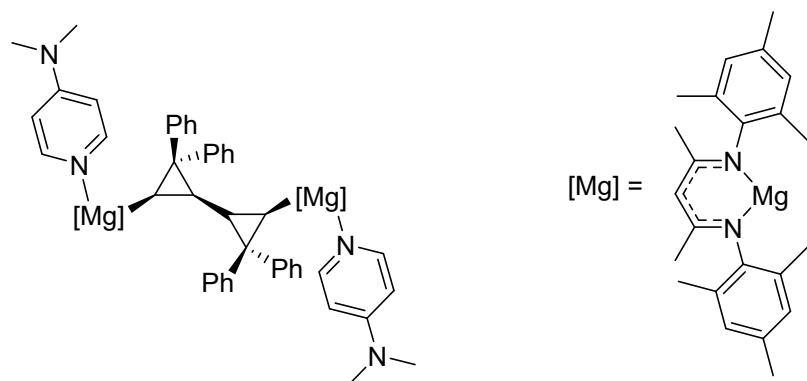
¹³C{¹H} NMR (100 MHz, C₆D₆): δ 18.87 (CH₃Mes), 18.95 (CH₃Mes), 19.12 (CH₃Mes), 19.60 (CH₃Mes), 20.85 (CH₃Mes), 21.43 (CH₃Mes), 22.43 (CH₃cyclopropane), 23.38 (CHC(CH₃)), 23.72 (CHC(CH₃)), 28.18 (C^{IV}-cyclopropane), 35.89 (MgCH), 37.74 (CH₃DMAP), 49.57 (MgCHCH), 94.11 (C(CH₃)CHC(CH₃)), 106.32 (CH_{meta}DMAP), 121.88 (CH^{naphthyl}), 123.04 (CH^{naphthyl}), 124.86 (CH^{naphthyl}), 125.63 (CH^{naphthyl}), 126.42 (CH^{naphthyl}), 127.07 (CH^{naphthyl}), 127.36 (CH^{naphthyl}), 129.07 (CH^{Mes}), 129.97 (CH^{Mes}), 130.21 (CH^{Mes}), 130.82 (C^{IV}-Mes), 131.37 (CH^{Mes}), 132.35 (C^{IV}-Mes), 132.69 (C^{IV}-Mes), 132.83 (C^{IV}-Naphthyl), 133.70 (C^{IV}-Naphthyl), 134.48 (C^{IV}-Naphthyl), 147.24 (C^{IV}-Mes), 149.00 (CH_{ortho}DMAP), 154.70 (C^{IV}-DMAP), 166.13 (C(CH₃)CHC(CH₃)), 166.37 (C(CH₃)CHC(CH₃)).



COMPLEX **3d**:

¹H NMR (400 MHz, C₆D₆): δ 0.79 (s, 2H, MgCH), 1.50 (s, 12H, CHC(CH₃)), 1.92 (s, 12H, CH₃^{Mes}), 2.07 (s, 12H, CH₃^{Mes}), 2.17 (s, 12H, CH₃^{Mes}), 4.82 (s, 2H, C(CH₃)CHC(CH₃)), 6.21-6.26 (m, 2H, ArH^{Ph}), 6.35-6.40 (m, 2H, ArH^{Ph}), 6.45-6.51 (m, 1H, ArH^{Ph}), 6.66-6.70 (m, 4H, ArH^{Mes}), 6.72-6.75 (m, 4H, ArH^{Mes}), 6.77-6.83 (m, 2H, ArH^{Ph}), 7.16-7.22 (m, 3H, ArH^{Ph}).

Note: This intermediate could be observed by ¹H NMR before conversion to the double inserted complex **4c** which formed alongside some minor unidentified species.



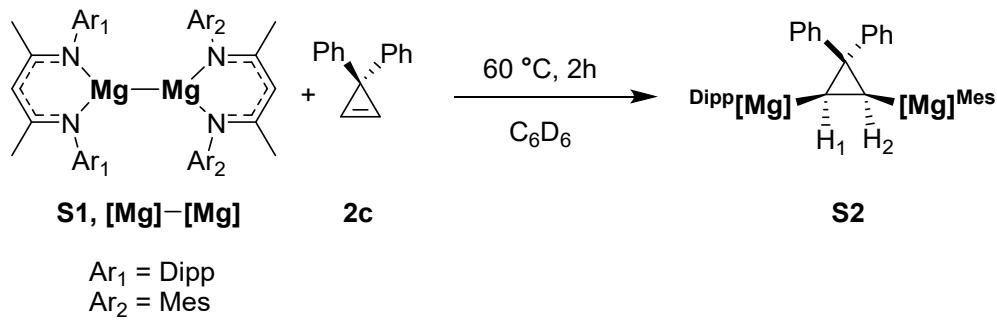
COMPLEX 4c.(DMAP)₂:

Yield: 16 mg, 0.012 mmol (57 %).

¹H NMR (400 MHz, C₆D₆): δ 0.22 (d, ³J_{HH} = 10.5 Hz, 2H, MgCH), 1.30 (d, ³J_{HH} = 10.5 Hz, 2H, MgCHCH), 1.60 (bs, 6H, CH₃^{Mes}), 1.69 (s, 6H, CHC(CH₃)), 1.75 (s, 6H, CHC(CH₃)), 1.93 (s, 12H, CH₃^{DMAP}), 1.98 (s, 6H, CH₃^{Mes}), 2.07 (s, 6H, CH₃^{Mes}), 2.14 (s, 6H, CH₃^{Mes}), 2.16 (s, 6H, CH₃^{Mes}), 2.37 (s, 6H, CH₃^{Mes}), 5.12 (s, 2H, C(CH₃)CHC(CH₃)), 5.69 (d, ³J_{HH} = 6.5 Hz, 4H, ArH^{DMAP}), 6.65-6.69 (m, 4H, ArH^{Mes}), 6.74-6.79 (m, 6H, ArH^{Mes}&ArH^{Ph}), 6.86-6.90 (m, 2H, ArH^{Ph}), 6.92-6.95 (m, 4H, ArH^{Ph}), 6.96-6.98 (m, 2H, ArH^{Ph}), 6.99-7.03 (m, 5H, ArH^{Ph}), 7.11-7.14 (m, 5H, ArH^{Ph}), 7.50 (d, ³J_{HH} = 6.5 Hz, 4H, ArH^{DMAP}).

¹³C{¹H} NMR (100 MHz, C₆D₆): δ 18.48 (CH₃^{Mes}), 18.98 (CH₃^{Mes}), 19.19 (CH₃^{Mes}), 19.25 (CH₃^{Mes}), 20.97 (CH₃^{Mes}), 21.43 (CH₃^{Mes}), 23.80 (CHC(CH₃)), 23.88 (CHC(CH₃)), 36.63 (MgCH), 38.01 (CH₃^{DMAP}), 40.21 (C^{IV}-cyclopropane), 45.06 (MgCHCH), 93.88 (C(CH₃)CHC(CH₃)), 106.32 (CH_{meta}^{DMAP}), 123.85 (CH^{Mes}), 126.36 (CH^{Mes}), 126.90 (CH^{Ph}), 128.57 (CH^{Ph}), 129.33 (CH^{Ph}), 130.05 (CH^{Mes}), 130.41 (CH^{Mes}), 131.78 (CH^{Mes}), 132.53 (CH^{Mes}), 132.62 (CH^{Mes}), 134.10 (CH^{Mes}), 147.58 (C^{IV}-Mes), 147.71 (C^{IV}-Mes), 149.02 (CH_{ortho}^{DMAP}), 154.70 (C^{IV}-DMAP), 156.30 (C^{IV}-Ph), 167.34 (C(CH₃)CHC(CH₃)).

2-3- Procedure for the formation of S2



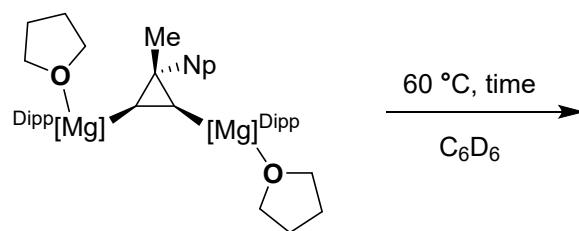
In a glovebox, in a J-Young NMR tube, to a solution of **S1** (10 mg, 0.012 mmol, 1 equiv.) in C_6D_6 (0.600 mL), cyclopropane **2c** was added by micropipette (4.5 μL , 0.025 mmol, 2 equiv.). The reaction required heating for 2h at 60°C for **S1** to be fully consumed. **S2** was characterized *in situ* (along with unidentified products). Attempts to isolate **S2** by recrystallisation were unsuccessful. As such only diagnostic *in situ* data is reported.

Diagnostic signals for **S2**:

^1H NMR (400 MHz, C_6D_6): δ 0.31 (d, ${}^3J_{\text{HH}} = 13.6$ Hz, 1H, H₁), 0.38 (d, ${}^3J_{\text{HH}} = 13.6$ Hz, 1H, H₂), 3.01-3.19 (m, 4H, $\text{CH}(\text{CH}_3)_2$), 4.93 (s, 1H, $\text{C}(\text{CH}_3)\text{CHC}(\text{CH}_3)$), 4.96 (s, 1H, $\text{C}(\text{CH}_3)\text{CHC}(\text{CH}_3)$), 6.26-6.32 (m, 2H, ArH^{Ph}), 6.40-6.45 (m, 2H, ArH^{Ph}), 6.58-6.64 (m, 1H, ArH^{Ph}).

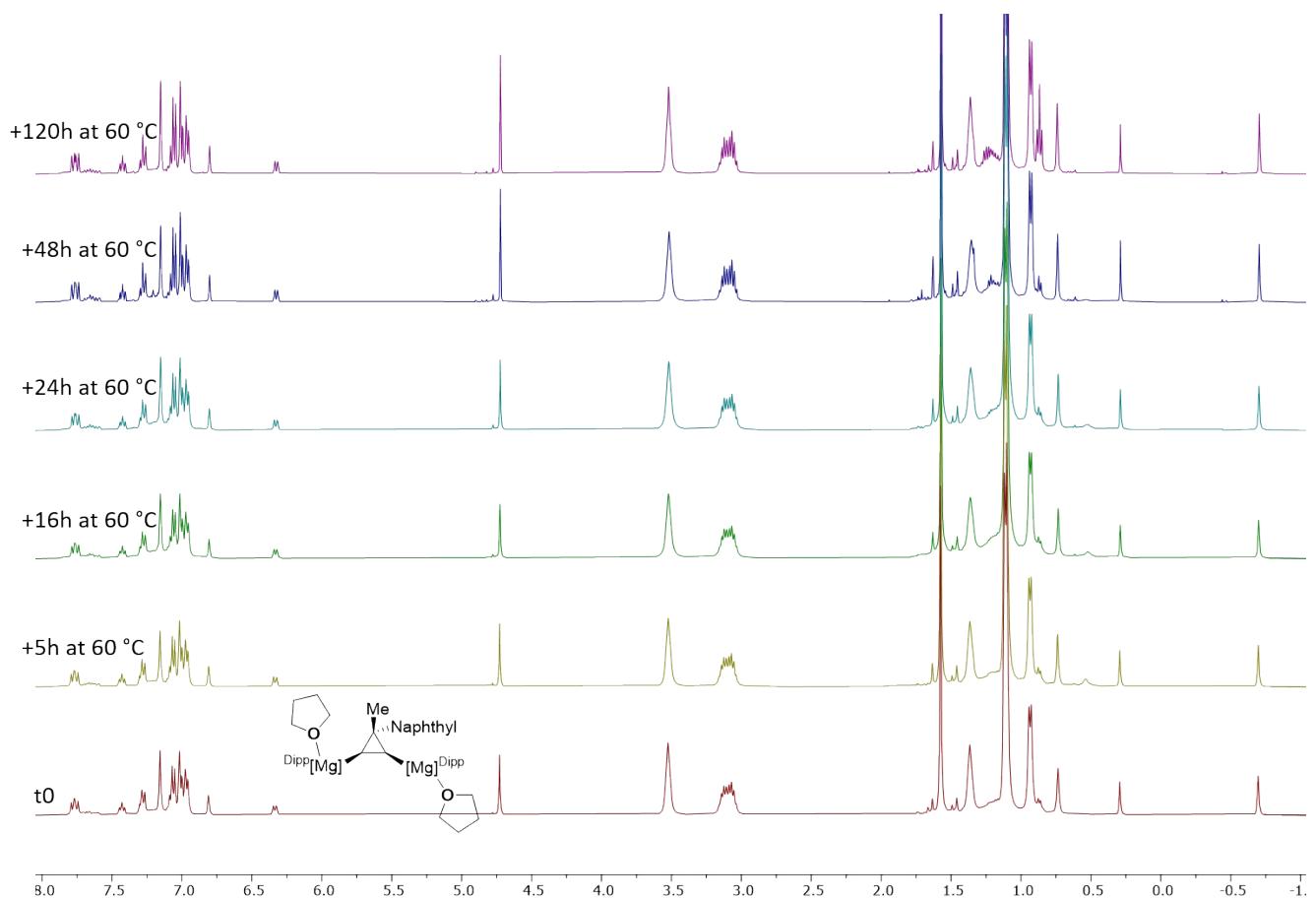
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ 28.30 ($\text{CH}(\text{CH}_3)_2$), 36.47 ($\text{C}^{\text{IV-cyclopropane}}$), 37.31 (MgCH), 37.40 (MgCH), 95.10 ($\text{C}(\text{CH}_3)\text{CHC}(\text{CH}_3)$), 95.46 ($\text{C}(\text{CH}_3)\text{CHC}(\text{CH}_3)$), 121.94 (CH^{Ph}), 122.86 (CH^{Ph}), 123.28 (CH^{Ph}), 128.18 (CH^{Ph}), 128.51 (CH^{Ph}), 152.50 ($\text{C}^{\text{IV-Ph}}$), 157.54 ($\text{C}^{\text{IV-Ph}}$), 168.62 ($\text{C}(\text{CH}_3)\text{CHC}(\text{CH}_3)$), 168.84 ($\text{C}(\text{CH}_3)\text{CHC}(\text{CH}_3)$).

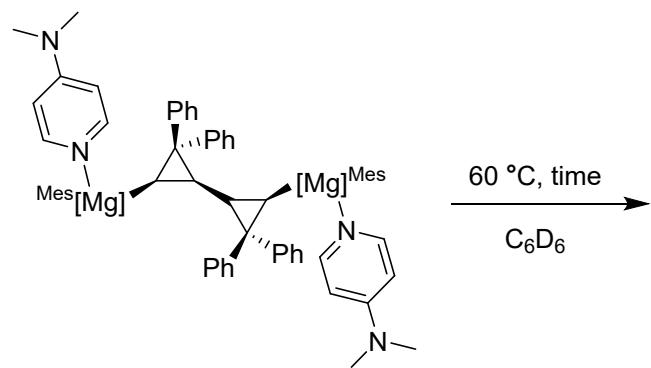
2-4- Monitoring of solutions of isolated inserted complexes $\mathbf{3b.(THF)_2}$ and $\mathbf{4c.(DMAP)_2}$ at $60\text{ }^\circ\text{C}$ overtime



In a glovebox, a solution of $\mathbf{3b.(THF)_2}$ (10 mg, 0.0083 mmol) in C_6D_6 (0.600 mL) was transferred in a J-Young NMR tube and the reaction mixture was monitored as a function of time at $60\text{ }^\circ\text{C}$. The complex is stable after 5 days at $60\text{ }^\circ\text{C}$ with no evidence for epimerization or decomposition.

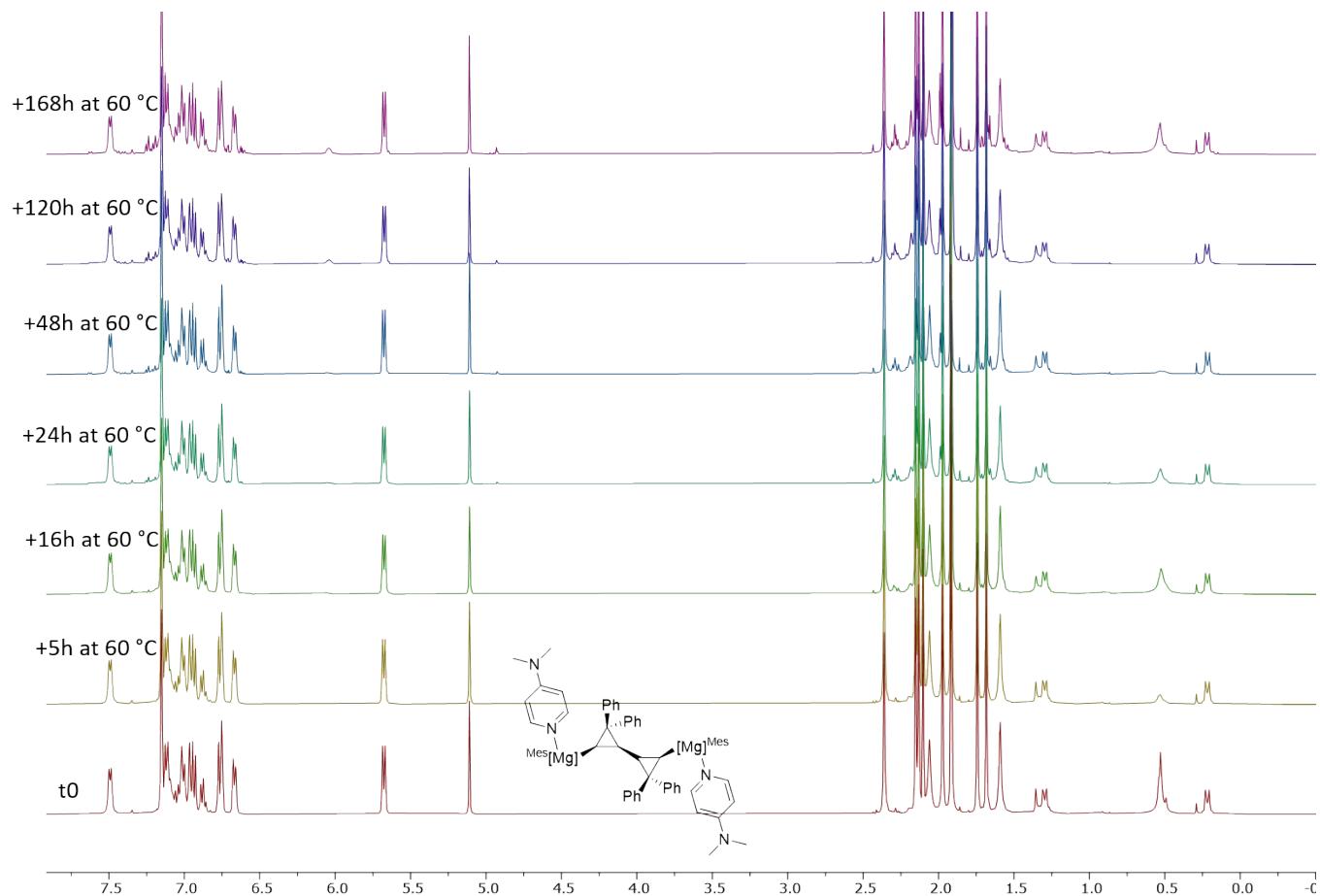
Figure S1: Stack plot of compound $\mathbf{3b.(THF)_2}$ in solution (C_6D_6) at $60\text{ }^\circ\text{C}$ over time.





In a glovebox, a solution of **4c.(DMAP)₂** (10 mg, 0.0074 mmol) in C₆D₆ (0.600 mL) was transferred in a J-Young NMR tube and the reaction mixture monitored as a function of time at 60 °C. The complex is stable after 7 days at 60 °C with no evidence for epimerization or decomposition.

Figure S2: Stack plot of compound **4c.(DMAP)₂** in solution (C₆D₆) at 60 °C over time.



3- NMR spectra of complexes

Figure S3: ^1H NMR spectrum of complex **3a.(DMAP)₂**

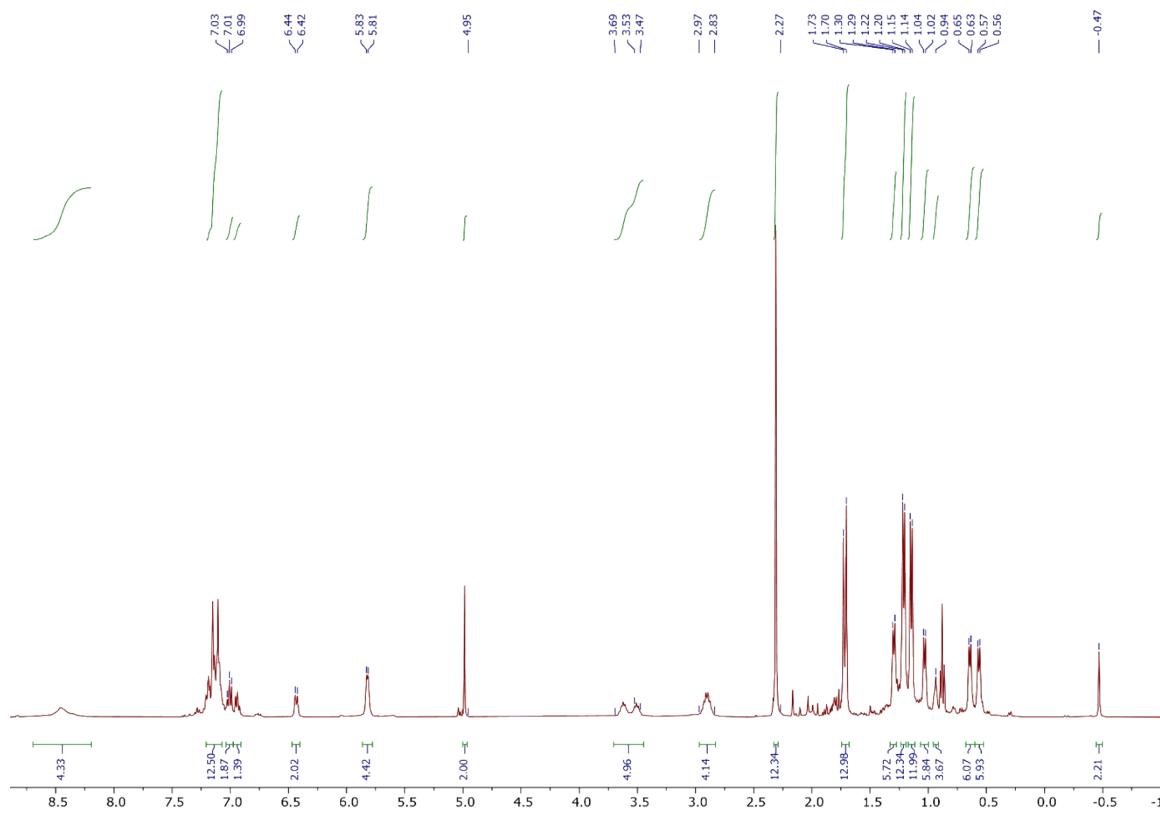


Figure S4: ^{13}C NMR spectrum of complex **3a.(DMAP)₂**

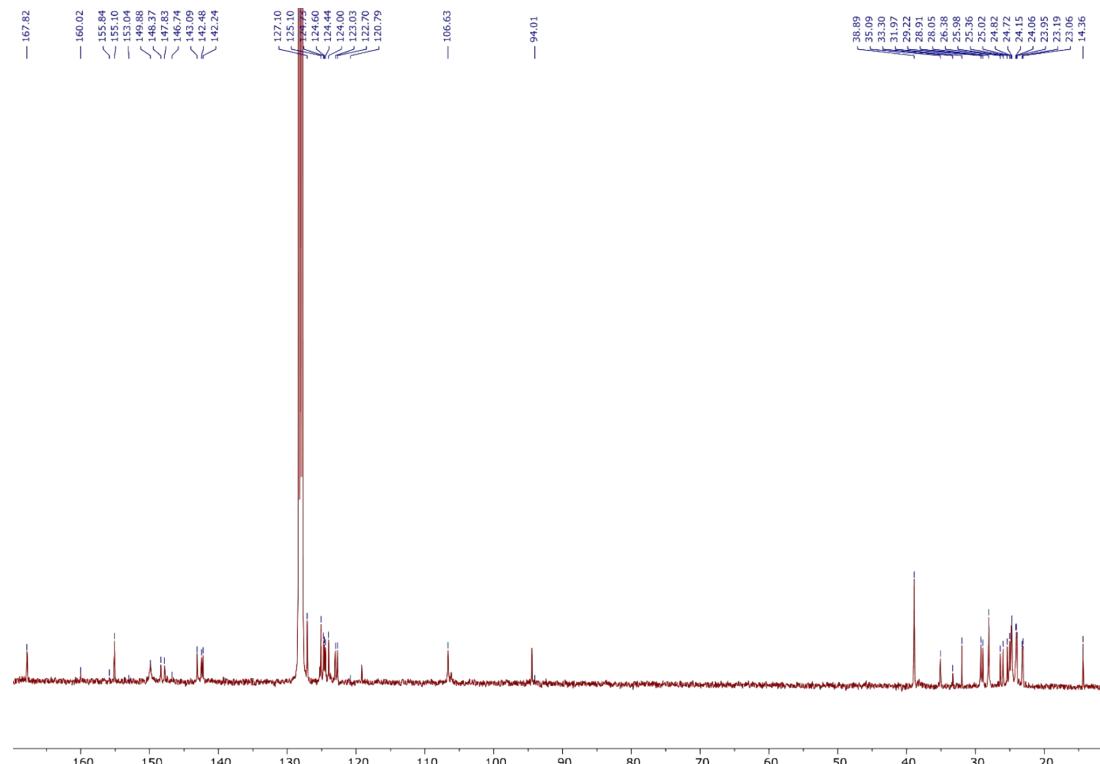


Figure S5: ^1H NMR spectrum of complex **3b.(THF)₂** (* residual hexane and silicon grease)

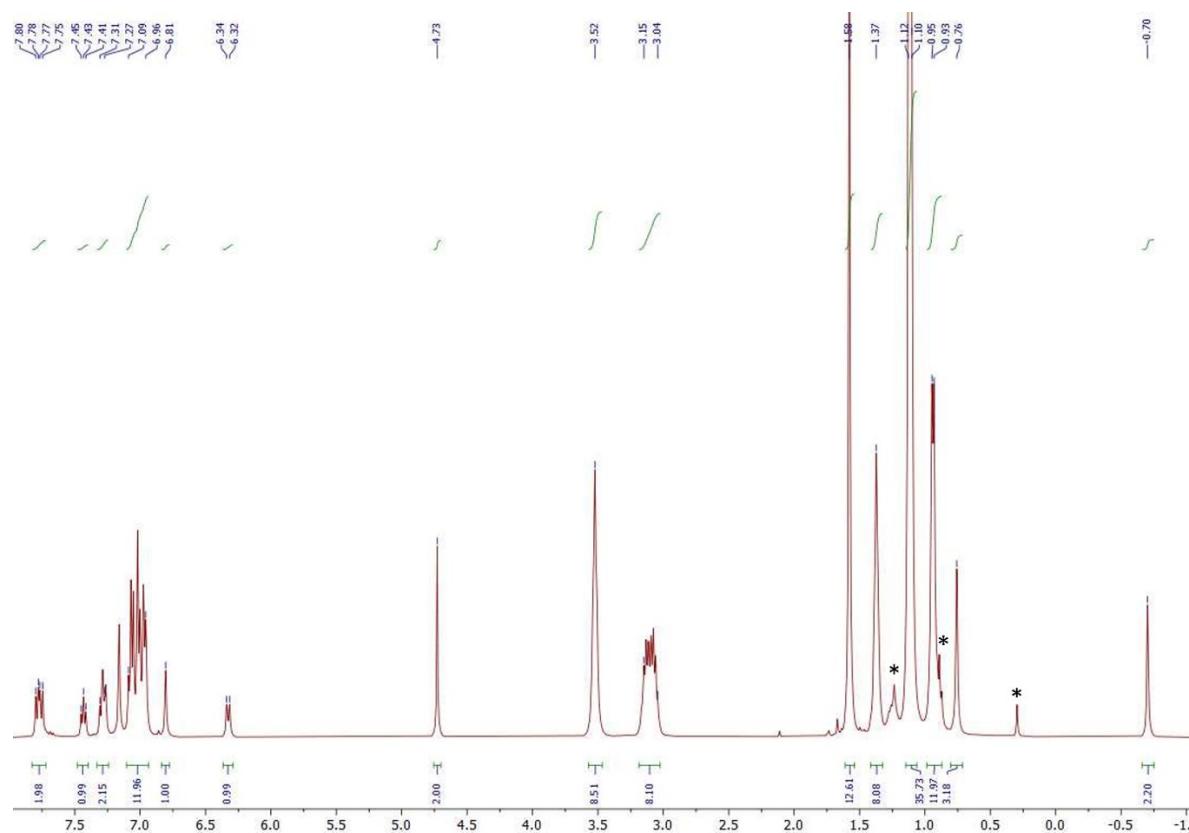


Figure S6: ^{13}C NMR spectrum of complex **3b.(THF)₂** (* residual hexane)

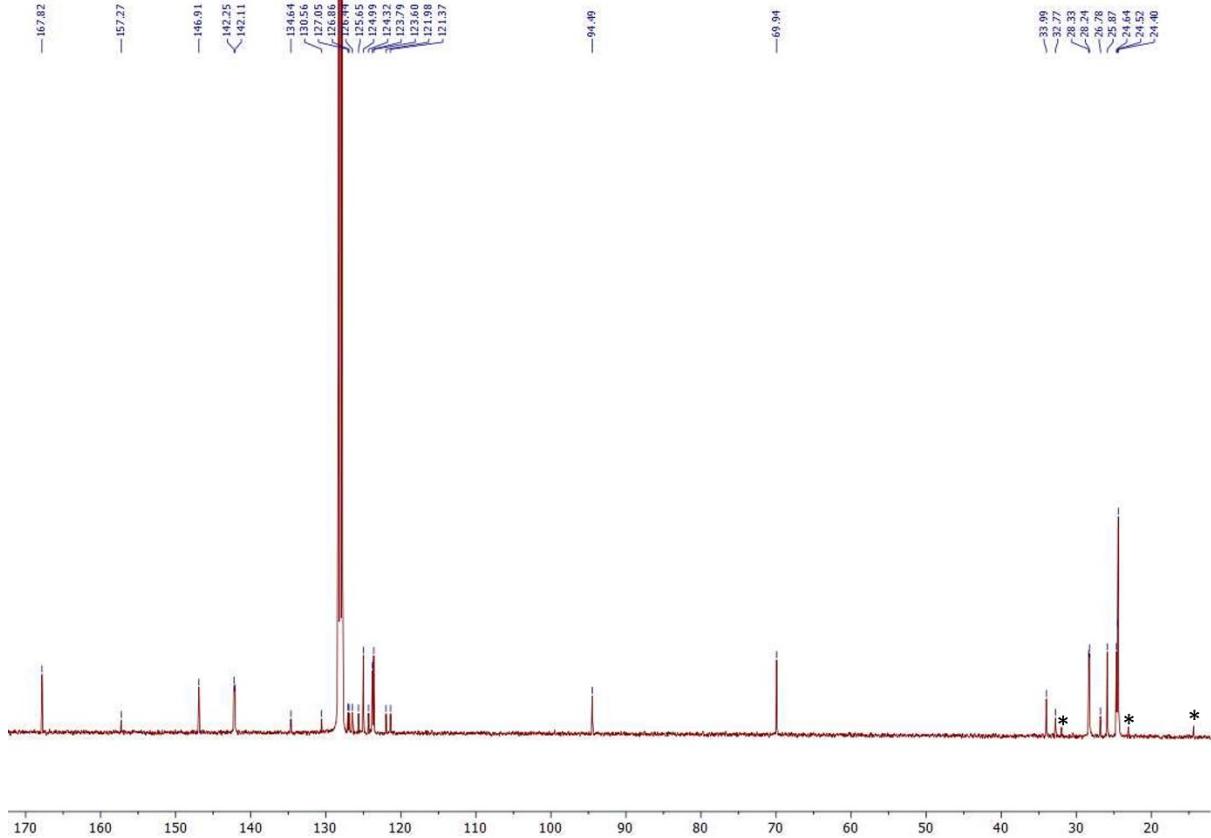


Figure S7: ^1H NMR spectrum of complex **3c.(THF)** (* residual hexane unidentified products)

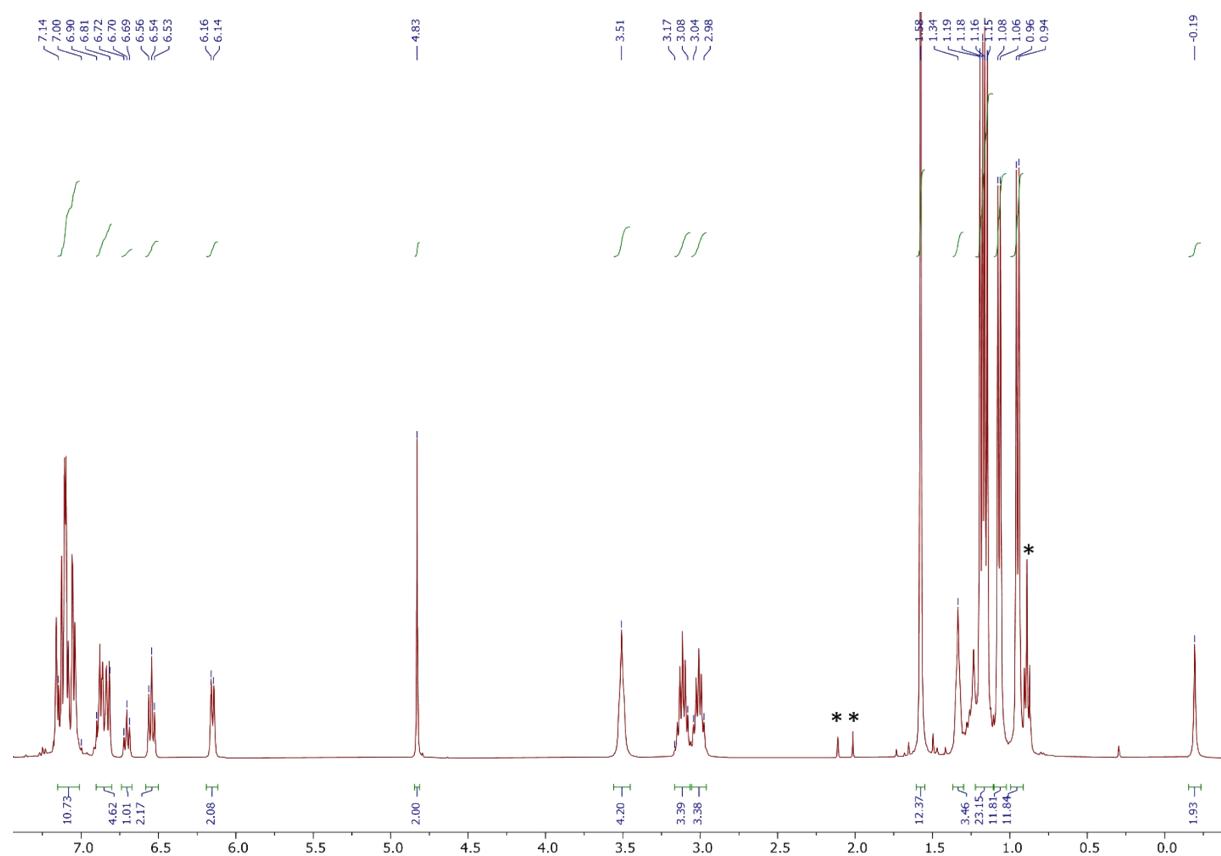


Figure S8: ^{13}C NMR spectrum of complex **3c.(THF)** (* residual hexane)

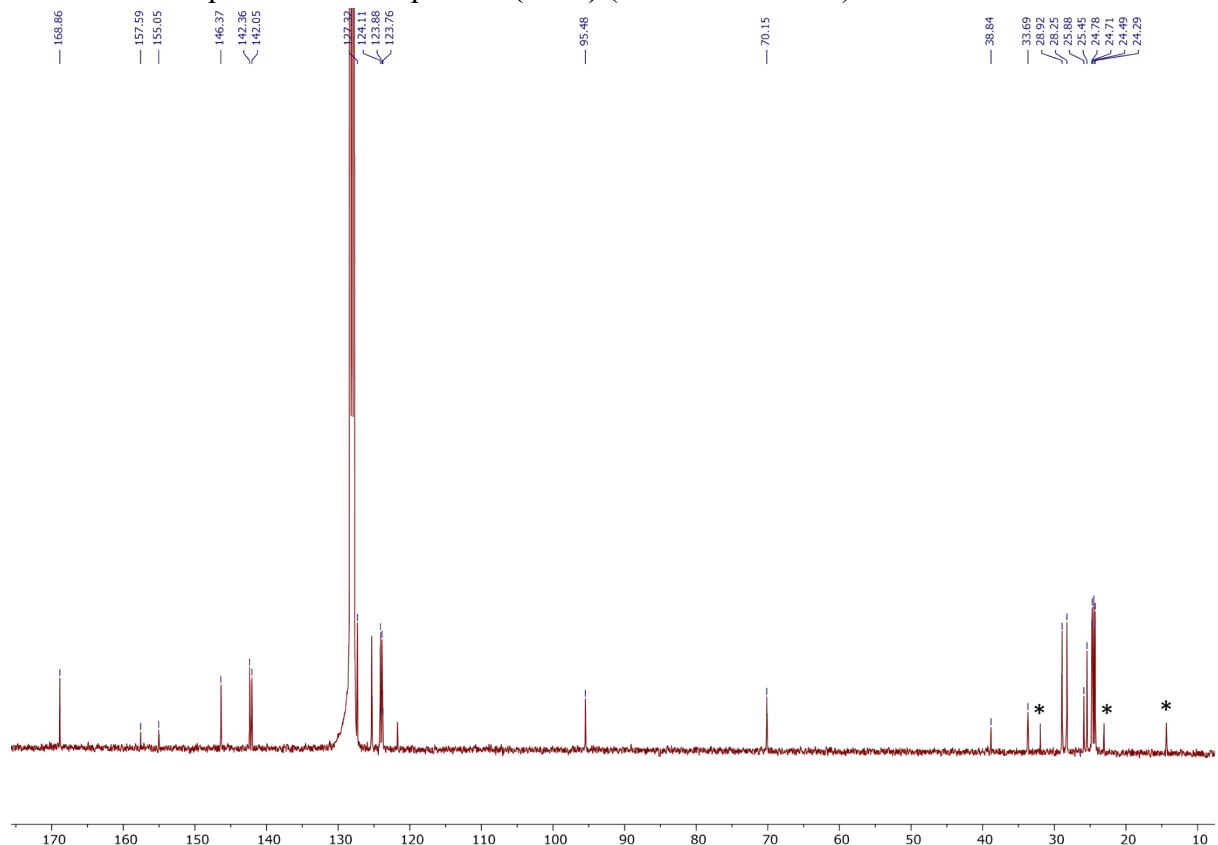


Figure S9: ^1H NMR spectrum of complex **4a.(DMAP)₂** (* residual hexane)

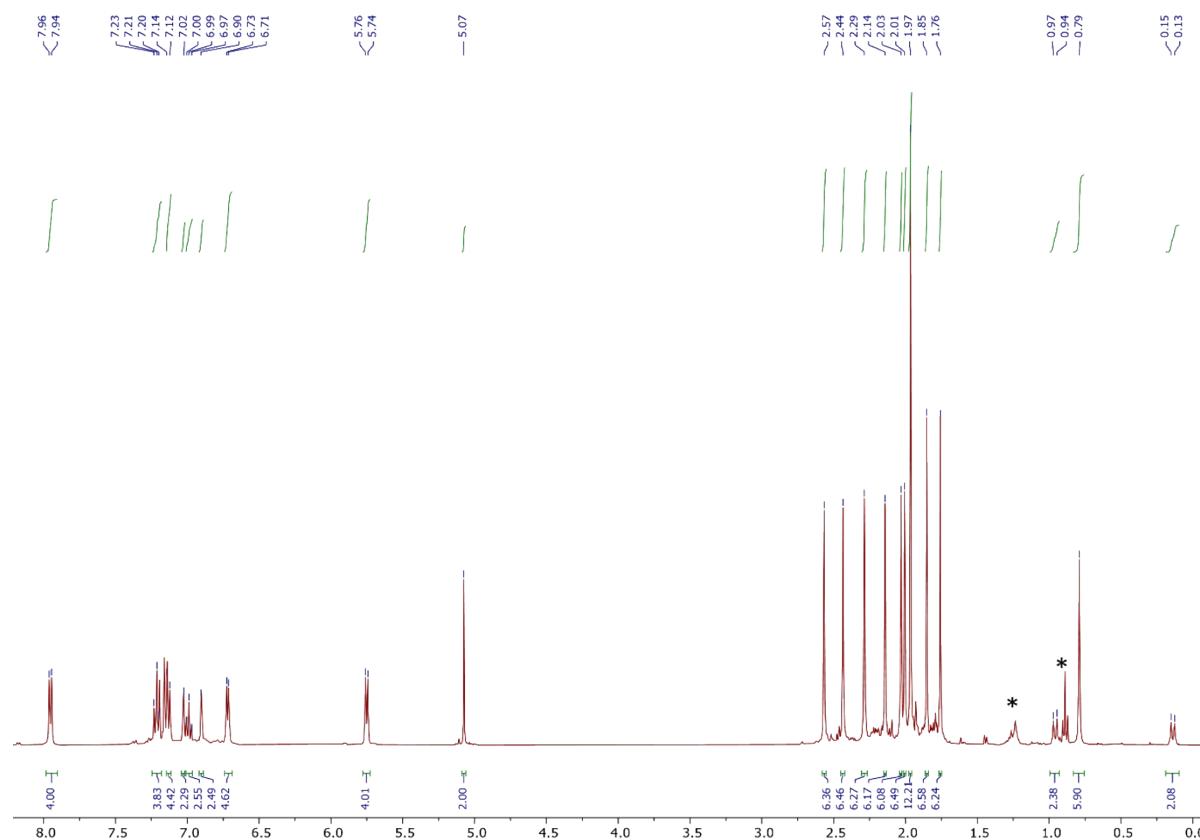


Figure S10: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **4a.(DMAP)₂** (* residual hexane)

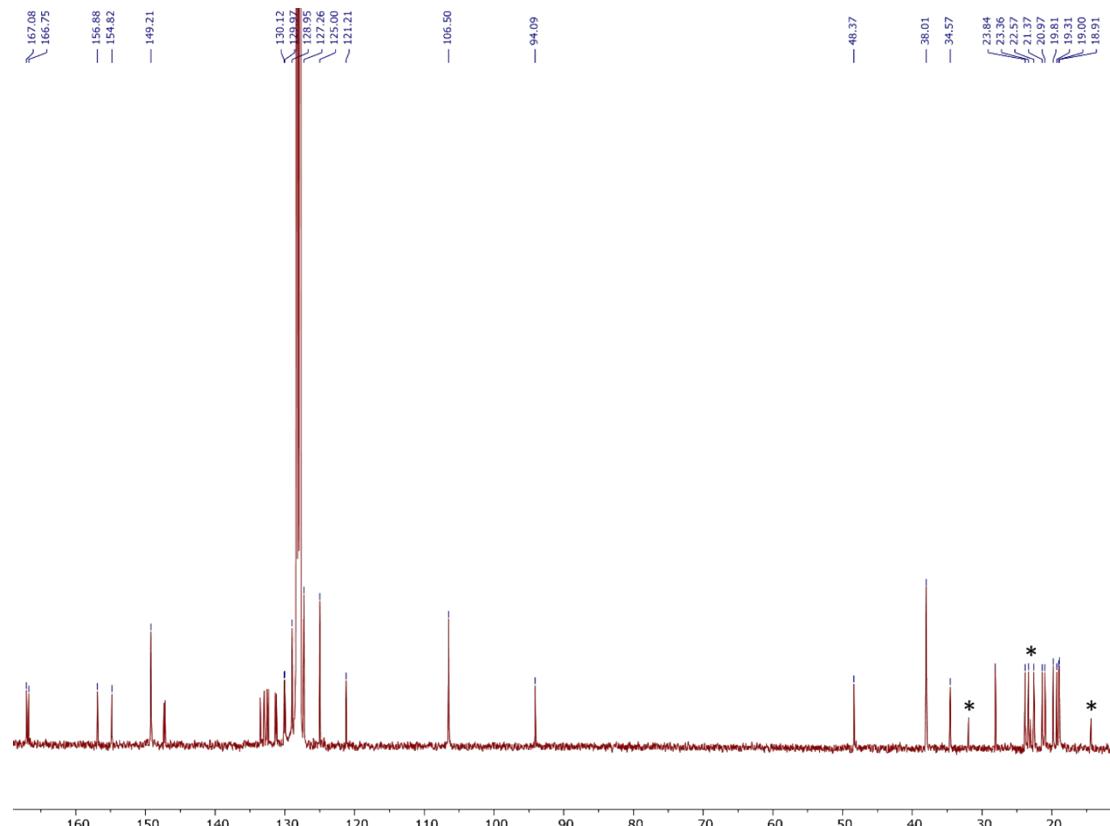


Figure S11: ^1H NMR spectrum of complex **4b.DMAP**

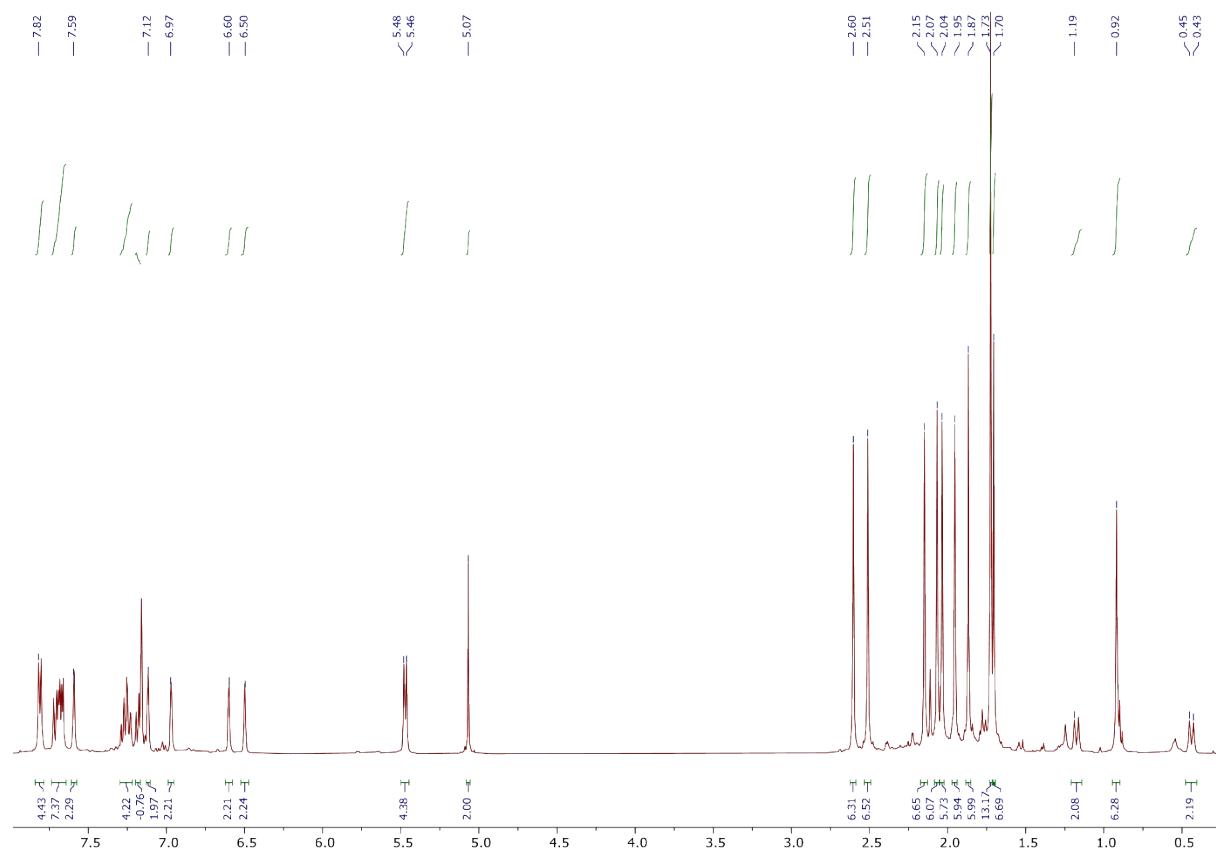


Figure S12: ^{13}C { ^1H } NMR spectrum of complex **4b.DMAP**

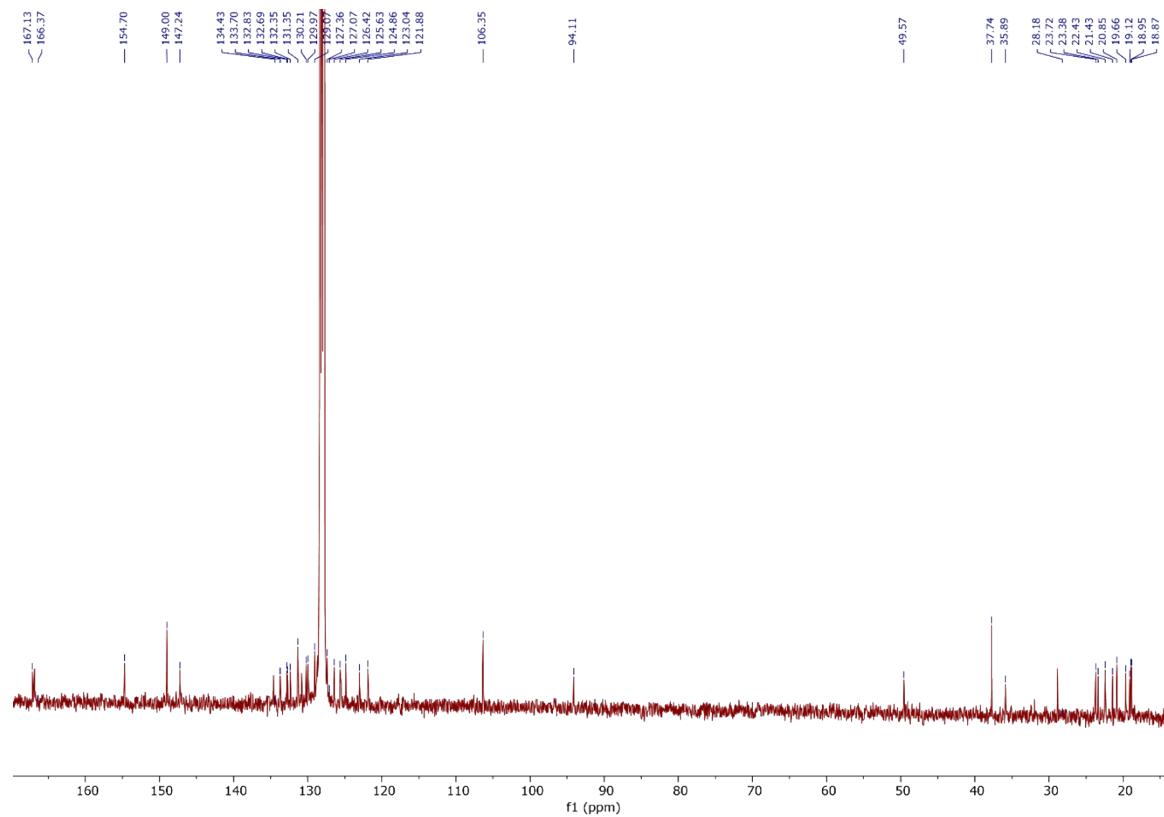


Figure S13: ^1H NMR spectrum of complex **3d** (* residual cyclopropane/unidentified product)

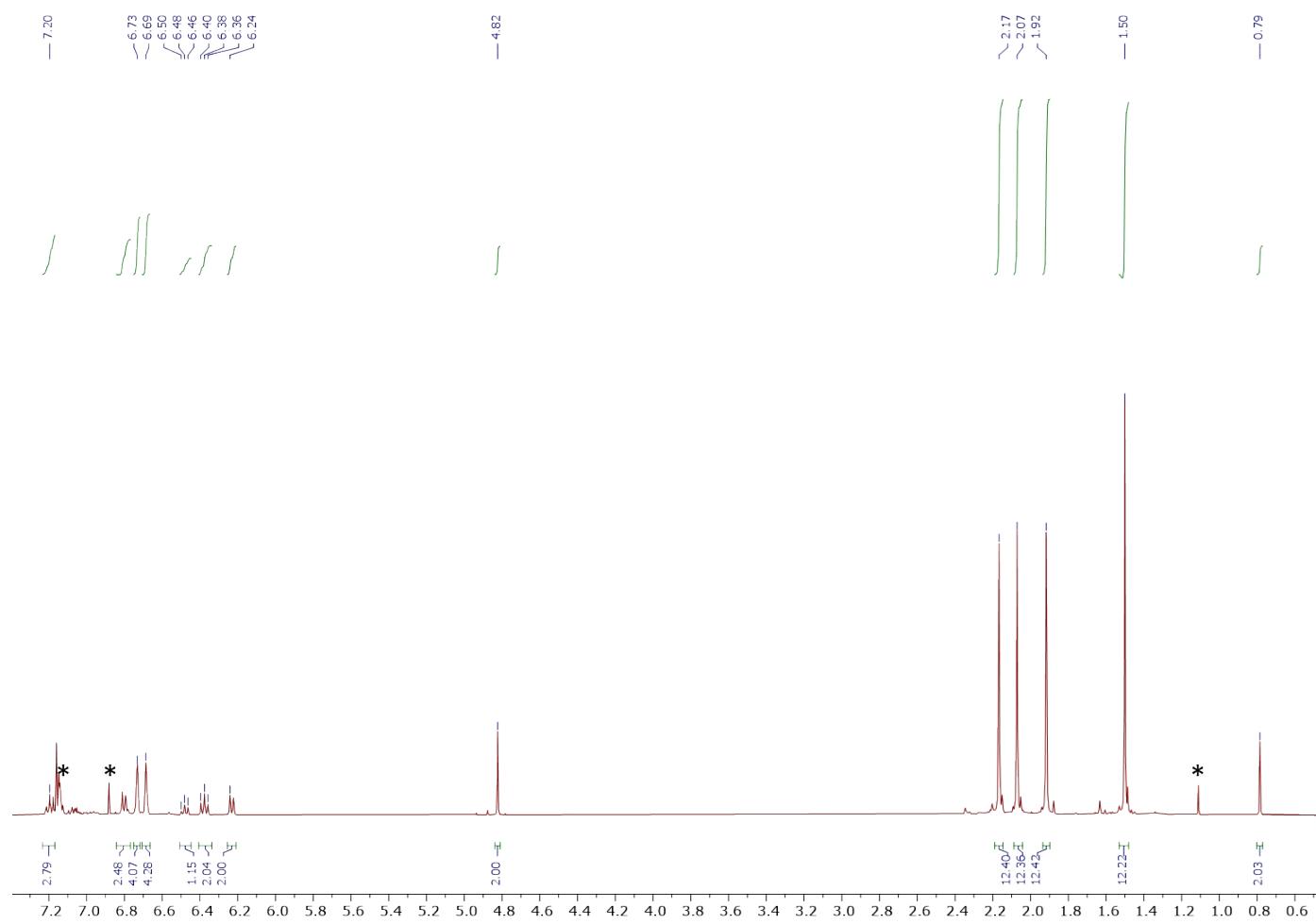


Figure S14: ^1H NMR spectrum of complex **4c.DMAP**

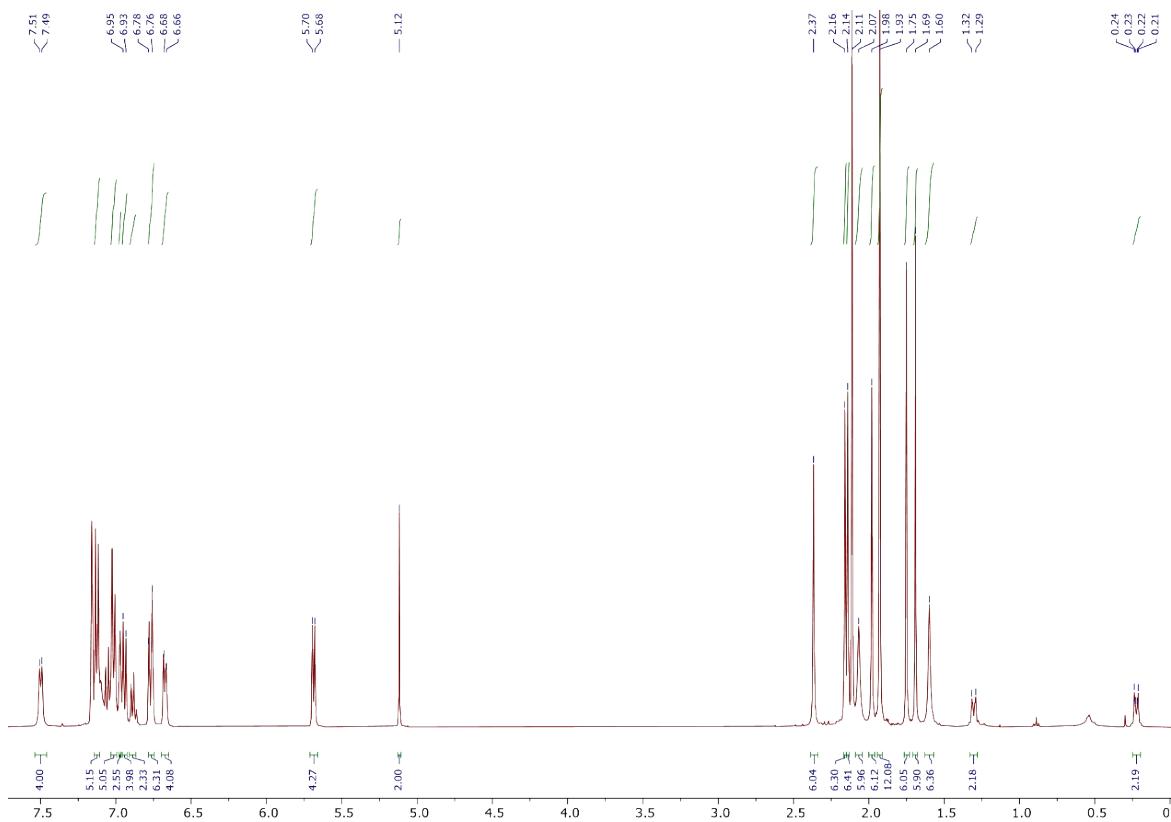


Figure S15: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **4c.DMAP**

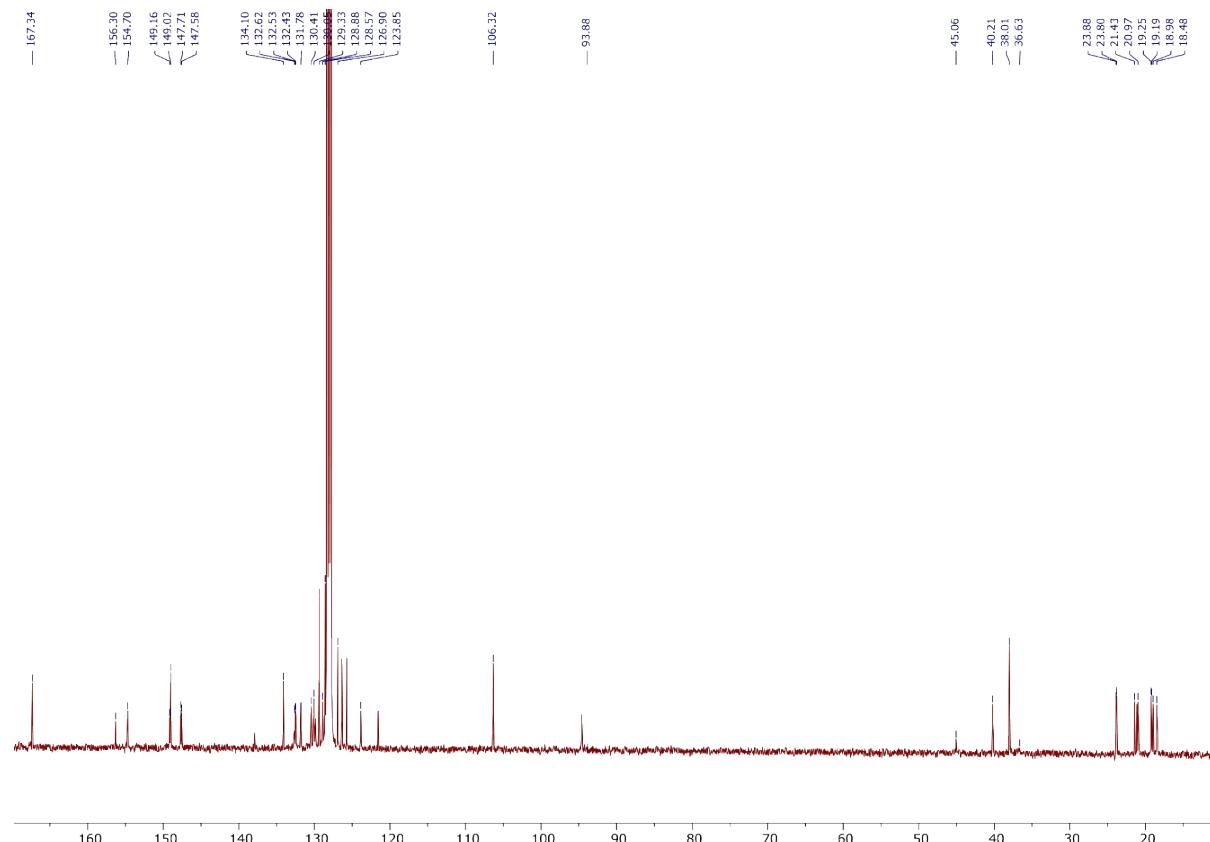


Figure S16: HSQC NMR spectrum of complex **4c.DMAP**

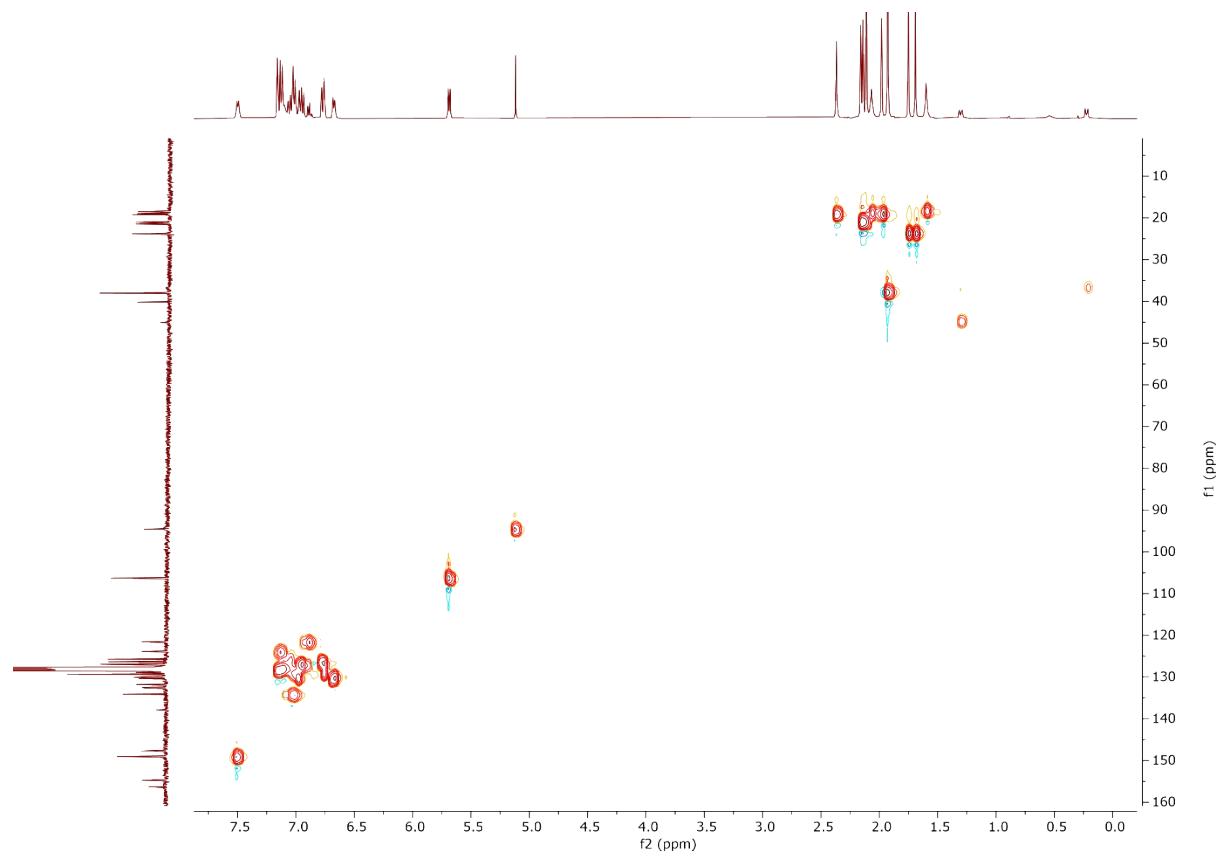


Figure S17: In situ ^1H NMR spectrum of complex **S2**

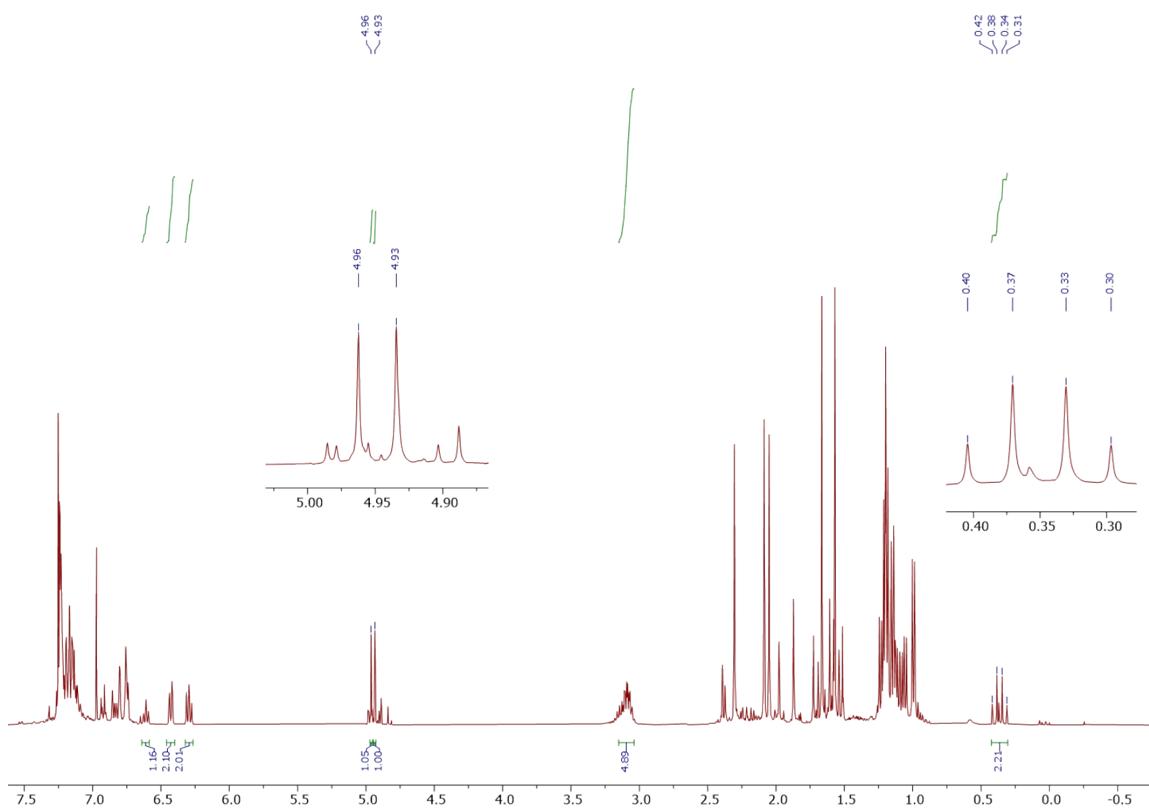


Figure S18: In situ $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **S2**

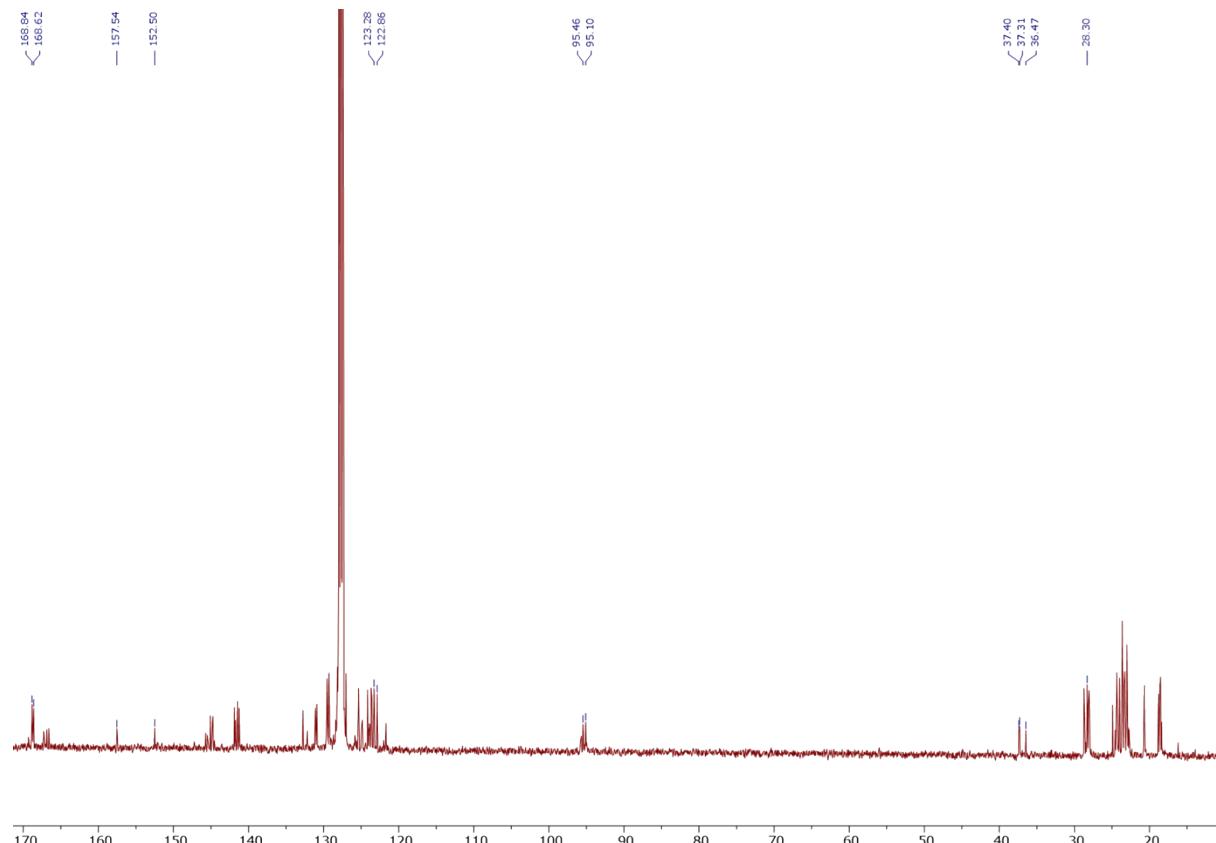


Figure S19: In situ HSQC NMR spectrum of complex S2

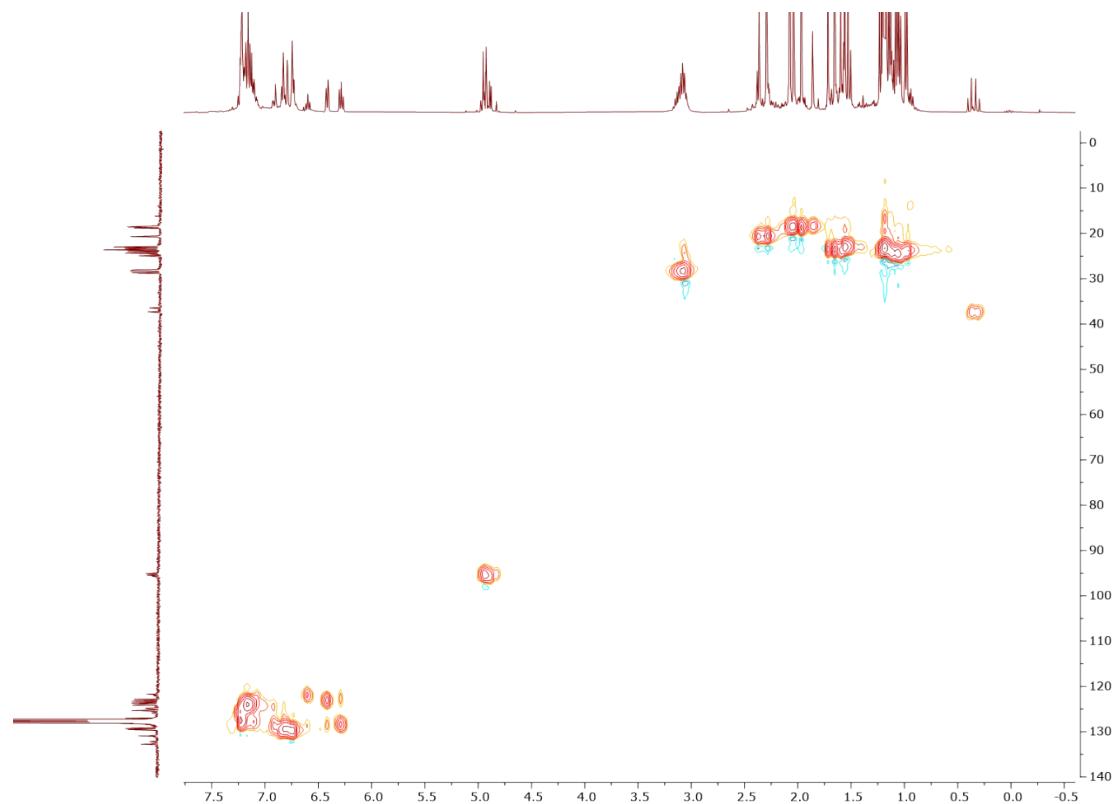


Figure S20: In situ HMBC NMR spectrum of complex S2

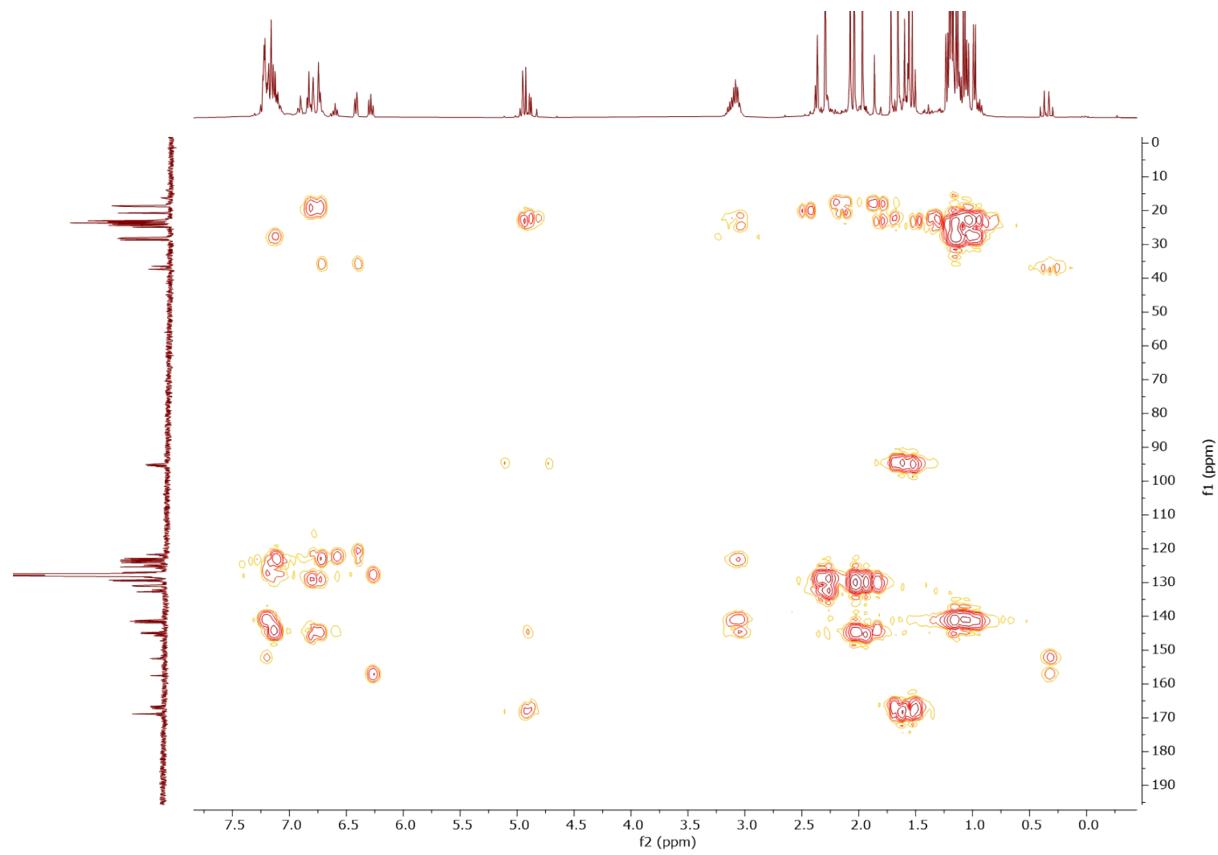


Figure S21: Stack plot of the reaction of **1a** (bellow) with **2a** to form **3a** (top).

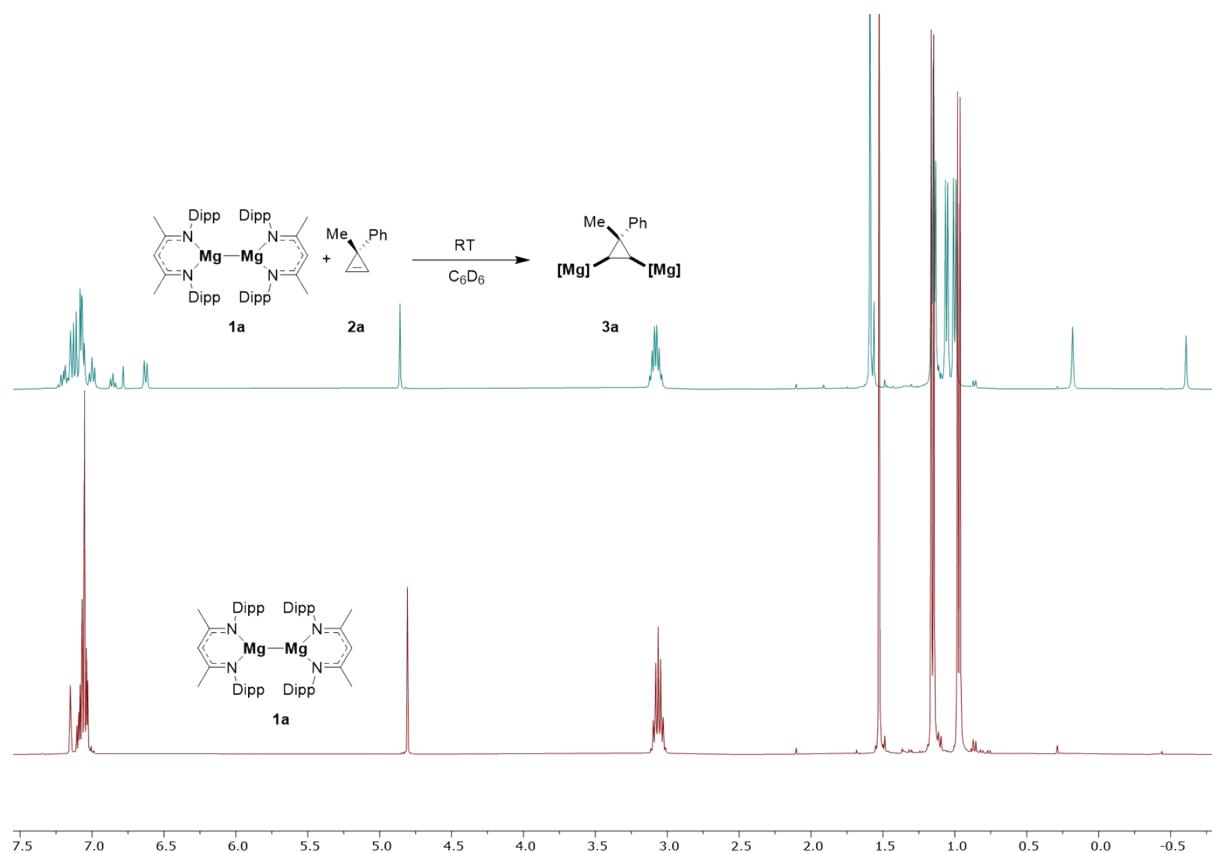


Figure S22: Stack plot of the reaction of **1a** (bellow) with **2b** to form **3b** (top).

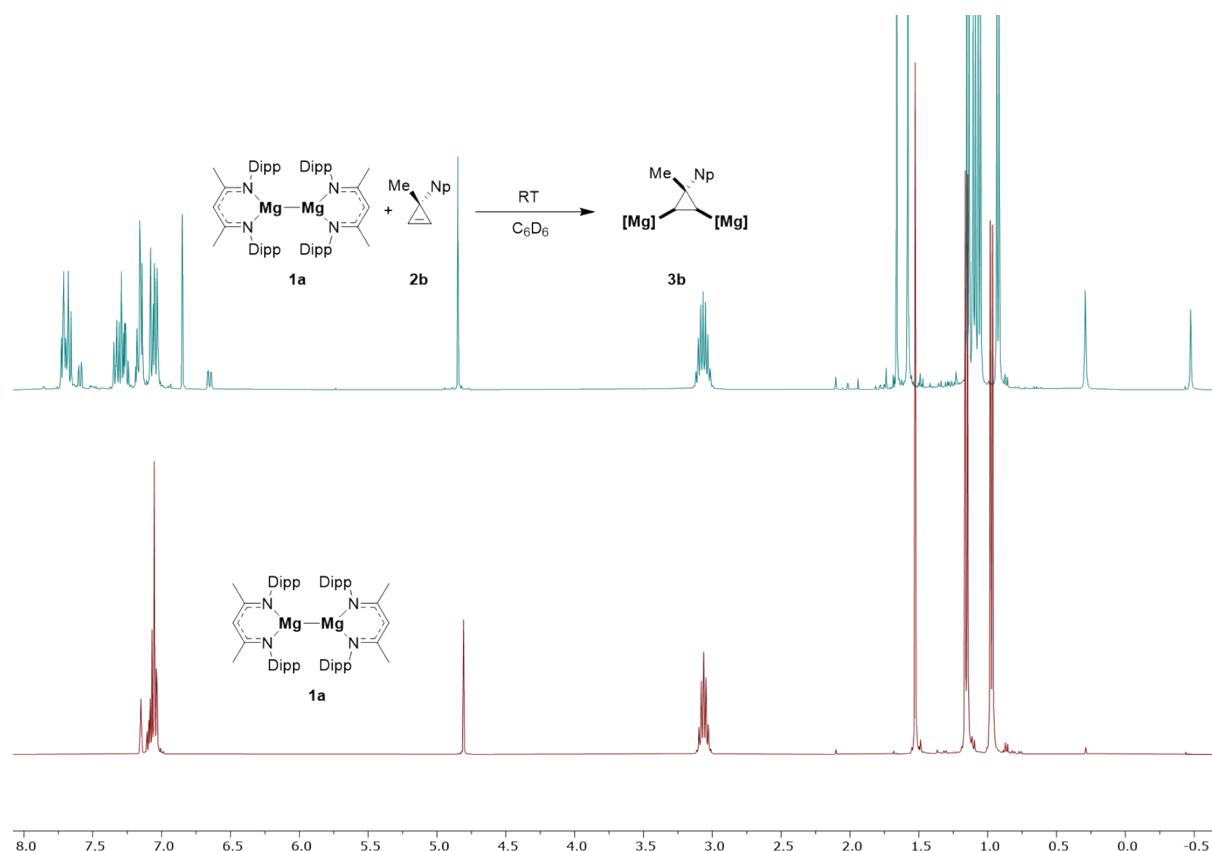


Figure S23: Stack plot of the reaction of **1a** (bellow) with **2c** to form **3c** (top).

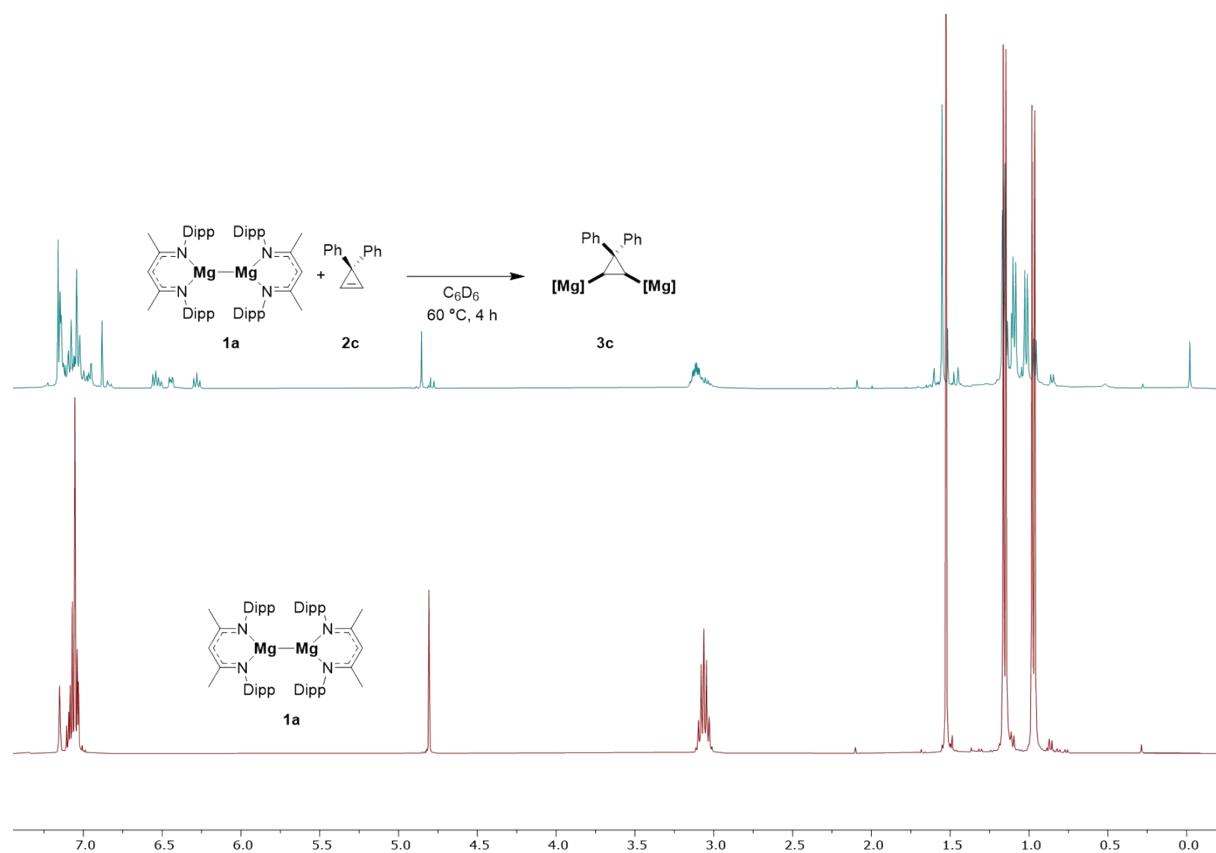


Figure S24: Stack plot of the reaction of **1b** (bellow) with **2a** to form **4a** (top).

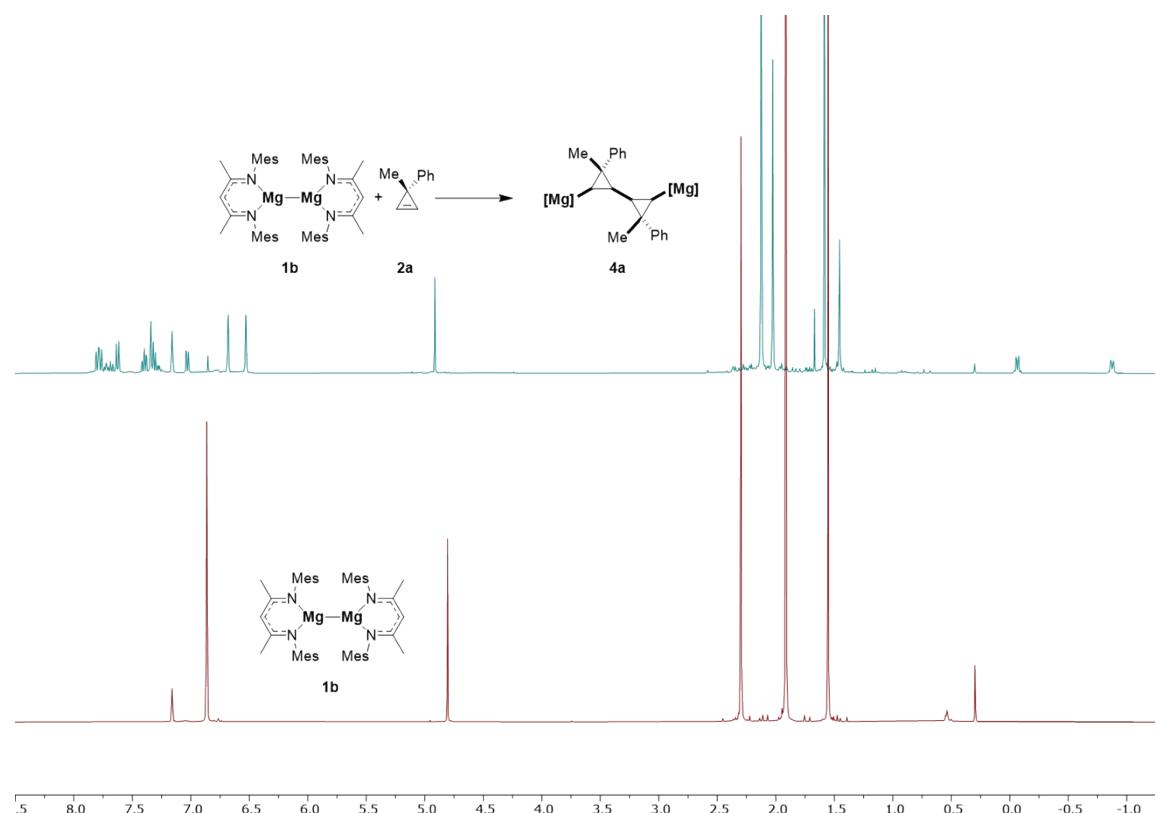


Figure S25: Stack plot of the reaction of **1b** (below) with **2b** to form **4b** (top).

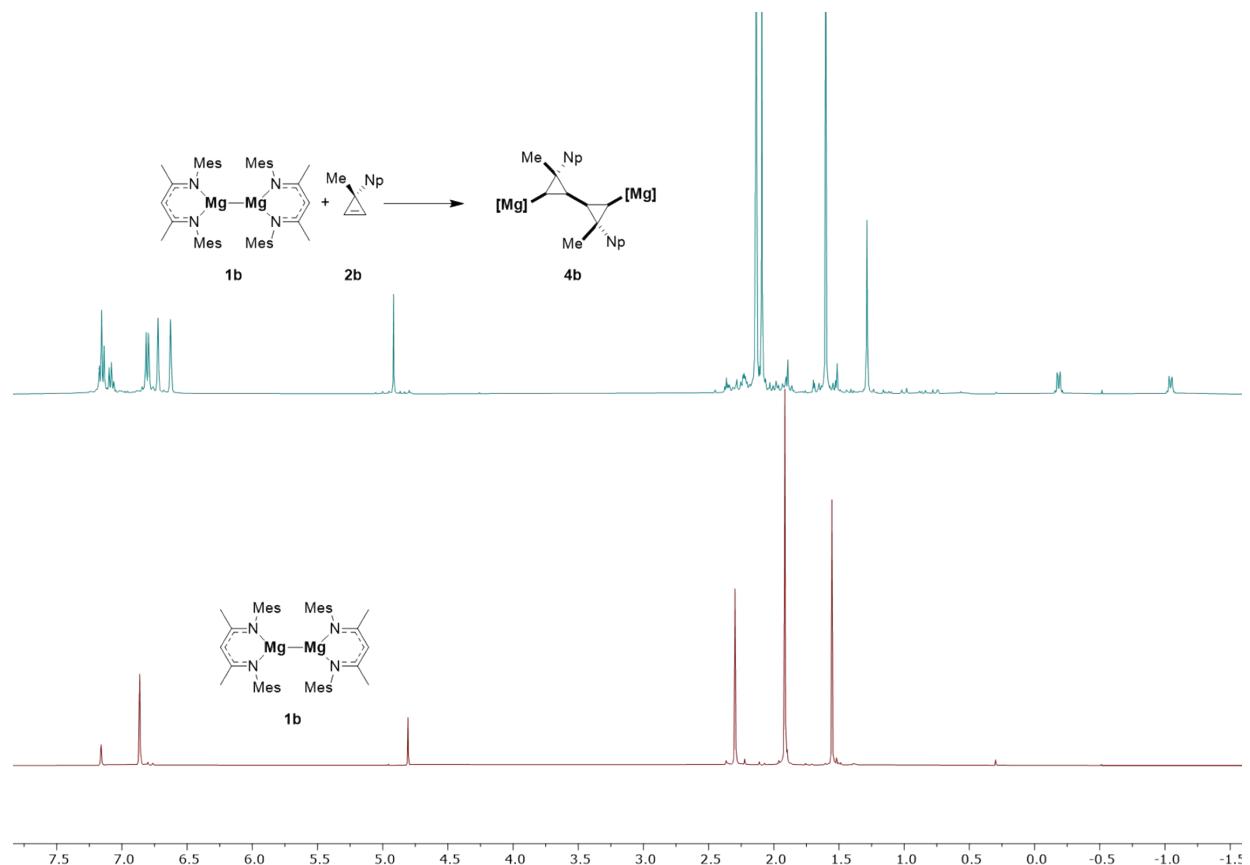
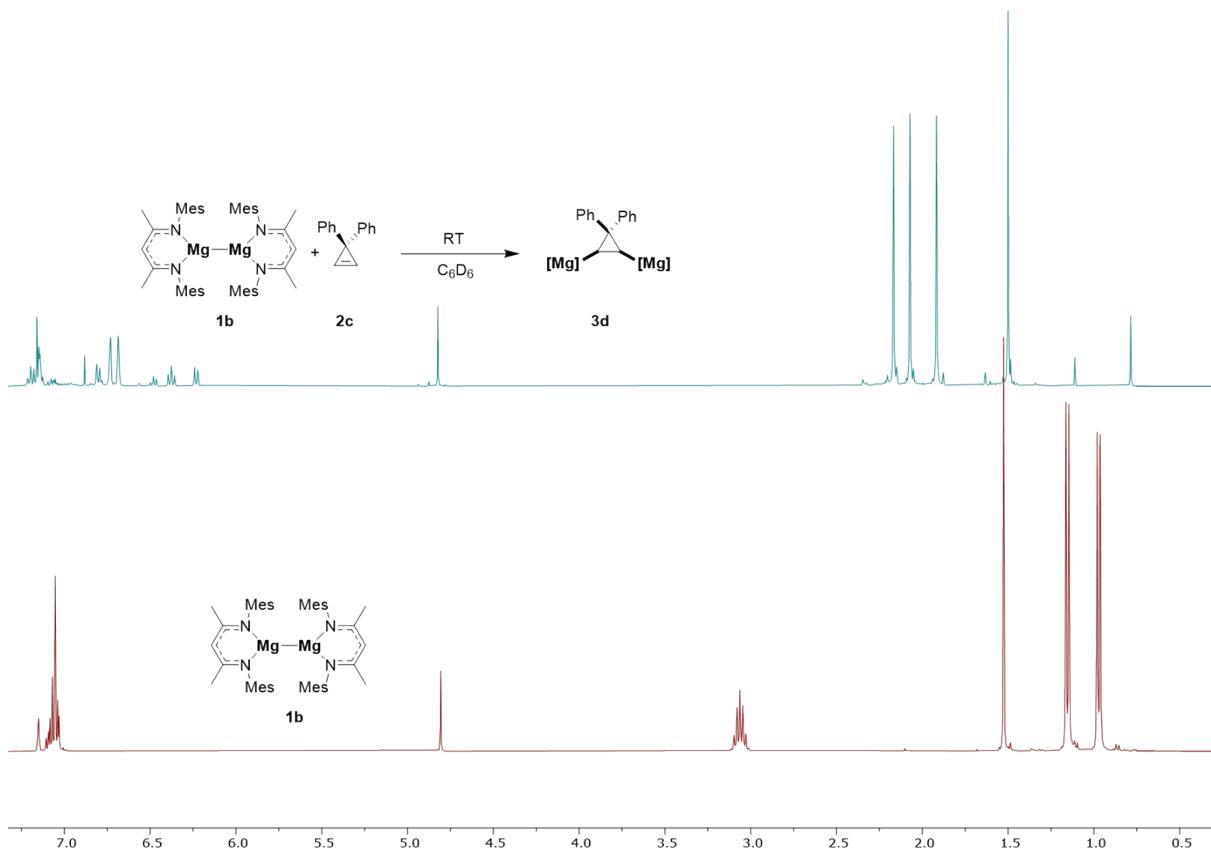


Figure S26: Stack plot of the reaction of **1b** (below) with **2c** to form **3d** (top).



4- X-ray Crystallographic Data

4-1- The X-ray crystal structure of 3a.(DMAP)₂

$C_{82}H_{112}Mg_2N_8 \cdot 4(C_7H_8)$, $M = 1626.94$, triclinic, $P-1$ (no. 2), $a = 13.7599(11)$, $b = 18.6960(13)$, $c = 22.2335(14)$ Å, $\alpha = 93.739(6)$, $\beta = 107.276(7)$, $\gamma = 110.812(7)^\circ$, $V = 5011.0(7)$ Å³, $Z = 2$, $D_c = 1.078$ g cm⁻³, $\mu(\text{Mo-K}\alpha) = 0.074$ mm⁻¹, $T = 173$ K, colourless needles, Agilent Xcalibur 3 E diffractometer; 20952 independent measured reflections ($R_{\text{int}} = 0.0533$), F^2 refinement,^{4,5} $R_1(\text{obs}) = 0.0872$, $wR_2(\text{all}) = 0.2439$, 8944 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$], completeness to $\theta_{\text{full}}(25.2^\circ) = 98.0\%$], 1157 parameters. CCDC 2173920.

The crystal of **3a.(DMAP)₂** that was studied was found to be a two component twin in a *ca.* 60:40 ratio, with the two lattices related by the approximate twin law [1.00 0.00 0.00 -0.97 -1.00 0.00 -0.96 0.00 -1.00]. The N43-bound 2,6-diisopropylphenyl group and the C81-based bridging cyclopropyl ligand (and the associated methyl and phenyl substituents) were found to be disordered, and in each case two orientations were identified, of *ca.* 66:34 and 53:47% occupancy respectively. The geometries of each pair of orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientations were refined anisotropically (those of the minor occupancy orientations were refined isotropically). The included toluene solvent was found to be distributed over six sites, two in general positions (based on C100 and C110) and four adjacent to centres of symmetry (based on C120, C130, C140 and C150) and thus only 50% occupancy. All bar the C110-based molecule were found to be disordered, and in each case two orientations were identified, of ca. 70:30, 28:22, 28:22, 30:20 and 28:22% occupancy for the C100, C120, C130, C140 and C150 molecules respectively. The geometries of each pair of orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientations were refined isotropically).

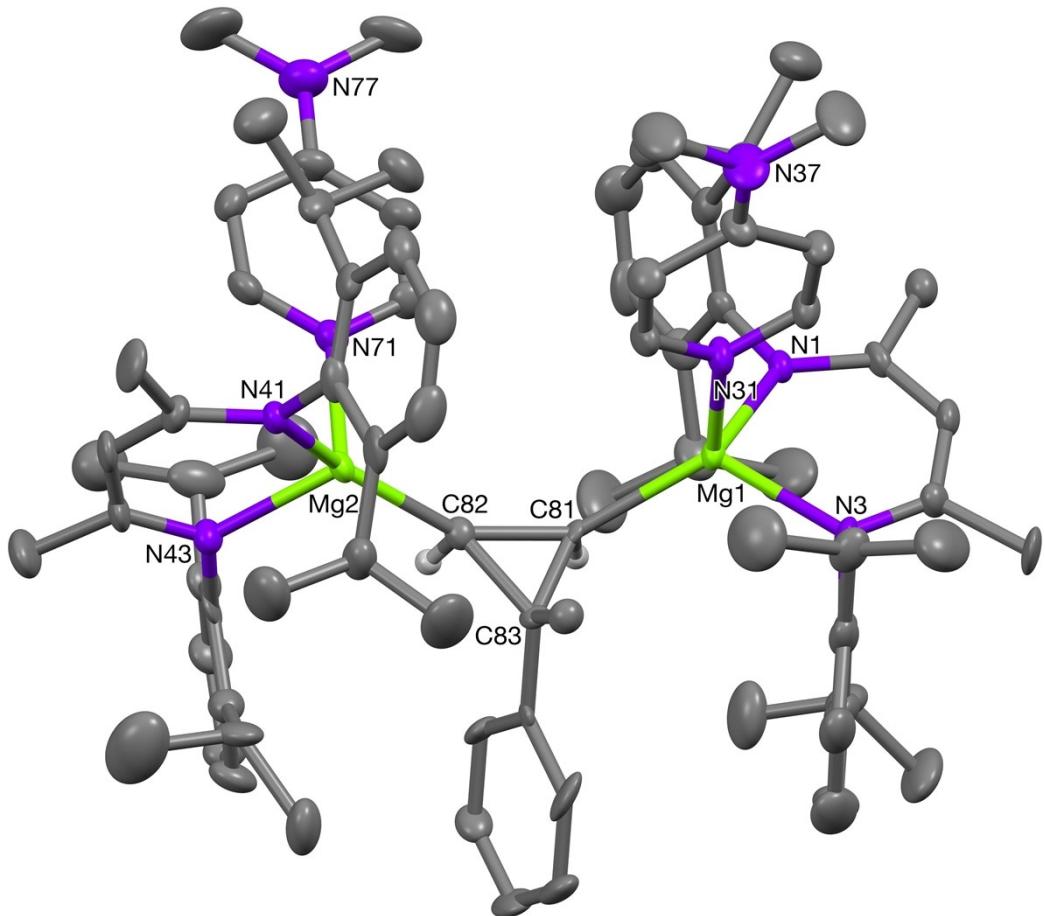


Fig. S27: The crystal structure of **3a.(DMAP)₂** (30% probability ellipsoids).

4-2- The X-ray crystal structure of 4c.(DMAP)₂

Crystal Data for C₉₅H₁₁₄Mg₂N₈, M=1416.56, monoclinic, space group I2/a (no. 15), a = 27.0624(13) Å, b = 15.1465(4) Å, c = 25.3866(13) Å, β = 121.506(7)°, V = 8872.0(9) Å³, Z = 4, ρ_{calc}g/cm³ = 1.061, μ(Cu Kα) = 0.596 mm⁻¹, T = 173.00(14), yellow blocks, F² refinement, R₁(obs) = 0.0612, wR₂(all) = 0.1836, 8461 independent observed reflections (R_{int} = 0.0583), 5234 independent measured reflections [|F_o| > 4σ(|F_o|), 2θ_{full} = 146.878], 461 parameters. CCDC 2173921.

4c.(DMAP)₂ was found to crystallise in the *I2/a* space group. The molecule was found to lie across a C₂ rotation axis which bisects the cyclopropane to cyclopropane C–C bond (C2–C2'). Accordingly, half the molecule was found in the asymmetric unit with the second half generated by symmetry relation, for a total of four molecules within the unit cell.

Two molecules of solvent were found to co-crystallise with the **4c.(DMAP)₂** in the asymmetric unit and found to be disordered across an element of symmetry in two orientations. Attempts to model the disordered molecules were unsuccessful. The SQUEEZE programme as implemented in PLATON⁶ was used to handle the disordered residual electron density. Prior to application of SQUEEZE, the disordered solvent most represented n-pentane. The SQUEEZE routine removed a total of 45 e- per asymmetric unit which is consistent with two half-occupancy molecules of pentane per asymmetric unit (2x0.5 pentane molecules corresponds to 42 e-).

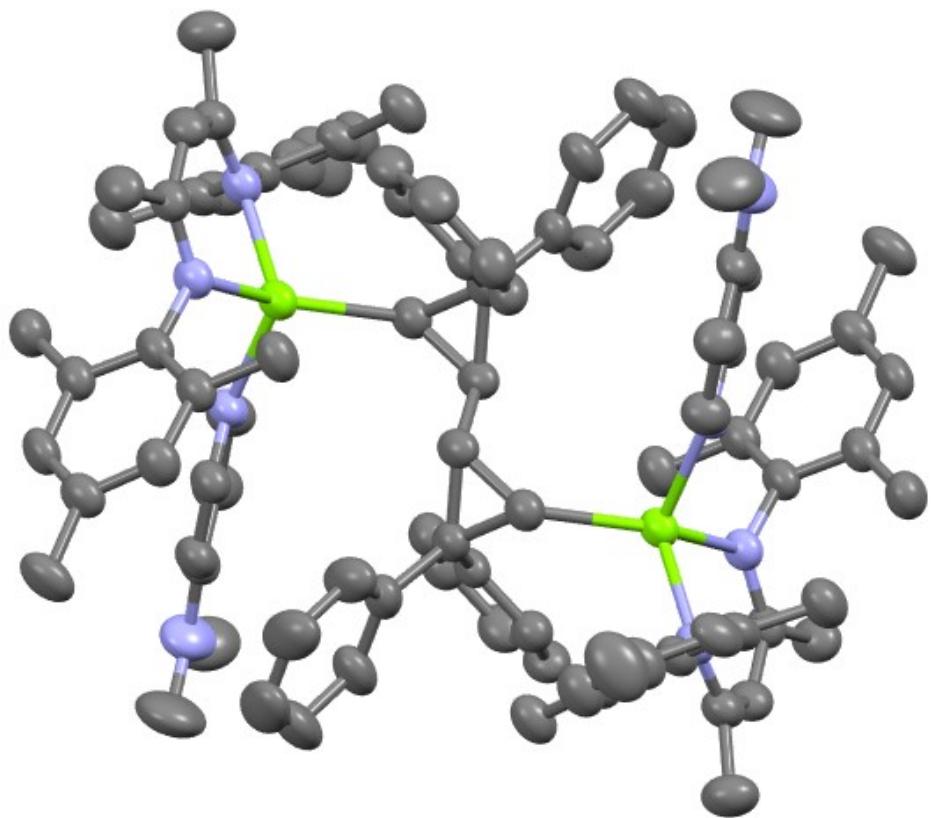


Fig. S28: The crystal structure of **4c.(DMAP)₂** (30% probability ellipsoids).

5- Computational details

5.1 Computational methods

All DFT computations were carried out with the Gaussian 09 (Revision D.01) program package.⁷ Geometry optimizations were performed in gas phase using B3PW91 density functional.⁸⁻¹² Pople's double- ζ basis set 6-31G(d,p) was adopted for H, C, N atoms.¹³ For Mg, the SDDAll basis set with effective core potential (ECP) was employed.^{14,15} Frequency analyses were performed at the same level to obtain thermal corrections at 298 K and to confirm the stationary points with zero imaginary frequency and transition states with only one imaginary frequency. Solution-phase single-point were calculated using the PCM solvation model in benzene,¹⁶ B3PW91 functional with Grimme's D3(BJ) dispersion,^{17,18} and the triple- ζ basis set def2-TZVP with ECP was used for all atoms.^{19,20} All discussed energy differences were based on free energies at 298 K (standard states are the hypothetical states at 1 mol/L). NBO analysis was performed using the NBO 6.0 version program.²¹ Non-covalent interactions were analysed with the NCIPILOT 3.0 program.²² QTAIM analysis was conducted with the AIMAll package.²³ Three-dimensional structures were prepared with the CYLview program.²⁴ NCI plots were generated with the VMD visualized program.²⁵

5.2 QTAIM analysis of TS-1 and TS-2

Quantum theory of atoms in molecules (QTAIM) analysis of **TS-1** and **TS-2** reveals that two bond critical points (BCP) are exist between Mg and C atoms in **TS-1** while only one BCP in **TS-2**, indicating that **TS-1** is predicted to be the later transition state than **TS-2**, which is consistent with the computational structures that Mg–C bond distances in **TS-1** are shorter than **TS-2** (Figure 2). The electron density at the BCP (ρ) between Mg and Mg in **TS-1** and **TS-2** are found to be small to 0.023. This result suggests that the insertion reaction is primarily an ionic addition as proposed by our mechanistic studies. QTAIM analysis shows that the syn-addition transition state from Me face (**TS-1**) has more non-covalent interactions between **1b** and **2a** than **TS-2**. These non-covalent interactions could contribute to the lower free energy barrier for **TS-1** and Me-facial selective product (**Int-2**).

	TS-1		TS-2	
	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
Mg1–Mg2	0.0229	-0.0039	Mg1–Mg2	0.0230
Mg1–C1	0.0250	0.1049	Mg1–C1	0.0255
Mg2–C1	0.0225	-0.0074	C3–H(Mes)	0.0048
C2–H(Mes)	0.0034	0.0120	H1–H(Mes)	0.0065
C3–H(Mes)	0.0100	0.0258	H2–H(Mes)	0.0062
C3–H(Mes)	0.0068	0.0224	H3–C(Mes)	0.0030
H1–C(Mes)	0.0082	0.0238	C7–H(Mes)	0.0012
C4–H(Mes)	0.0046	0.0190	H6–C(Mes)	0.0051
H3–H(Mes)	0.0023	0.0076	H7–C(Mes)	0.0058
H5–C(Mes)	0.0065	0.0186	H8–C(Mes)	0.0070
C5–H(Mes)	0.0036	0.0121		
C6–C(Mes)	0.0033	0.0094		

Table S1. QTAIM parameters on **TS-1** and **TS-2**.

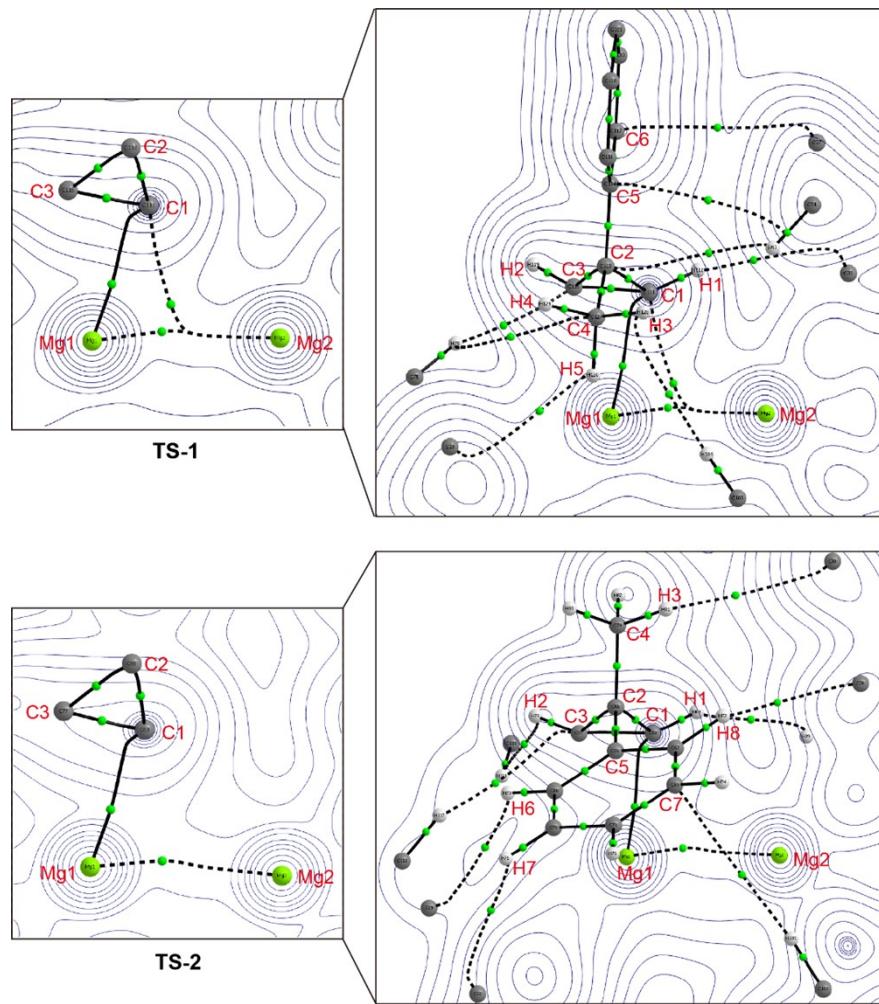


Figure S29. QTAIM molecular graphs for **TS-1** and **TS-2** showing key bond paths (black or dotted lines) and bond critical points (BCPs, green points).

5.3 DFT study on the first and second insertion between **1b** and **2c**

The reaction starts with the formation of a weak van der Waals complex **Int-1_1b2c** between the substrates **1b** and **2c**, which is calculated to lie above the reactants by 3.4 kcal mol⁻¹. Subsequently, **Int-1_1b2c** experiences a stereoselective syn-addition transition state **TS-1_1b2c** to form the first insertion intermediate **Int-2_1b2c** ($\Delta G^\circ(298K) = -33.4$ kcal mol⁻¹). **Int-2_1b2c** then combines with the second molecular **2c** to generate the intermediate **Int-5_1b2c**. Finally, the second insertion occurs via syn-addition transition state **TS-4_1b2c** to form the second insertion product **Int-6_1b2c** ($\Delta G^\circ(298K) = -80.5$ kcal mol⁻¹). DFT calculations indicate that the activation free energy for the first insertion is 6.6 kcal mol⁻¹ (**TS-1_1b2c**) and the second is 15.8 kcal mol⁻¹ (**TS-4_1b2c**), which are energetically feasible under the experimental conditions.

The concerted anti-addition pathway for the first insertion is also studied. Anti-addition of **Int-1_1b2c** via transition state **TS-3_1b2c** gives the intermediate **Int-4_1b2c**, which is predicted to be more thermodynamically stable than the syn-addition intermediate ($\Delta G^\circ(298K) = -39.4$ kcal mol⁻¹). However, the free energy barrier for the anti-addition via **TS-3_1b2c** is much higher than the syn-addition via **TS-1_1b2c** (26.6 kcal mol⁻¹ versus 6.6 kcal mol⁻¹), suggesting that anti-addition is energetically unfavourable.

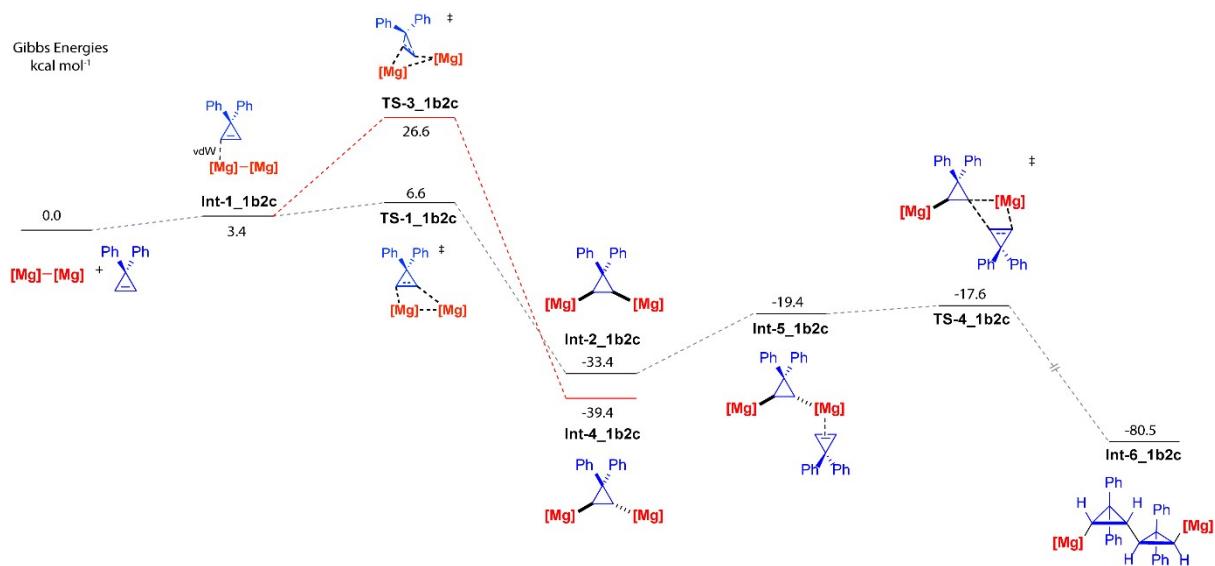
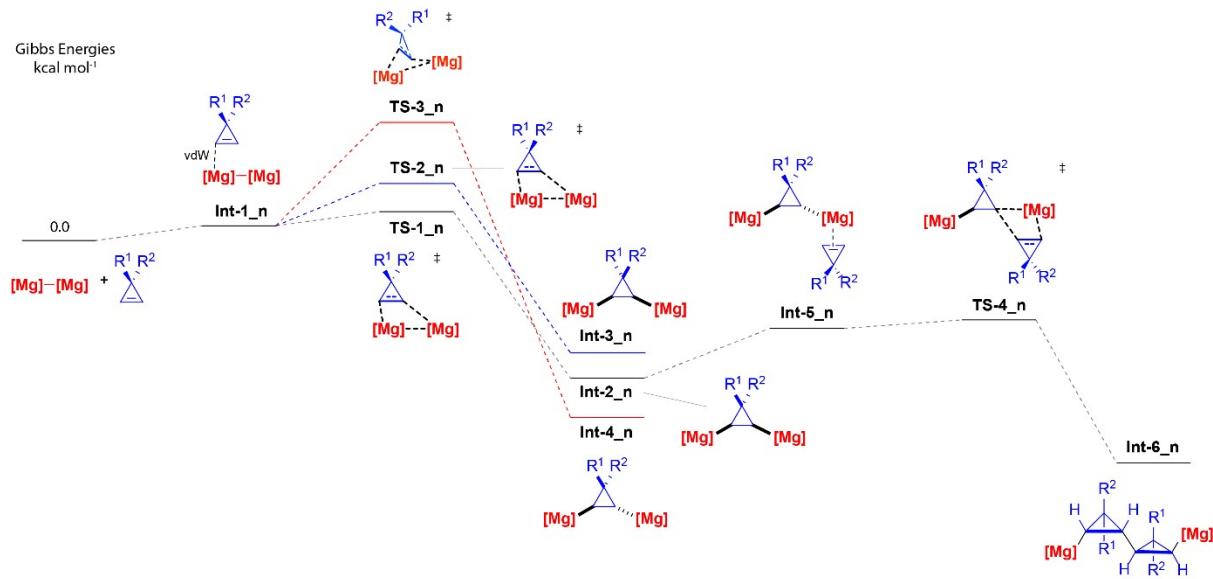


Figure S30. Free energy profile for mechanism of the first and second insertion between **1b** and **2c**. Computed at the PCM (benzene) / B3PW91-D3(BJ) / def2-TZVP// B3PW91 / SDDAll-6-31G(d,p) level. Gibbs energies, values in kcal mol⁻¹.

5.4 Mechanism of the insertion reaction for all the other substrates

The DFT studies reveal that the stereo- and facial-selectivity for the substrates used in experimental studies (**1a/1b** and **2a/2b/2c**) are predicted to be similar. For all the substrates, the insertion reactions proceed under kinetic control and occur through syn-addition pathway (**TS-1_n**) which is favoured over anti-addition pathway (**TS-3_n**). For the cyclopropenes with different R groups ($R^1 \neq R^2$, **2a** and **2b**), the insertion reactions (**1a2a**, **1a2b**, **1b2a** and **1b2b**) favour addition to the less hindered face. In all cases, approach of the Mg–Mg reagent occurs toward the face with the methyl substituent (**TS-1_n**). This approach leads to lower free energy barriers ($> 3 \text{ kcal mol}^{-1}$) for the insertion step than the alternative approach to the face with phenyl or naphthyl substituent (**TS-2_n**).

Considering the chemoselectivity, with **1b2c** the second insertion step requires free energy barriers $15.8 \text{ kcal mol}^{-1}$ (**TS-4_1b2c**), while with **1a2c** higher activation free energies of 22 kcal mol^{-1} (**TS-4_1a2c**) are needed. These calculations suggest that the formation of the double insertion products should be more favourable for **1b** relative to **1a**, which is consistent with the experimental findings.



Substrates	Int-1_n	TS-1_n	TS-2_n	TS-3_n	Int-2_n	Int-3_n	Int-4_n	Int-5_n	TS-4_n	Int-6_n
1a + 2a	4.6	9.2	14.7	33.6	-29.1	-28.3	-30.3			
1a + 2b	4.7	8.4	12.9	32.8	-30.9	-31.0	-31.8			
1a + 2c	3.8	12.4	/	29.7	-28.6	/	-33.3	-25.6	-6.6	-77.3
1b + 2a	3.8	5.7	9.3	30.7	-29.0	-26.5	-34.2			
1b + 2b	2.8	5.1	8.6	30.0	-30.3	-33.2	-34.9			

Figure S31. Free energy profile for mechanism of the first and second insertion between **1a/1b** and **2a/2b/2c**. Computed at the PCM (benzene) / B3PW91-D3(BJ) / def2-TZVP//B3PW91 / SDDAll-6-31G(d,p) level. Gibbs energies, values in kcal mol⁻¹.

5.5 Computed energies of the stationary points

Table S2. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs)

	TCG ^{a,b} (a.u.)	SPE ^a (a.u.)	SPE ^c (a.u.)
1a	1.163961	-2479.576335	-2879.168331
1b	0.826963	-2008.014557	-2407.355934
2a	0.132208	-386.854691	-387.019352
2b	0.175683	-540.441450	-540.673306
2c	0.179288	-578.516550	-578.767760
Int-1	0.972931	-2394.869859	-2794.382951
Int-1_1a2a	1.310432	-2866.432449	-3266.194644
Int-1_1a2b	1.350360	-3020.018099	-3419.844909
Int-1_1a2c	1.358363	-3058.094558	-3457.945215
Int-1_1b2b	1.013916	-2548.457875	-2948.03608
Int-1_1b2c	1.020781	-2586.531699	-2986.132816
TS-1	0.986047	-2394.848573	-2794.393135
TS-1_1a2a	1.322220	-2866.404406	-3266.199048
TS-1_1a2b	1.365491	-3019.991243	-3419.854048
TS-1_1a2c	1.374354	-3058.054754	-3457.94737
TS-1_1b2b	1.028984	-2548.435295	-2948.047431
TS-1_1b2c	1.032756	-2586.502103	-2986.139630
Int-2	0.982112	-2394.911009	-2794.444365
Int-2_1a2a	1.320350	-2866.478918	-3266.258263
Int-2_1a2b	1.361198	-3020.066028	-3419.912471
Int-2_1a2c	1.370865	-3058.130182	-3458.009346
Int-2_1b2b	1.025872	-2548.499342	-2948.10075
Int-2_1b2c	1.034689	-2586.573104	-2986.205342
TS-2	0.983459	-2394.838268	-2794.384713
TS-2_1a2a	1.324131	-2866.392212	-3266.192196
TS-2_1a2b	1.367368	-3019.979313	-3419.848808
TS-2_1b2b	1.031437	-2548.426495	-2948.044343
Int-3	0.985178	-2394.904849	-2794.443553
Int-3_1a2a	1.318779	-2866.472796	-3266.255383
Int-3_1a2b	1.362338	-3020.060453	-3419.913749
Int-3_1b2b	1.029336	-2548.498208	-2948.108886
TS-3	0.981329	-2394.80942	-2794.348551
TS-3_1a2a	1.320899	-2866.370249	-3266.158915
TS-3_1a2b	1.363846	-3019.957001	-3419.813608
TS-3_1a2c	1.369171	-3058.032316	-3457.914665
TS-3_1b2b	1.024867	-2548.395854	-2948.003666
TS-3_1b2c	1.031935	-2586.471106	-2986.10695
Int-4	0.979130	-2394.92024	-2794.449805
Int-4_1a2a	1.318905	-2866.482797	-3266.258755
Int-4_1a2b	1.364536	-3020.071339	-3419.917228
Int-4_1a2c	1.368830	-3058.142993	-3458.01475
Int-4_1b2b	1.022189	-2548.505601	-2948.104396
Int-4_1b2c	1.032394	-2586.587554	-2986.212654
Int-5_1a2c	1.566908	-3636.648093	-4036.789077

Int-5_1b2c	1.233456	-3165.069927	-3564.970351
TS-4_1a2c	1.581300	-3636.597593	-4036.773055
TS-4_1b2c	1.241709	-3165.052900	-3564.975702
Int-6_1a2c	1.582236	-3636.724642	-4036.886715
Int-6_1b2c	1.241799	-3165.163574	-3565.076057

^aComputed at the B3PW91/SDDAll-6-31G(d,p) level.

^bA standard state at 1atm and 298 K was used.

^cComputed at the PCM (benzene) / B3PW91-D3(BJ) / def2-TZVP// B3PW91 / SDDAll-6-31G(d,p) level.

References:

1. S. J. Bonyhady, C. Jones, S. Nembenna, A. Stasch, A. J. Edwards, G. J. McIntyre, *Chem. Eur. J.* **2010**, *16*, 938–955.
2. C. Bakewell, A. J. P. White, M. R. Crimmin, *J. Am. Chem. Soc.* **2016**, *138*, 12763–12766.
3. K. Kramer, P. Leong, M. Lautens, *Org. Lett.*, **2011**, Vol. 13, No. 4.
- 4- SHELXTL v5.1, Bruker AXS, Madison, WI, 1998.
5. SHELX-2013, G.M. Sheldrick, *Acta Cryst.*, 2015, C71, 3-8.
6. A.L. Spek (2003, 2009) PLATON, A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands. See also A.L.Spek, *Acta Cryst.*, 2015, C71, 9-18
7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, M. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, revision D.01*, Gaussian, Inc., Wallingford, CT, 2016.
8. A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648.
9. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.
10. J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev. B* **1992**, *46*, 6671–6687.
11. J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev. B* **1993**, *48*, 4978.
12. J. P. Perdew, K. Burke and Y. Wang, *Phys. Rev. B* **1996**, *54*, 16533–16539.
13. W. J. Hehre, L. Radom, P. V. R. Schleyer and J. A. Pople, *Ab Initio Molecular Orbital Theory*; Wiley: New York, NY, USA, 1986.
14. T. H. Dunning and P. J. Hay, *Modern Theoretical Chemistry*; Plenum: New York, NY, USA, 1–28.
15. G. Igel-Mann, H. Stoll and H. Preuss, *Mol. Phys.* **1988**, *65*, 1321–1328.

16. J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* **2005**, *105*, 2999–3094.
17. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.
18. S. Grimme, S. Ehrlich and L. J. Goerigk, *Comput. Chem.* **2011**, *32*, 1456–1465.
19. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.
20. D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theor. Chim. Acta* **1990**, *77*, 123–141.
21. E. D. Glendening, C. R. Landis and F. Weinhold, *J. Comput. Chem.* **2013**, *34*, 1429–1437.
22. E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen and W. Yang, *J. Am. Chem. Soc.* **2010**, *132*, 6498–6506.
23. AIMAll (Version 13.10.19), Todd A. Keith, TK Gristmill Software, Overland Park KS, USA, 2013 (aim.tkgristmill.com)
124. C. Y. Legault, CYLview, 1.0b, Université de Sherbrooke: Quebec, Canada, 2009, <http://www.cylview.org>.
25. W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graphics*, **1996**, *14*, 33–38.

5-6- Cartesian coordinates of the stationary points

1a			
Mg	1.19276800	0.86895900	0.28723700
Mg	-1.19448100	-0.86994900	0.28319200
N	3.07854900	0.87762700	1.23380200
N	1.54676900	2.75245000	-0.57299700
N	-1.54572100	-2.74997200	-0.58567100
N	-3.08141800	-0.88351200	1.22672100
C	4.97978700	2.02234400	2.32496900
C	3.73942700	2.02120000	1.45403300
C	3.41296100	3.26503600	0.88465100
C	2.48751300	3.58468800	-0.12843200
C	2.61814400	4.97005500	-0.72438900
C	3.72662400	-0.32994900	1.65433500
C	3.37446200	-0.96010400	2.87019400
C	4.06535700	-2.11352200	3.25851800
C	5.06662200	-2.66211000	2.46871700
C	5.37797700	-2.06147700	1.25492100
C	4.72725800	-0.90111600	0.82746900
C	2.27584500	-0.43097200	3.77910700
C	1.19241700	-1.49410200	4.00744400
C	2.82645300	0.07101900	5.12221400
C	5.09416600	-0.31399600	-0.52903400
C	4.60180300	-1.22686300	-1.66199400
C	6.59887800	-0.04806200	-0.67794400
C	0.71316200	3.16167500	-1.66230600
C	-0.43431400	3.95756900	-1.43095000
C	-1.26906200	4.26171400	-2.51060300
C	-0.98782400	3.81387500	-3.79574900
C	0.14995300	3.04799200	-4.01589800
C	1.01264000	2.70745800	-2.96893400
C	-0.79899000	4.47846400	-0.04822300
C	-2.03057800	3.75478400	0.50760000
C	-1.03052100	5.99712300	-0.03434500
C	2.26389200	1.89695100	-3.27717700
C	1.93694600	0.55489800	-3.94394200
C	3.25035600	2.70107200	-4.13811800
C	-2.61700100	-4.96688300	-0.74952600
C	-2.48746800	-3.58418100	-0.14709900
C	-3.41490000	-3.26929500	0.86573200
C	-3.74242500	-2.02826600	1.44051600
C	-4.98405700	-2.03357100	2.30959300
C	-0.70924000	-3.15397600	-1.67467900
C	-1.00429400	-2.69194500	-2.97957200
C	-0.13911800	-3.02782300	-4.02597800
C	0.99704100	-3.79641100	-3.80685600
C	1.27414600	-4.25156700	-2.52338600
C	0.43667200	-3.95239000	-1.44444500
C	-2.25355400	-1.87798200	-3.28668600
C	-3.23996800	-2.67719500	-4.15227700
C	-1.92328500	-0.53383300	-3.94747900
C	0.79711100	-4.48075300	-0.06348000
C	2.02730300	-3.76040800	0.49965000
C	1.02791600	-5.99957300	-0.05693200
C	-3.73068500	0.32206600	1.65109400
C	-4.73070800	0.89571500	0.82517400
C	-5.38226100	2.05437400	1.25593100
C	-5.07243300	2.65088200	2.47216000
C	-4.07192100	2.09982900	3.26118400
C	-3.38017600	0.94801500	2.86958700
C	-5.09587900	0.31310000	-0.53375300
C	-4.59999900	1.22859800	-1.66305100
C	-6.60065100	0.04965600	-0.68641200
C	-2.28253400	0.41602800	3.77800300
C	-2.83479300	-0.09098600	5.11854800
C	-1.19969800	1.47861500	4.01153900
H	4.85350100	1.39064200	3.20669000
H	5.22730400	3.03668000	2.64359500
H	5.83835600	1.62270200	1.77572100
H	4.05994400	4.08226600	1.18171500
H	2.59384100	4.92930900	-1.81657200
H	3.54636100	5.44892800	-0.40880600
H	1.78273800	5.60634300	-0.41670900
H	3.81291900	-2.58819500	4.20352300
H	5.59400900	-3.55571900	2.79148700

H	6.14725600	-2.50066400	0.62458900	H	-5.84160800	-1.63021100	1.76148400
H	1.80974200	0.42126300	3.27195800	H	-0.36449900	-2.68227800	-5.03185500
H	0.75888300	-1.82247000	3.05748100	H	1.65996600	-4.04376400	-4.63161300
H	0.38534100	-1.09879700	4.63254600	H	2.16112900	-4.85635300	-2.35267700
H	1.59496400	-2.37787500	4.51399300	H	-2.75140000	-1.66850000	-2.33388000
H	3.31079700	-0.73786500	5.68061600	H	-2.80532600	-2.91840900	-5.12887100
H	2.01789000	0.46676500	5.74707200	H	-4.15416900	-2.09936100	-4.32857000
H	3.56323900	0.86835200	4.98684900	H	-3.52471000	-3.61981700	-3.67469200
H	4.57841800	0.64561400	-0.62907300	H	-1.26800900	0.07581100	-3.31814000
H	5.08544700	-2.20905600	-1.61335800	H	-2.83828500	0.03844400	-4.13227600
H	4.83400500	-0.79003200	-2.63963400	H	-1.42211000	-0.67131000	-4.91181200
H	3.52109900	-1.38955700	-1.60913200	H	-0.04316300	-4.26740700	0.60519900
H	6.98268300	0.59253200	0.12196500	H	2.90857000	-3.93702100	-0.12586600
H	6.80354900	0.44860800	-1.63265200	H	2.26095700	-4.11313600	1.50924300
H	7.17900700	-0.97727300	-0.66321600	H	1.86990600	-2.67882800	0.54992900
H	-2.15721300	4.86456400	-2.33909600	H	0.18707500	-6.54864500	-0.49268400
H	-1.64872400	4.06494900	-4.62100800	H	1.17165700	-6.35652700	0.96867900
H	0.37863700	2.70832400	-5.02304100	H	1.92472100	-6.27227900	-0.62388000
H	0.03950600	4.26204400	0.62172100	H	-6.15098300	2.49551000	0.62629400
H	-2.90992100	3.93389600	-0.11992000	H	-5.60045500	3.54320500	2.79744200
H	-2.26769000	4.10260900	1.51808200	H	-3.82074900	2.57121800	4.20816700
H	-1.87277300	2.67306400	0.55339300	H	-4.58129300	-0.64692500	-0.63573000
H	-0.18859200	6.54894300	-0.46450300	H	-5.08220000	2.21139700	-1.61232100
H	-1.17755400	6.34852200	0.99271600	H	-4.83100100	0.79505900	-2.64244400
H	-1.92568900	6.27248100	-0.60259500	H	-3.51913700	1.38944100	-1.60763400
H	2.76049700	1.68449400	-2.32439800	H	-6.98702300	-0.59236100	0.11112800
H	1.28269500	-0.05897700	-3.31768700	H	-6.80399200	-0.44438600	-1.64276200
H	2.85330500	-0.01456000	-4.13072500	H	-7.17956100	0.97960800	-0.67066200
H	1.43598000	0.69557400	-4.90792700	H	-1.81546300	-0.43422200	3.26845000
H	2.81715900	2.94499900	-5.11467700	H	-3.32000000	0.71575800	5.67928900
H	4.16592600	2.12552500	-4.31477200	H	-2.02698300	-0.48891100	5.74299500
H	3.53255800	3.64250300	-3.65669900	H	-3.57128900	-0.88791800	4.97926300
H	-2.58219200	-4.92241000	-1.84124000	H	-0.76492900	1.81033600	3.06330900
H	-3.54966800	-5.44383500	-0.44427700	H	-0.39338600	1.08132400	4.63637200
H	-1.78674500	-5.60707300	-0.43589200	H	-1.60313300	2.36053200	4.52060900
H	-4.06242200	-4.08797400	1.15762600				
H	-4.85848400	-1.40691700	3.19503400				
H	-5.23267900	-3.04950100	2.62221500				

1b

Mg 0.26096900 0.06688400 1.40986800

Mg	-0.26597400	-0.07274300	-1.40975100	C	1.72537000	2.86270700	-2.58613200
N	-0.31291300	1.36219200	2.92480300	H	-0.12859200	3.28024400	4.92504000
N	1.35934600	-1.08969500	2.73647300	H	-0.08406000	2.05604200	6.21019600
N	-1.72445900	-0.97770700	-2.57315200	H	-1.54573400	2.29586600	5.23137800
N	0.67433700	0.70302000	-3.08719800	H	1.06062600	0.27644900	5.77673200
C	-0.45149700	2.27247800	5.20574800	H	1.92837300	-2.81268000	4.83675900
C	0.04325400	1.24981400	4.20455400	H	2.31248000	-1.47624700	5.94083300
C	0.86614600	0.22568600	4.71182500	H	3.34328400	-1.82289000	4.53749600
C	1.47479200	-0.85419000	4.04341100	H	-0.97427000	5.59878300	1.27800200
C	2.30907300	-1.78784000	4.89505700	H	-4.43346000	3.18970100	2.04153100
C	-1.15342000	2.44300000	2.52693500	H	4.94141200	-3.04863100	0.63242300
C	-0.58056800	3.64530500	2.06901400	H	1.48287800	-5.47005100	1.35765500
C	-1.42161100	4.66960700	1.62740200	H	-2.89748300	-2.70528600	-4.40290100
C	-2.81142900	4.53535600	1.61742300	H	-2.83664500	-1.50108700	-5.70614800
C	-3.35307200	3.32459400	2.05380000	H	-3.88598300	-1.26248100	-4.29401400
C	-2.55155300	2.27288600	2.50399000	H	-1.06030000	-0.27413500	-5.77683100
C	2.02693800	-2.21470600	2.16934200	H	1.10299700	2.24065600	-5.35787800
C	3.32401000	-2.06692200	1.64073200	H	0.60805300	0.92642200	-6.44440100
C	3.93714900	-3.16695800	1.03612000	H	2.08965700	0.79707700	-5.47458700
C	3.30101800	-4.40539900	0.93093300	H	-3.29378200	-4.80096900	-0.56791200
C	2.00614900	-4.51885200	1.44093600	H	-5.71188900	-1.27410200	-0.31136600
C	1.35351300	-3.44642900	2.05382300	H	5.19229900	1.13339100	-2.37866800
C	-2.91074400	-1.63345000	-4.62553700	H	2.78143500	4.66312100	-2.09674500
C	-1.78759400	-0.91912600	-3.90350200	C	0.91465800	3.81654900	2.03393100
C	-0.86671400	-0.22476700	-4.71170700	H	1.18422400	4.82866200	1.72001200
C	0.26765400	0.52455000	-4.34399600	H	1.37576200	3.62870200	3.00927400
C	1.05433900	1.15321300	-5.47479600	H	1.37828300	3.11513400	1.32865400
C	-2.71768100	-1.71048300	-1.85945800	C	-3.17189900	0.97114300	2.93652400
C	-2.49881800	-3.06556600	-1.54398800	H	-2.87181100	0.14866300	2.27489200
C	-3.46262300	-3.75068200	-0.80021400	H	-2.86762500	0.68406900	3.94856400
C	-4.62877300	-3.13054200	-0.34728900	H	-4.26338000	1.03278800	2.91475000
C	-4.81279700	-1.78169900	-0.65715900	C	-3.69874500	5.66807700	1.17093800
C	-3.87666400	-1.05640700	-1.39823600	H	-4.63201500	5.29868500	0.73485700
C	1.84214800	1.48149900	-2.83614500	H	-3.96904200	6.31822200	2.01267500
C	3.09911900	0.85178200	-2.74702600	H	-3.20295200	6.29535200	0.42376900
C	4.22252200	1.62429000	-2.44259400	C	4.03096300	-0.73935100	1.70456400
C	4.13727200	2.99918700	-2.21479000	H	4.08750900	-0.34880400	2.72604500
C	2.87640600	3.59491200	-2.28496100	H	5.04951000	-0.82077900	1.31526900

H	3.50690900	0.01862600	1.10895900	H	0.33992400	2.19868000	0.00041200
C	-0.05525900	-3.60079700	2.56169500	C	2.19564800	1.13284500	0.00023100
H	-0.39483200	-4.63529300	2.46135800	C	2.82648100	-0.10828100	-0.00001100
H	-0.15022700	-3.31193300	3.61373000	C	2.04736200	-1.26509400	-0.00021700
H	-0.75188600	-2.96663300	1.99883900	H	2.52352300	-2.24237400	-0.00036300
C	3.99752800	-5.58697900	0.30775300	C	-1.50277200	0.14151800	-0.00003400
H	4.71656000	-5.27230600	-0.45482900	H	-1.80012700	2.11121300	-0.88596900
H	4.55241800	-6.16382200	1.05852500	C	-2.10269200	1.53923700	-0.00050500
H	3.28435100	-6.27057600	-0.16308500	H	-1.80031300	2.11167300	0.88472500
C	0.37977300	3.53691600	-2.61853300	H	-3.19371000	1.47461100	-0.00057700
H	-0.26838700	3.16692600	-1.81402000	C	-2.27667100	-0.98564900	-0.64719400
H	0.48200500	4.61792600	-2.48981900	H	-2.55291200	-1.44194600	-1.58622200
H	-0.15258900	3.35466400	-3.55789700	C	-2.27659100	-0.98513000	0.64790700
C	3.22855100	-0.63382400	-2.95324500	H	-2.55192200	-1.44049200	1.58765700
H	4.27704700	-0.94224700	-2.92014900	H	0.06692600	-2.08841800	-0.00036600
H	2.69373800	-1.19072000	-2.17345100	H	2.78711500	2.04489200	0.00045400
H	2.80883100	-0.95721200	-3.91161600	H	3.91093800	-0.17488500	0.00004800
C	5.36871100	3.81709800	-1.92454700				
H	5.13604600	4.68410700	-1.29865900				
H	6.13137600	3.22482500	-1.40960800				
H	5.82215400	4.19659900	-2.84902500				
C	-4.09662000	0.40524000	-1.68344600				
H	-5.07515800	0.73064200	-1.31989700				
H	-3.33614200	1.02328400	-1.18976100				
H	-4.03771800	0.63291500	-2.75294700				
C	-1.23995400	-3.76192900	-1.98734500				
H	-0.35468000	-3.31961600	-1.51299300				
H	-1.26506900	-4.82151300	-1.71869300				
H	-1.08409200	-3.68863600	-3.06883600				
C	-5.63897900	-3.88353300	0.47880100				
H	-5.65627100	-4.94669100	0.21976800				
H	-5.40979500	-3.81434000	1.54970100				
H	-6.64871500	-3.48595600	0.33753600				

2a

C	0.65875600	-1.17752300	-0.00023200
C	0.00535800	0.06505800	-0.00011800
C	0.80354700	1.21752700	0.00020600

2b

C	0.80656700	-1.42933200	-0.00016800
C	1.19663700	-0.05944200	-0.00008300
C	0.19759100	0.89572300	0.00005100
H	0.44792300	1.95242300	0.00014500
C	-1.17793300	0.54781100	0.00004800
C	-1.54908900	-0.83136800	-0.00008800
C	-0.51413600	-1.80139500	-0.00019300
H	-0.78332100	-2.85537000	-0.00030500
C	-2.92380800	-1.17693300	-0.00009100
H	-3.19956400	-2.22903000	-0.00019300
C	-3.89447100	-0.20178400	0.00003100
H	-4.94534000	-0.47791800	0.00002800
C	-3.52932400	1.16444500	0.00018300
H	-4.30324600	1.92724000	0.00029600
C	-2.20285400	1.52930400	0.00018300
H	-1.92157400	2.57993300	0.00029900
C	2.65831000	0.31054000	-0.00009700
H	2.55957200	2.29937600	0.88472500
C	2.97006100	1.79904800	-0.00059100

H	2.55933500	2.29884300	-0.88610300	Mg	-0.71715200	-0.83720000	-0.95350300
H	4.05213700	1.95223200	-0.00077400	Mg	-1.73591200	0.97381500	1.03228500
C	3.64239600	-0.64001600	0.64788900	N	-0.39166600	-2.88530800	-1.01483800
H	4.01108400	-1.02411400	1.58747300	N	-0.02096900	-0.60751300	-2.89417700
C	3.64249000	-0.64058200	-0.64692800	N	-3.66024400	1.58509000	1.50263600
H	4.01103900	-1.02546200	-1.58624800	N	-0.92284400	2.17321500	2.51880400
H	1.57732800	-2.19427400	-0.00021800	C	0.40782400	-5.02898700	-1.91741700

2c

C	-0.00002100	2.41025100	0.64739600	C	0.61629500	-2.92366700	-3.21950100
C	-0.00004600	2.41042600	-0.64711400	C	0.50254200	-1.58302000	-3.63666200
H	0.01174200	2.94155700	-1.58704000	C	1.01159400	-1.26631300	-5.02726800
C	0.00007200	1.04202300	0.00007400	C	-0.82510100	-3.61953500	0.12853100
H	-0.01184100	2.94102500	1.58753100	C	0.02487900	-3.75008800	1.24367600
C	-1.28360800	0.24644700	0.03732600	C	-0.44225300	-4.42202100	2.37586900
C	-1.39088600	-0.91074400	0.82101400	C	-1.72825500	-4.96193900	2.43946500
C	-2.41330000	0.67313100	-0.66877800	C	-2.55943700	-4.79847800	1.32950600
C	-2.59018500	-1.61522800	0.89522300	C	-2.13597400	-4.13272400	0.17667600
C	-3.61301100	-0.03237900	-0.60248200	C	-0.12238300	0.70663600	-3.43860900
C	-3.70689500	-1.18069200	0.18181400	C	0.90738900	1.64141400	-3.21772600
H	-0.52439000	-1.26146800	1.37498500	C	0.76173800	2.93856300	-3.71572900
H	-2.35201400	1.57514600	-1.27335200	C	-0.37820400	3.34102500	-4.41410000
H	-2.65230100	-2.50706700	1.51346900	C	-1.39202600	2.40010200	-4.60509000
H	-4.47513400	0.31552700	-1.16564100	C	-1.29055000	1.09233400	-4.12482700
H	-4.64154600	-1.73204300	0.23712100	C	-5.42919300	2.78727000	2.71730400
C	1.28365600	0.24639100	-0.03732200	C	-3.97618500	2.43312400	2.48066000
C	2.41363500	0.67343500	0.66812300	C	-3.03615500	3.04463200	3.33288200
C	1.39061600	-0.91121600	-0.82044400	C	-1.63263900	2.93610700	3.35252800
C	3.61329700	-0.03215100	0.60176600	C	-0.91311000	3.75697200	4.40241800
C	2.58985800	-1.61578700	-0.89468900	C	-4.69813800	1.03519800	0.69434600
C	3.70684000	-1.18091200	-0.18191000	C	-5.07067000	1.67921100	-0.50135800
H	2.35260500	1.57579100	1.27221200	C	-6.05542800	1.09772900	-1.30374300
H	0.52392300	-1.26217300	-1.37394700	C	-6.67131400	-0.10845900	-0.96425600
H	4.47564800	0.31603700	1.16440100	C	-6.27017900	-0.73627200	0.21679800
H	2.65172600	-2.50796000	-1.51247800	C	-5.28961000	-0.19244500	1.04999200
H	4.64144400	-1.73234000	-0.23724300	C	0.49876200	2.17040500	2.63241300

Int-1

C	2.53642500	1.21793600	3.51650600	H	2.85903800	2.07821100	-2.42119100
C	1.13931500	1.21378600	3.44090000	H	1.89734700	0.98963500	-1.41236900
H	0.99939200	-5.27370100	-1.02946500	C	-2.41912600	0.11650600	-4.32637000
H	0.91990600	-5.42002400	-2.79814200	H	-3.21792400	0.56254800	-4.92509200
H	-0.54561000	-5.55590200	-1.80687900	H	-2.09067700	-0.80041600	-4.82709500
H	1.07494500	-3.59199300	-3.93890100	H	-2.85386700	-0.19054200	-3.36706100
H	0.20224900	-0.88851600	-5.66061800	C	-0.52425800	4.75385200	-4.91649400
H	1.44163500	-2.14860200	-5.50418300	H	0.44801100	5.19930500	-5.14847700
H	1.77090500	-0.47844200	-4.99632200	H	-1.13861500	4.79612400	-5.82117900
H	0.22052400	-4.52295400	3.23380600	H	-1.00506200	5.39578000	-4.16759300
H	-3.57232900	-5.19675200	1.36009700	C	0.33729500	0.19872800	4.21101400
H	1.56554400	3.65438400	-3.55138800	H	-0.21905900	-0.46422200	3.53647100
H	-2.29280600	2.69030900	-5.14353500	H	0.98835500	-0.42585100	4.82879400
H	-5.86925300	3.24186800	1.82376700	H	-0.40392800	0.66851500	4.86625100
H	-5.53862100	3.48231300	3.55137000	C	0.59092600	4.07386100	0.96542600
H	-6.02020400	1.89044700	2.92902400	H	1.32625500	4.72808500	0.48930500
H	-3.45640800	3.70624100	4.08119400	H	0.03131500	3.56566500	0.17037900
H	-0.31475300	3.11564100	5.05749900	H	-0.12913600	4.70357600	1.49892300
H	-1.61684300	4.32193300	5.01577400	C	4.81733600	2.15295100	2.93641300
H	-0.21381600	4.45931200	3.93730700	H	5.31188300	2.08870900	1.96113900
H	-6.34763300	1.60459000	-2.22201300	H	5.16177800	3.08006200	3.40987800
H	-6.73247500	-1.68011600	0.50133600	H	5.17699200	1.31937400	3.54609800
H	3.24049500	3.76488400	1.40694300	C	-4.86153600	-0.91504600	2.29918200
H	3.02672500	0.48840100	4.15909400	H	-5.46374600	-1.81398700	2.45608200
C	1.40769200	-3.15739000	1.22419200	H	-3.81119200	-1.22607800	2.23531100
H	1.94394000	-3.38500300	2.14943100	H	-4.94819400	-0.28706100	3.19220900
H	2.00689900	-3.52637100	0.38541100	C	-4.40860200	2.96581900	-0.91670300
C	-3.07646600	-3.94614300	-0.98401300	H	-3.33842600	2.81614300	-1.10812500
H	-3.30883000	-2.88521100	-1.13920900	H	-4.85753700	3.35759600	-1.83347200
H	-2.65301700	-4.31398000	-1.92445000	H	-4.48255600	3.73867900	-0.14429400
H	-4.02034000	-4.46949400	-0.80874600	C	-7.71094000	-0.72996900	-1.86033100
C	-2.19621600	-5.71479400	3.65756400	H	-8.25922200	0.03012800	-2.42528500
H	1.36863000	-2.06570400	1.12017200	H	-7.25369900	-1.40995900	-2.59016600
H	-3.27920900	-5.63017500	3.78989400	H	-8.43804600	-1.31290200	-1.28654000
H	-1.96135500	-6.78391900	3.57983800	C	4.67653500	-0.94215700	0.46323000
H	-1.71553300	-5.34331500	4.56781000	H	3.99370800	-0.35451700	1.05996600
C	2.14169500	1.25349200	-2.44893600	C	6.09558900	-1.45893900	0.35989600
H	2.64243800	0.38161000	-2.88277900	C	7.18854100	-0.47654200	0.01390100

C	6.91032100	0.65916500	-0.76408000	C	0.33342700	-5.50716700	1.47716000
C	8.50891900	-0.65483700	0.45051600	C	0.37949700	-5.33052400	0.09868500
C	7.90583200	1.57549800	-1.08963800	C	-0.20271400	-4.21584100	-0.51089500
C	9.50860800	0.26164700	0.12516400	C	6.99930800	-0.68272000	0.37608900
C	9.21409200	1.38258700	-0.64633500	C	5.69167000	0.06338900	0.54328500
H	5.89717300	0.82222000	-1.12019800	C	5.79245800	1.32046900	1.15965500
H	8.76868300	-1.51892200	1.05340900	C	4.79953600	2.25912000	1.49009200
H	7.65846700	2.44437400	-1.69447100	C	5.32185900	3.54007600	2.11391500
H	10.52292100	0.09484700	0.47886400	C	4.64916700	-1.81096200	-0.43393900
H	9.99258100	2.09678000	-0.90007400	C	4.58728100	-2.93602400	0.42229000
C	4.94452600	-1.62089100	-0.60720600	C	4.64549500	-4.21292400	-0.14249400
H	4.64489300	-2.02041500	-1.56480300	C	4.78660900	-4.39090700	-1.51448000
C	6.50994900	-2.64681500	1.21502600	C	4.87084800	-3.27922300	-2.34376600
H	7.27487300	-3.25776700	0.72037900	C	4.80786600	-1.98060200	-1.82808200
H	6.91347300	-2.32985600	2.18445100	C	2.64587200	3.19073600	1.64797400
H	5.64381300	-3.28542600	1.40565600	C	1.94722500	3.13292300	2.87736100
				C	1.17662600	4.23627900	3.25796300
				C	1.06854400	5.35867000	2.44453800

Int-1_1a2a

Mg	-0.18429500	-0.34656300	-0.52580100	C	1.72489000	5.38538200	1.21990200
Mg	2.64642500	0.41598000	0.29283900	C	2.52398700	4.31748600	0.80159600
N	-1.75503400	0.65839600	-1.54533200	H	-4.49250900	1.66665000	-1.70656100
N	-1.39396800	-2.07376900	-0.29728200	H	-4.85166200	0.32717000	-2.79919500
N	4.55078100	-0.49455700	0.12411400	H	-3.66115800	1.56917300	-3.24899600
N	3.49130900	2.10000200	1.26625500	H	-4.38270800	-1.41302500	-1.65390800
C	-4.05101600	0.96808400	-2.42562000	H	-2.95972700	-4.28081000	-1.08194500
C	-2.96793300	0.14189700	-1.75725100	H	-4.45824400	-3.36575500	-0.83736000
C	-3.36933200	-1.15172700	-1.37239200	H	-3.40495200	-3.77338800	0.53373300
C	-2.65767900	-2.17308100	-0.71928700	H	-2.17501300	5.22327200	-1.06266800
C	-3.42072600	-3.46566000	-0.51523700	H	-0.29591200	3.76737300	-4.61371700
C	-1.55290500	2.00624900	-1.98585900	H	-0.34815600	-4.70406300	3.34456600
C	-2.00657100	3.08341300	-1.18939600	H	0.86810500	-6.07954200	-0.51834200
C	-1.82961200	4.38648700	-1.66311400	H	6.99936200	-1.60438100	0.96662700
C	-1.23374700	4.63180200	-2.89442000	H	7.84466400	-0.07018900	0.69294800
C	-0.77232400	3.56640600	-3.65903400	H	7.15259400	-0.98408800	-0.66358600
C	-0.90692600	2.24464800	-3.22194800	H	6.80051400	1.61694800	1.42337400
C	-0.82627800	-3.24368300	0.30639300	H	5.36690400	4.33639600	1.36306300
C	-0.89160300	-3.42051000	1.70705600	H	6.33022400	3.39455000	2.50585900
C	-0.30215000	-4.55788800	2.26823100	H	4.67628500	3.90099100	2.91670200

H	4.59080800	-5.08398900	0.50465300	H	0.46724000	6.20662700	2.76180000
H	4.99461300	-3.42006500	-3.41474800	H	4.84058900	-5.39220000	-1.93376000
H	0.64849800	4.21765300	4.20635100	C	6.22700000	-0.85445600	-3.60831400
H	1.62410600	6.25793800	0.58060500	H	6.32917100	0.05239700	-4.21449400
C	-2.66244000	2.84994900	0.16461900	H	7.11801200	-0.93935200	-2.97847200
C	-0.39880200	1.09646500	-4.08482600	H	6.22529800	-1.70849400	-4.29442500
H	-0.12489100	0.28059800	-3.40243300	C	3.71563800	-0.67006300	-3.68945000
H	-3.02765300	1.81836300	0.18386900	H	3.60140600	-1.55836400	-4.32092900
C	-1.60459800	-2.42532900	2.61084500	H	2.79557200	-0.55491700	-3.10737100
H	-2.11046100	-1.70027500	1.96487300	H	3.81307700	0.19951300	-4.34839600
C	-0.16518000	-4.07227700	-2.02599300	C	5.42123000	-3.69765000	2.70716400
H	-0.91329800	-3.32261700	-2.30294900	H	5.14481500	-4.75271700	2.60550100
C	3.22663400	4.37785200	-0.54790100	H	6.45723500	-3.59196400	2.36877800
H	4.04269700	3.64869100	-0.53061300	H	5.38876400	-3.45777600	3.77546800
C	2.05153100	1.91757200	3.79047300	C	3.02353800	-2.98558100	2.39597000
H	2.19917700	1.04321600	3.14214200	H	2.68244100	-4.00246200	2.18019800
C	4.93938100	-0.79526400	-2.77340300	H	2.93202000	-2.81675200	3.47518300
H	4.98681600	0.10976300	-2.15881700	H	2.33430000	-2.30517300	1.88415700
C	4.46966100	-2.77683700	1.93176700	C	2.26968400	3.96343300	-1.67296400
H	4.74634100	-1.74604200	2.17505200	H	1.42252400	4.65202600	-1.74403600
C	-6.53318500	0.20430600	2.41761000	H	2.78571100	3.95923000	-2.64022700
H	-6.48807300	0.93446200	3.21218700	H	1.85437700	2.96425700	-1.50183500
C	-7.41699100	-0.79844400	1.71295800	C	3.84588300	5.74846500	-0.85043800
C	-8.51440100	-0.28044600	0.81491400	H	4.44907400	5.69467500	-1.76306300
C	-5.98944100	-0.39483800	1.40576400	H	3.08187400	6.51577800	-1.01618100
C	-9.68764700	-1.01248300	0.58363600	H	4.49232900	6.09454600	-0.03717600
C	-8.39010300	0.96411900	0.17696100	C	0.78239700	1.66910200	4.61200600
C	10.69314100	-0.52342200	-0.25003500	H	-0.11259600	1.66362700	3.98326200
H	-5.15967900	-0.54107400	0.72670500	H	0.84999500	0.70077100	5.11771300
C	-9.39171600	1.45485400	-0.65482800	H	0.64533100	2.42711900	5.39137000
C	10.55207700	0.71278600	-0.87470600	C	3.26749000	1.99408200	4.72714000
H	-9.82631700	-1.97885600	1.05751500	H	3.21677500	2.89156200	5.35439800
H	-7.49293900	1.55487100	0.33803400	H	3.29370000	1.12229000	5.39074800
H	11.59102200	-1.11520500	-0.40928100	H	4.20895100	2.01722500	4.17395800
H	-9.26558200	2.42276600	-1.13354100	C	-0.61027400	-1.65109400	3.48518200
H	11.33520400	1.09458700	-1.52390800	H	-0.05283300	-2.32743400	4.14296500
H	0.78298100	-6.38620200	1.93154900	H	0.11717700	-1.10842500	2.87246700
H	-1.12209100	5.65099100	-3.25495600	H	-1.13382200	-0.92454800	4.11594800

C	-2.67790200	-3.09196500	3.48355500	N	2.62160300	3.43290200	-0.47242000
H	-3.23243200	-2.33439000	4.04791900	N	1.46278200	1.75898500	-2.70541100
H	-3.39769100	-3.65707300	2.88316600	C	4.99676200	-4.47854100	2.03175200
H	-2.23774700	-3.78434900	4.20950800	C	3.88788100	-3.44690700	1.97546400
C	1.19927700	-3.55432600	-2.49536100	C	3.09727000	-3.36227400	3.13527800
H	1.45572500	-2.60403200	-2.01453300	C	1.87484000	-2.69707800	3.35406800
H	1.99710200	-4.26020500	-2.24592700	C	1.14175200	-3.07330900	4.62408900
H	1.20619500	-3.40114200	-3.58072000	C	4.40100800	-3.17222800	-0.31073000
C	-0.52926800	-5.36996300	-2.75956500	C	3.89718500	-4.26364400	-1.06318100
H	-1.48543600	-5.77838800	-2.41622800	C	4.61075800	-4.70127200	-2.18211600
H	-0.60872900	-5.18348100	-3.83600500	C	5.79939900	-4.09320000	-2.56746300
H	0.23154500	-6.14598500	-2.62233600	C	6.27070700	-3.00716900	-1.84235100
C	-3.86711700	3.76421700	0.42176300	C	5.58659400	-2.52096800	-0.72251200
H	-4.38286000	3.45638300	1.33749400	C	0.06771100	-1.24037900	2.81587800
H	-3.56735300	4.80893900	0.55827300	C	-1.07105100	-1.75217100	2.14885100
H	-4.58875400	3.73105800	-0.40117200	C	-2.31579200	-1.15979600	2.38656700
C	-1.63398700	2.98892300	1.29420600	C	-2.44932600	-0.08224500	3.25323300
H	-1.22075500	4.00125200	1.32933900	C	-1.32621300	0.41054300	3.90667600
H	-2.09358500	2.77572300	2.26642800	C	-0.06145600	-0.15306700	3.71294700
H	-0.78921800	2.30487800	1.15751900	C	3.43677700	5.61425400	-1.30464700
C	-1.48474900	0.55110300	-5.02554800	C	2.85763600	4.23066000	-1.52145800
H	-1.85331200	1.34112600	-5.68998100	C	2.55365700	3.91755300	-2.85853900
H	-1.07993600	-0.25207000	-5.65170300	C	1.81471800	2.84446000	-3.39403300
H	-2.33626000	0.14461800	-4.47528600	C	1.40764100	2.98639500	-4.84507200
C	0.85164100	1.45775800	-4.89306300	C	2.72245600	4.03272800	0.82579800
H	1.26618400	0.55879900	-5.35997100	C	1.63184100	4.78989400	1.32378000
H	0.62602400	2.16208800	-5.70156100	C	1.74512600	5.39653300	2.57747600
H	1.62651600	1.90272600	-4.26232700	C	2.90079900	5.27559500	3.33963600
C	-7.67323500	-2.14425900	2.37416900	C	3.95341400	4.50980500	2.85699500
H	-8.56683200	-2.12165800	3.00978200	C	3.88503800	3.87048400	1.61399900
H	-7.81204500	-2.94223700	1.63453700	C	0.64245200	0.77203800	-3.33929800
H	-6.82173200	-2.41616800	3.00292000	C	-0.74992800	0.76536400	-3.08639100
				C	-1.53429400	-0.24508100	-3.65217400
				C	-0.97364300	-1.23614600	-4.44769800
Mg	2.36738900	-1.09414700	0.82098600	C	0.39371000	-1.21800900	-4.69498500
Mg	2.10122400	1.40467300	-0.73502300	C	1.22062800	-0.22517200	-4.16079300
N	3.68872400	-2.73985300	0.85579000	H	5.90837100	-4.11712600	1.55142900
N	1.35494400	-1.79360700	2.52404700	H	4.70452900	-5.38975000	1.49993500

Int-1_1a2b

Mg	2.36738900	-1.09414700	0.82098600
Mg	2.10122400	1.40467300	-0.73502300
N	3.68872400	-2.73985300	0.85579000
N	1.35494400	-1.79360700	2.52404700

H	5.21994900	-4.74979000	3.06532800	C	-7.49186900	-1.24163700	0.95012000
H	3.41249500	-4.00890500	3.94600200	C	-6.15840500	-0.78140100	0.39989300
H	1.20736500	-2.26818000	5.36258400	H	-5.49298900	0.06161300	0.28653500
H	1.56235900	-3.97698300	5.06805000	C	-7.62441700	-1.48511200	2.44521800
H	0.07825100	-3.23460300	4.43035500	H	-7.94614200	-0.58098100	2.97592900
H	4.22866900	-5.53905300	-2.76011900	H	-8.35173100	-2.27617900	2.66384000
H	7.19512200	-2.52365000	-2.14849500	H	-6.66085600	-1.79222200	2.85933500
H	-3.19686600	-1.55430700	1.88641700	C	-1.55272900	-2.64937700	-0.17641100
H	-1.43199200	1.25153900	4.58723300	H	-2.61728000	-2.39444900	-0.13482800
H	2.66624800	6.30346300	-0.94424500	H	-1.02983500	-1.81265700	-0.64888600
H	3.83725500	6.01610300	-2.23726400	H	-1.44950900	-3.52159700	-0.83034500
H	4.22557100	5.60721100	-0.54956300	C	-1.69170700	-4.17754700	1.82684700
H	2.82118900	4.68566100	-3.57480700	H	-1.26866900	-4.44251900	2.80068100
H	1.95086300	2.27488800	-5.47416700	H	-2.76174000	-3.98943400	1.97018800
H	1.60883900	3.99310000	-5.21447700	H	-1.59121500	-5.04766100	1.16832200
H	0.34413200	2.76801600	-4.97447900	C	1.50251000	1.81258900	3.90745400
H	0.91167200	5.97936000	2.96163900	H	1.73253900	1.76800300	2.83857600
H	4.85452300	4.40576400	3.45637800	H	0.68225300	2.52589400	4.03957300
H	-2.60581600	-0.25069100	-3.46793100	H	2.37970700	2.21668200	4.42263500
H	0.83225700	-1.99198300	-5.31970800	C	0.88760600	0.51900600	5.97423500
C	2.58588800	-4.95529100	-0.71415800	H	0.11178300	1.25336500	6.21683600
C	6.15438700	-1.31420900	0.00864900	H	0.57375000	-0.43968800	6.39937200
H	5.44236700	-1.04003300	0.79516900	H	1.80342900	0.83412800	6.48598600
H	2.25000500	-4.56798700	0.25233500	C	7.49771700	-1.62631300	0.68489900
C	-0.99018600	-2.95372800	1.21762000	H	7.40924100	-2.44392800	1.40638800
H	0.06866700	-3.20895100	1.10173400	H	8.25606700	-1.91369600	-0.05200400
C	1.12852100	0.43241500	4.45944600	H	7.87336100	-0.74762100	1.22122000
H	1.98461700	-0.22985500	4.29459200	C	6.29731800	-0.11388900	-0.93743200
C	2.71107000	-0.26569600	-4.46506100	H	7.00379600	-0.32126200	-1.74835800
H	3.15450300	0.66060700	-4.08549600	H	5.33566100	0.14563300	-1.39136900
C	-1.42567300	1.84250500	-2.24967200	H	6.66822000	0.76361300	-0.39809900
H	-0.63933200	2.49732500	-1.85934400	C	2.73120000	-6.47752800	-0.57689800
C	5.07022800	3.03169000	1.16154400	H	2.99201300	-6.94853300	-1.53101900
H	4.79673100	2.56093400	0.21057600	H	3.50410600	-6.75146800	0.14774900
C	0.32612900	4.93744100	0.55393900	H	1.78638200	-6.92002900	-0.24291100
H	0.47676000	4.51615000	-0.44444400	C	1.50475900	-4.61712900	-1.75160400
C	-6.45392700	-2.02195500	0.17235300	H	1.34331500	-3.53780600	-1.83020700
H	-6.21841000	-2.97759300	-0.27222700	H	1.78714400	-4.98105600	-2.74598600

H	0.55140600	-5.08635100	-1.48409700	C	-8.72175900	-0.55866000	-1.16598800
C	3.00398200	-0.34325500	-5.97107900	C	-9.94949200	-0.64588600	0.89846400
H	2.67868700	-1.29942300	-6.39529900	C	-9.84574500	-0.16462300	-1.84725100
H	2.50194700	0.45072100	-6.53317800	H	-7.78684100	-0.68264900	-1.70426900
H	4.08094200	-0.25789800	-6.15204600	C	-11.13133400	-0.23977900	0.22661400
C	3.38867600	-1.43248500	-3.73787100	H	-10.01663700	-0.82674600	1.96712800
H	3.23363300	-1.37418800	-2.65623600	C	-11.08500000	0.00831600	-1.17917100
H	2.98914200	-2.39386000	-4.07739500	H	-9.79678900	0.02109000	-2.91795900
H	4.46749900	-1.43766300	-3.92261000	C	-12.36454900	-0.07073600	0.90811700
C	-2.36256400	2.70996700	-3.10404800	C	-12.26673600	0.41418000	-1.84855400
H	-1.83121100	3.17526900	-3.93996400	C	-13.49584600	0.32428800	0.23229500
H	-3.18276400	2.11592500	-3.52263400	H	-12.40126800	-0.25936300	1.97862900
H	-2.80574200	3.50961300	-2.50000600	C	-13.44757300	0.56942700	-1.15965400
C	-2.17949300	1.25260700	-1.05103200	H	-12.22445900	0.60148900	-2.91909900
H	-2.98342700	0.58208800	-1.37449500	H	-14.43320400	0.44964900	0.76750900
H	-1.51412400	0.67943500	-0.39842900	H	-14.34753100	0.88101000	-1.68268400
H	-2.63307300	2.04946100	-0.45222700				
C	-0.79323900	4.13445000	1.23322300				
H	-0.53483900	3.07464000	1.31916600				
H	-0.98721500	4.50923000	2.24456700				
H	-1.72644600	4.21379600	0.66448300				
C	-0.10197600	6.40132600	0.37828300				
H	-0.34720600	6.87101900	1.33714700				
H	0.68143700	7.00320900	-0.09246300				
H	-0.99590900	6.46199600	-0.25195800				
C	5.37136600	1.91563100	2.17138000				
H	5.65362000	2.32158100	3.14874700				
H	4.49792800	1.27212300	2.31709700				
H	6.20135500	1.29155300	1.82483600				
C	6.32358000	3.88464500	0.91527000				
H	6.14861000	4.65506400	0.15847000				
H	6.64871600	4.38768000	1.83281800				
H	7.15394900	3.25921400	0.56864300				
H	-3.42385800	0.36734500	3.42399700				
H	6.34860800	-4.45757700	-3.43143500				
H	2.97631200	5.76726000	4.30576100				
H	-1.59834400	-2.01526600	-4.87618000				
C	-8.74783100	-0.81065900	0.23562700				

Int-1_1a2c

Mg	-2.93084100	0.66453400	-0.29191000
N	1.24958200	-0.03393000	1.91665400
N	0.65680200	-2.45924400	0.20659500
Mg	-0.32723700	-0.62654000	0.62080900
N	-4.94829800	0.03750600	-0.43216700
N	-3.43264400	2.58509600	-1.03602400
C	3.46095200	-0.20931700	3.02248000
C	2.35251700	-0.75191300	2.13965400
C	2.61316600	-2.01841500	1.58076900
C	1.84281000	-2.81062200	0.71213400
C	2.43913400	-4.15989700	0.36715200
C	1.18456300	1.24724500	2.55430000
C	1.86276000	2.35131700	1.98747400
C	1.80915100	3.58068500	2.65049800
C	1.11940200	3.72504100	3.84824800
C	0.44048400	2.63753100	4.38605800
C	0.44553300	1.39072900	3.75239600
C	0.00258700	-3.42771500	-0.62377700
C	0.18840400	-3.40131800	-2.02465400
C	-0.48156600	-4.34590900	-2.80886500

C	-1.31362200	-5.30056900	-2.23690800	H	-5.57696200	-4.39472600	-1.51473300
C	-1.48181500	-5.32390900	-0.85681100	H	-6.16096900	-3.25181200	2.56535100
C	-0.82691200	-4.40777200	-0.02924000	H	-0.01714100	4.69479600	-3.29301100
C	-7.35811600	0.25822700	-0.91962300	H	-1.12826200	6.25810300	0.52537000
C	-5.95093100	0.81524700	-0.85493500	C	2.62832800	2.22800500	0.67718500
C	-5.81349000	2.14941100	-1.26900300	C	-0.30164100	0.21409800	4.36784400
C	-4.67430300	2.96943700	-1.34738500	H	-0.62448900	-0.42893100	3.53768100
C	-4.94909200	4.39447100	-1.79110000	H	2.86113700	1.16910300	0.52677900
C	-5.28488000	-1.31385800	-0.09379700	C	1.11342100	-2.39641900	-2.69578700
C	-5.28664600	-2.30500000	-1.10384900	H	1.62316100	-1.84030300	-1.90204500
C	-5.57977400	-3.62433100	-0.74859300	C	-1.00997000	-4.48400900	1.48011800
C	-5.88875900	-3.96828000	0.56298900	H	-0.21485300	-3.88678000	1.93775200
C	-5.90677600	-2.98334700	1.54288700	C	-3.08552700	4.48066400	1.15883500
C	-5.61253800	-1.65009400	1.23922000	H	-3.99420000	3.91440700	0.93164800
C	-2.41341900	3.58457000	-1.14531100	C	-1.74845100	2.59139700	-3.41115000
C	-1.59148100	3.61837900	-2.29653600	H	-2.08838900	1.65910800	-2.94006300
C	-0.64430400	4.64136700	-2.40839000	C	-5.67757700	-0.60133700	2.33987800
C	-0.48447900	5.59202100	-1.40658100	H	-5.54560500	0.37752900	1.86718200
C	-1.26852000	5.52210200	-0.26116000	C	-4.98573000	-1.95605800	-2.55472100
C	-2.24371800	4.53238100	-0.10907600	H	-5.09828300	-0.87240100	-2.66102100
H	4.07392300	0.50738600	2.46509900	H	4.76945200	-1.57052000	-0.19482300
H	4.11737800	-1.01426500	3.35807700	C	7.08500800	0.23255600	-1.92722300
H	3.07128900	0.32013700	3.89366900	C	5.91476300	0.68422600	-2.54792500
H	3.54474500	-2.47016500	1.90107800	C	8.30254600	0.80959900	-2.31373000
H	3.44589600	-4.26121000	0.77519500	C	5.95299100	1.68492400	-3.51713900
H	2.47916500	-4.31139700	-0.71469300	C	8.34562300	1.80534700	-3.28701900
H	1.82085100	-4.96923100	0.76833800	C	7.17068800	2.25032600	-3.89188700
H	2.32729200	4.43661700	2.22770300	C	7.04035700	-0.88660700	-0.91357800
H	-0.10652100	2.76224000	5.31550400	H	4.96256800	0.23650000	-2.27310100
H	-0.34271100	-4.33562200	-3.88716000	H	9.22363200	0.47496600	-1.84454700
H	-2.12692400	-6.07624000	-0.41128200	H	5.02945800	2.02233800	-3.98057100
H	-7.41784200	-0.56848900	-1.63446700	H	9.30205100	2.23457600	-3.57430700
H	-8.07170000	1.02678800	-1.22013500	H	7.20410900	3.02919600	-4.64875400
H	-7.66601300	-0.14905900	0.04731500	C	8.00187200	-0.78387900	0.24682400
H	-6.73712900	2.62841500	-1.57082600	C	6.60999100	-2.25434500	-1.39408700
H	-4.97653300	5.06288400	-0.92355500	C	8.23290100	0.44254300	0.88547800
H	-5.91573800	4.46182400	-2.29380100	C	8.64551000	-1.92028300	0.74811800
H	-4.17352100	4.77619600	-2.45758600	C	9.07858000	0.52624800	1.98912300

H	6.90503200	-3.11809100	-1.97095300	H	0.36844000	2.04186300	-3.43719500
C	5.73434600	-1.61989800	-0.68171900	H	-0.57212100	1.43092100	-4.80956400
C	9.49730200	-1.83995600	1.84795100	H	-0.10405200	3.12658900	-4.75636400
C	9.71697100	-0.61463000	2.47475600	C	-2.82290100	2.99795300	-4.43185400
H	7.74600100	1.33858100	0.51036000	H	-2.57721300	3.96371100	-4.88843700
H	8.46994400	-2.88231100	0.27210500	H	-2.88821000	2.25453100	-5.23445900
H	9.23895300	1.48688500	2.47182200	H	-3.81139100	3.07861900	-3.97435400
H	9.99103200	-2.73630400	2.21444000	C	0.32540900	-1.38525800	-3.53808000
H	10.37921400	-0.54882000	3.33368000	H	-0.22575500	-1.88523000	-4.34247100
H	-1.82300900	-6.02859700	-2.86281500	H	-0.40035800	-0.83991900	-2.92605200
H	1.10500700	4.68421000	4.35915200	H	1.00063600	-0.65546100	-3.99777900
H	0.25559000	6.38044600	-1.51567000	C	2.19307400	-3.07709900	-3.54994800
H	-6.12383700	-4.99840900	0.81771700	H	2.89039000	-2.33192300	-3.94797800
C	-7.03598200	-0.58843100	3.05596700	H	2.77271700	-3.80298700	-2.97126800
H	-7.07592400	0.23240100	3.78046300	H	1.75771500	-3.60764300	-4.40380900
H	-7.86545300	-0.45752100	2.35399800	C	-2.34919900	-3.86833900	1.90232900
H	-7.21282400	-1.51917600	3.60604500	H	-2.44426100	-2.83378800	1.55508800
C	-4.54119900	-0.78322900	3.35371900	H	-3.19063800	-4.42327200	1.47680800
H	-4.60514000	-1.75889200	3.84860400	H	-2.45444400	-3.87416000	2.99337800
H	-3.56252100	-0.72047600	2.86665300	C	-0.87876400	-5.91185200	2.02703000
H	-4.58627400	-0.01027900	4.12853100	H	0.05663600	-6.38576900	1.71179600
C	-5.95774000	-2.61272500	-3.54381200	H	-0.89801900	-5.89839500	3.12215100
H	-5.83331100	-3.70043200	-3.58083500	H	-1.70298000	-6.55387100	1.69784800
H	-7.00207000	-2.40663200	-3.28709000	C	3.95895900	2.99143000	0.67489000
H	-5.77748000	-2.23350900	-4.55551200	H	4.53100400	2.74674400	-0.22600600
C	-3.53665300	-2.30462400	-2.91379500	H	3.80814600	4.07647000	0.67546300
H	-3.35755800	-3.38072000	-2.83103600	H	4.57410700	2.74116200	1.54555200
H	-3.30415500	-1.99807900	-3.94019600	C	1.75446500	2.67201100	-0.50268700
H	-2.82560100	-1.81287900	-2.24082200	H	1.47195700	3.72476100	-0.41005300
C	-2.34497100	3.72328600	2.26859500	H	2.29058400	2.54683300	-1.45066200
H	-1.41548900	4.23154700	2.54162100	H	0.82398900	2.09593900	-0.55593200
H	-2.96741900	3.64626100	3.16783300	C	0.59973000	-0.63897000	5.27428800
H	-2.07290500	2.70976300	1.95318200	H	1.01313500	-0.03303800	6.08876900
C	-3.52427100	5.86397700	1.65570500	H	0.02514800	-1.45711300	5.72325300
H	-4.23661200	5.75750400	2.48082100	H	1.43218200	-1.08228400	4.72353400
H	-2.68050200	6.45045100	2.03513900	C	-1.55808400	0.63302400	5.13790500
H	-4.00645000	6.44855700	0.86519400	H	-2.14016500	-0.25268000	5.41115300
C	-0.43527400	2.28452900	-4.13829200	H	-1.31078900	1.15248800	6.07050300

H	-2.19745600	1.29101500	4.54260900	C	2.15622600	-0.17014800	-4.18936200
Int-1_1b2b							
Mg	0.80705700	0.09453000	0.68664800	C	1.09262200	-0.63269900	-4.96816800
Mg	3.34397700	-0.00858400	-0.65072300	C	0.70367400	-1.97371600	-4.97034300
N	-0.25804500	-1.23883100	1.86981100	C	1.40504500	-2.85756400	-4.14780200
N	-0.69409200	1.52071000	0.85158700	C	2.47489500	-2.44038700	-3.35213000
N	5.29496200	0.48006300	-0.15123300	H	-2.23382300	-2.99261700	2.71050600
N	3.91655900	-0.62708500	-2.54358600	H	-3.07590800	-1.73598500	3.64097400
C	-2.10198700	-2.06286200	3.27308500	H	-1.46913400	-2.30963100	4.13168800
C	-1.44964300	-1.00013700	2.41412500	H	-3.11865000	0.24489100	2.77312000
C	-2.17150400	0.20035900	2.24752800	H	-2.38570800	3.39836700	2.02194400
C	-1.82581600	1.36893200	1.53658600	H	-3.71557800	2.22969000	2.15341900
C	-2.82966900	2.50172500	1.57748900	H	-3.14218600	2.78201500	0.56654700
C	0.37813300	-2.49318500	2.10817100	H	0.70797400	-5.58381100	0.73425200
C	0.18550900	-3.55952200	1.20849000	H	2.61166000	-3.95715900	4.20992200
C	0.86345000	-4.76078000	1.42986100	H	-0.79769500	4.22015700	-2.86487200
C	1.73290700	-4.93400200	2.50860100	H	1.07498300	5.75492900	0.66898600
C	1.92631800	-3.85264400	3.37039000	H	7.75222000	1.77727000	-0.17650100
C	1.27035400	-2.63263800	3.18879100	H	8.48950700	0.53515300	-1.20865700
C	-0.44572700	2.75507100	0.18085300	H	7.98418500	0.15758400	0.45109300
C	-0.81386100	2.90783200	-1.16965300	H	7.23229700	-0.24427400	-2.78227600
C	-0.50680400	4.10454200	-1.82206300	H	5.11131000	-2.14117700	-4.53909600
C	0.16221200	5.14867200	-1.18059600	H	6.50606400	-1.04800000	-4.65165400
C	0.53846200	4.96163300	0.15105200	H	4.88683900	-0.51189300	-5.14441100
C	0.25203700	3.78322300	0.84415900	H	5.41546900	3.97868400	2.82261100
C	7.72425100	0.71822200	-0.45263500	H	5.98065500	0.02350200	4.36802100
C	6.34950200	0.32719400	-0.95262500	H	0.55164600	0.07936900	-5.58931100
C	6.28277100	-0.18300500	-2.26360100	H	1.11110400	-3.90558700	-4.12003200
C	5.16752800	-0.62005400	-3.00435800	C	-0.71643900	-3.40193300	0.01372000
C	5.44311800	-1.10566500	-4.41178500	H	-0.79559300	-4.34069500	-0.54123300
C	5.48494300	1.01748600	1.15590000	H	-1.72741100	-3.08738200	0.29299400
C	5.37087400	2.40531300	1.36692000	C	1.53464800	-1.47895900	4.11920100
C	5.50084200	2.90471300	2.66513600	H	2.03057200	-0.65255100	3.59402700
C	5.73131800	2.07059900	3.76084600	H	0.61285700	-1.07015300	4.54604500
C	5.81615800	0.69642000	3.52798600	H	2.18472900	-1.78383200	4.94378100
C	5.69245200	0.15197900	2.24747100	C	2.42324200	-6.25160800	2.74692900
C	2.86458400	-1.08739700	-3.38889400	H	-0.33115900	-2.63988600	-0.67541700
				H	3.38440400	-6.11522600	3.25195300
				H	1.81514800	-6.91113100	3.37894200

H	2.60808500	-6.78315200	1.80838000	H	-4.90067300	-1.67720200	-2.45749100
C	-1.50582000	1.79320800	-1.90790900	C	-6.13661200	-1.71255900	-0.31487600
H	-2.40518900	1.44666000	-1.38844600	C	-4.71430600	-1.19518200	-0.21926300
H	-1.79605600	2.11278200	-2.91252700	H	-3.96690800	-0.78419000	0.44770700
H	-0.84926500	0.92030300	-2.01463200	C	-6.44667300	-3.10471200	0.21351800
C	0.70259500	3.60784000	2.26985100	H	-6.73647000	-3.08276500	1.27112600
H	1.18170100	4.51733400	2.64219300	H	-7.26296500	-3.57857100	-0.34516700
H	-0.12821200	3.36310600	2.94020300	H	-5.56353000	-3.74186500	0.12133100
H	1.42781100	2.78924700	2.35932600	C	-7.26731700	-0.71735700	-0.25575200
C	0.44958300	6.44352500	-1.89493300	C	-8.50864000	-1.04454900	0.25718300
H	-0.36619000	7.16429700	-1.75641400	C	-7.07687000	0.60987900	-0.73671400
H	1.36387400	6.91396200	-1.52025800	C	-9.57232300	-0.10728700	0.31393300
H	0.56659100	6.28998200	-2.97204900	H	-8.70037300	-2.04457500	0.63468900
C	3.18146900	-3.41784400	-2.45112400	C	-8.08331900	1.54163400	-0.69723600
H	3.01046700	-3.17668500	-1.39405500	H	-6.10860400	0.88520600	-1.14383300
H	2.81992000	-4.43583500	-2.62026400	C	-10.84604700	-0.44457300	0.84100800
H	4.26584600	-3.41185200	-2.60213800	C	-9.36126300	1.21876600	-0.17297400
C	2.52206800	1.29021100	-4.18786000	H	-7.90934700	2.54795800	-1.07206000
H	2.33624100	1.74405800	-3.20590800	C	-11.86050300	0.48372500	0.88438600
H	3.58159500	1.45229500	-4.41158200	H	-11.00830500	-1.45404000	1.21202100
H	1.93078100	1.84136500	-4.92420500	C	-10.42519300	2.15361100	-0.11536200
C	-0.42138400	-2.45580400	-5.84869800	C	-11.64913100	1.79607700	0.40173400
H	-1.16052000	-1.66773300	-6.02261300	H	-12.83060800	0.21066700	1.29085700
H	-0.05103700	-2.77537000	-6.83100300	H	-10.25754300	3.16162400	-0.48797300
H	-0.93883100	-3.31165700	-5.40433600	H	-12.45778100	2.52075800	0.44103800
C	5.75770300	-1.33791700	2.04207400				
H	5.99363200	-1.85094700	2.97839300				
H	4.79921200	-1.73092000	1.68005800	Int-1_1b2c			
H	6.51142000	-1.62102600	1.29979300	Mg	1.92021300	0.01822900	1.41165400
C	5.09131500	3.33497600	0.21628600	Mg	1.79683000	-0.17249400	-1.45753000
H	4.11244200	3.12705200	-0.23365800	N	2.78430800	-1.17749100	2.87116800
H	5.08939800	4.37678800	0.54814300	N	1.27625000	1.38709900	2.83114400
H	5.83034900	3.23533700	-0.58579900	N	3.07155700	0.56758900	-2.91798900
C	5.90467300	2.63631400	5.14631100	N	0.58503400	-1.07297700	-2.88060300
H	5.35170900	3.57257600	5.26932500	C	3.45665500	-1.87517500	5.13227400
H	5.55641800	1.93621300	5.91198400	C	2.78466800	-0.91090500	4.17746100
H	6.95933300	2.85178300	5.35960700	C	2.19202800	0.22871200	4.75438000
C	-5.09684300	-1.56015000	-1.40190600	C	1.49556000	1.28891900	4.14266600
			C	0.97626900	2.37148900	5.06551100	

C	3.42175700	-2.36427100	2.40397800	H	-2.63563700	3.42824900	1.55370000
C	2.67388900	-3.54721700	2.24618300	H	1.01327300	5.61833100	1.05858000
C	3.30499500	-4.68322500	1.73331900	H	3.98082600	2.04561100	-5.08610100
C	4.65142500	-4.68014300	1.36379200	H	3.71172900	0.70548600	-6.21923300
C	5.36421600	-3.48799400	1.50707200	H	4.95665500	0.59568100	-4.95793000
C	4.77509200	-2.32759900	2.01509200	H	1.93098200	-0.47049700	-5.88651700
C	0.54144900	2.50371500	2.33369300	H	-0.18627700	-2.84693800	-4.86875200
C	-0.85551900	2.41367400	2.19056600	H	0.17852500	-1.68955500	-6.16484400
C	-1.55420200	3.50026700	1.65600600	H	-1.15398900	-1.39515800	-5.02953200
C	-0.90680400	4.66791600	1.25065800	H	4.98153600	4.53067700	-1.59557300
C	0.48363300	4.72269600	1.37977800	H	7.35449800	0.97562200	-1.30901300
C	1.22203700	3.66203600	1.90767400	H	-3.84069400	-1.28120600	-1.65867100
C	3.94765800	0.95562100	-5.18361300	H	-1.46900700	-4.81884600	-1.19117600
C	2.93550600	0.36041100	-4.22753000	C	1.21163800	-3.58261400	2.60246500
C	1.89460500	-0.39087300	-4.80639900	H	0.80775200	-4.59290900	2.49397800
C	0.81251600	-1.05294200	-4.19517000	H	1.02750100	-3.25049400	3.62953400
C	-0.13488400	-1.78346800	-5.12388500	C	5.56915400	-1.05300900	2.12193100
C	4.17252600	1.34125600	-2.44681500	H	5.18165100	-0.28542200	1.43995100
C	4.02466200	2.72831800	-2.25354100	H	5.53110300	-0.62410200	3.12863500
C	5.09921700	3.45772400	-1.73833300	H	6.61811600	-1.22465600	1.86526700
C	6.31160600	2.85326200	-1.40025900	C	5.31953100	-5.92828100	0.84866000
C	6.42405100	1.47283200	-1.57838000	H	0.62907700	-2.92000100	1.94968800
C	5.37669300	0.70313400	-2.09051700	H	6.12663700	-5.69149300	0.14856000
C	-0.55882400	-1.77199200	-2.39251700	H	5.76075800	-6.51085000	1.66730800
C	-1.78579700	-1.09903600	-2.24826200	H	4.60776500	-6.58093300	0.33394200
C	-2.88740200	-1.79988700	-1.74562500	C	-1.58547400	1.15942800	2.59026600
C	-2.80312100	-3.14035600	-1.36683100	H	-1.40789700	0.89218500	3.63763600
C	-1.56405200	-3.77589600	-1.48960600	H	-2.66347500	1.27130800	2.44685100
C	-0.43986600	-3.11829800	-1.99096900	H	-1.25300100	0.30189800	1.99108300
H	3.00832100	-2.87133600	5.05931800	C	2.72218100	3.74808800	2.00053300
H	3.37748400	-1.53218800	6.16515300	H	3.07208200	4.74963000	1.73569800
H	4.51612900	-1.99575600	4.88419400	H	3.08890100	3.51344300	3.00510100
H	2.28336100	0.29929700	5.83190300	H	3.20394400	3.03827400	1.31603200
H	1.39247500	3.34702900	4.79391500	C	-1.67871400	5.83989400	0.70216900
H	1.22948500	2.16203100	6.10606000	H	-2.71563900	5.56862900	0.48466200
H	-0.11112500	2.46733300	4.98261400	H	-1.70007000	6.67263300	1.41583200
H	2.72349100	-5.59643600	1.61765100	H	-1.22893700	6.22083800	-0.22125600
H	6.41190600	-3.45588200	1.21237500	C	0.88076200	-3.83341400	-2.09426200

H	1.62920300	-3.38464500	-1.42888700	C	-5.95129100	0.14137800	2.28877600
H	0.77781800	-4.88522000	-1.81391900	C	-7.92354700	-1.11601600	-0.81920500
H	1.29585800	-3.78973600	-3.10674200	C	-8.18038500	-1.66182100	1.50684500
C	-1.91310000	0.35436900	-2.62037600	C	-8.88124800	-2.07242700	-1.14934800
H	-2.94318200	0.69998200	-2.49894700	H	-6.15452600	0.47394100	3.29570700
H	-1.27159700	0.98214400	-1.98896100	C	-9.14396700	-2.61399800	1.18126800
H	-1.61120300	0.54565900	-3.65561500	C	-9.49815100	-2.82461300	-0.15027100
C	-4.00448500	-3.88708100	-0.84699900	H	-7.45657900	-0.52789800	-1.60455800
H	-4.89063600	-3.24781800	-0.80714900	H	-7.90071800	-1.51297400	2.54722400
H	-4.24534000	-4.74574800	-1.48448100	H	-9.14642300	-2.22971600	-2.19163400
H	-3.82911700	-4.27913000	0.16164200	H	-9.61928300	-3.19152300	1.96991500
C	5.52569500	-0.78769300	-2.23650200	H	-10.24778300	-3.56792100	-0.40739000
H	6.54390600	-1.10369200	-1.99366400				
H	4.84233500	-1.32166900	-1.56395100				
H	5.29606700	-1.12980000	-3.25101100	TS-1			
C	2.72241000	3.41175400	-2.57471500	Mg	-0.37390600	-1.23608300	0.87514200
H	1.91818700	3.05972300	-1.91623600	Mg	0.04982700	1.50579300	-0.37673600
H	2.80699000	4.49407700	-2.44448700	N	0.42601900	-1.74504500	2.73556900
H	2.39448600	3.21651400	-3.60104900	N	-2.03888700	-2.48738000	1.09391700
C	7.46870900	3.66700500	-0.88204400	N	-1.21519600	3.13852000	-0.72756300
H	7.12490900	4.55363500	-0.34058300	N	1.70481700	2.55899300	-1.10312000
H	8.09908200	3.08222700	-0.20506600	C	0.57166200	-3.06506200	4.81186600
H	8.10946700	4.01551600	-1.70193300	C	-0.08186600	-2.72612000	3.48632400
C	-5.17671300	-0.43801600	1.42789200	C	-1.23212800	-3.47130800	3.17095700
H	-4.26591400	-0.96318700	1.18187300	C	-2.16741200	-3.31905200	2.12716200
C	-6.47806100	0.10078200	0.87108000	C	-3.42977600	-4.14823900	2.26338300
C	-6.46058200	1.38321700	0.07328500	C	1.48881200	-0.97693400	3.30032000
C	-5.25226800	1.95641300	-0.33775700	C	2.83351300	-1.33204300	3.08422100
C	-7.65111500	2.05546100	-0.23503100	C	3.83997500	-0.56561700	3.68009600
C	-5.22836000	3.15984800	-1.04108900	C	3.55697100	0.54428300	4.47677400
C	-7.63109700	3.26236700	-0.93041000	C	2.21618000	0.89519500	4.65151200
C	-6.41963100	3.81931800	-1.33927000	C	1.17810300	0.15759200	4.07871200
H	-4.31720900	1.45483200	-0.09967200	C	-3.10936500	-2.43589400	0.14928500
H	-8.60078200	1.62527200	0.07151100	C	-3.17570000	-3.36154100	-0.91202200
H	-4.27707100	3.57879200	-1.35849600	C	-4.22326100	-3.25740300	-1.83061700
H	-8.56617300	3.76945500	-1.15390300	C	-5.20343000	-2.26793600	-1.73213500
H	-6.40472400	4.75824800	-1.88589200	C	-5.11644200	-1.36728700	-0.66939400
C	-7.55660200	-0.89591300	0.51595700	C	-4.08738900	-1.43122900	0.27339400
			C	-1.82992100	5.40451200	-1.48538300	

C	-0.81869800	4.29741900	-1.26321100	C	3.19303500	-2.52649000	2.24203000
C	0.50163100	4.59611500	-1.64177500	H	4.27239000	-2.70088300	2.25553600
C	1.66822700	3.81699600	-1.54708300	H	2.69737400	-3.43892600	2.59041700
C	2.95388900	4.49931200	-1.96786600	C	-0.25497900	0.55900300	4.30042100
C	-2.58779000	3.04669700	-0.34222100	H	-0.77080200	0.72655700	3.34647300
C	-3.54454200	2.54711200	-1.24461500	H	-0.82322000	-0.21729500	4.82521000
C	-4.88783000	2.52000000	-0.85887300	H	-0.31731000	1.47874500	4.88867500
C	-5.30773200	2.95758300	0.39832300	C	4.65681100	1.32303200	5.15081200
C	-4.33189400	3.40312600	1.29330700	H	2.88870400	-2.38418700	1.19993700
C	-2.97957700	3.45322300	0.94904800	H	4.43246000	2.39417500	5.18005500
C	2.97649200	1.90904700	-1.07368700	H	4.79751200	0.99539100	6.18855900
C	3.44470600	1.22543700	-2.21350400	H	5.61431600	1.19263000	4.63759400
C	4.67520300	0.56710900	-2.14719800	C	-2.14851700	-4.45237900	-1.05492500
C	5.45290800	0.56607900	-0.98698900	H	-2.26264100	-5.22812900	-0.28775600
C	4.96016400	1.24081800	0.13141300	H	-2.23401000	-4.94173500	-2.02927500
C	3.73503600	1.91293100	0.11198900	H	-1.13503900	-4.05377400	-0.95030100
H	1.64121000	-3.26025500	4.69161100	C	-4.03351300	-0.45527900	1.41583900
H	0.10475100	-3.93929200	5.26815200	H	-4.89671100	0.21284000	1.40147400
H	0.48839300	-2.22581200	5.51063200	H	-4.00268100	-0.96442900	2.38532800
H	-1.49317200	-4.22742300	3.90159600	H	-3.13543500	0.17342000	1.36031000
H	-4.29888300	-3.49304100	2.38796900	C	-6.30418500	-2.16166100	-2.75537700
H	-3.37309600	-4.81139900	3.12780700	H	-6.58787700	-3.14506800	-3.14327700
H	-3.62344000	-4.75000400	1.37201400	H	-7.19965900	-1.69506400	-2.33345700
H	4.87740600	-0.85481200	3.52054200	H	-5.99394100	-1.55293300	-3.61417300
H	1.96710100	1.76453400	5.25812600	C	3.23855200	2.63038000	1.33804300
H	-4.27247600	-3.97587800	-2.64744600	H	2.36089100	2.13173400	1.76727200
H	-5.87149900	-0.59106600	-0.56279500	H	4.00689800	2.65051300	2.11423000
H	-2.65317500	5.06259700	-2.12031300	H	2.94415800	3.66165100	1.11676200
H	-1.36507000	6.27278800	-1.95494100	C	2.63132900	1.19440200	-3.47896200
H	-2.28226500	5.72073700	-0.54007500	H	3.08361500	0.52928100	-4.21787200
H	0.64743500	5.59032700	-2.04672400	H	1.61349600	0.83926200	-3.28677700
H	3.65695600	4.54438800	-1.12950200	H	2.53328100	2.18912400	-3.92956800
H	2.76460200	5.51580500	-2.31625800	C	6.79366900	-0.12026600	-0.95308500
H	3.45976900	3.94539500	-2.76393000	H	6.81301600	-0.99424200	-1.61135200
H	-5.62619400	2.15003100	-1.56794800	H	7.59366200	0.55307800	-1.28591000
H	-4.63043900	3.72888200	2.28845000	H	7.04941700	-0.45231500	0.05773500
H	5.02644800	0.03171600	-3.02666200	C	-1.95846900	3.94757800	1.93841200
H	5.54249000	1.24673100	1.05079800	H	-2.42907900	4.19741700	2.89318700

H	-1.18980400	3.18896500	2.12895400	C	3.20475200	-2.41233300	3.86873800
H	-1.43130100	4.83790300	1.57752000	C	2.73220600	-2.12938100	2.45271400
C	-3.13195500	2.06141000	-2.60796800	C	2.76805300	-3.26189400	1.61433000
H	-2.44935400	1.20651900	-2.53292000	C	2.62315400	-3.39229100	0.22157600
H	-4.00127900	1.74094100	-3.18803000	C	2.97513500	-4.75949300	-0.33156000
H	-2.60580100	2.83392700	-3.17936900	C	2.49332800	0.16015000	3.02559300
C	-6.76702600	2.97027300	0.77397900	C	3.66644100	0.95396600	2.95898500
H	-7.34600200	2.27310600	0.16102100	C	3.84283500	1.98240800	3.88943800
H	-6.91506400	2.69903000	1.82420300	C	2.89651900	2.24006000	4.87372900
H	-7.20453400	3.96674400	0.63396300	C	1.74436500	1.46722000	4.92463400
C	1.30209600	-1.26767100	-0.87317400	C	1.51604900	0.42988200	4.01391100
H	2.18342600	-0.66096200	-0.69805700	C	2.36025300	-2.64163100	-2.01024800
C	0.76645600	-1.97704800	-2.10900200	C	3.54635100	-2.18946600	-2.64246100
C	1.79496800	-2.35624100	-3.14209700	C	3.69058300	-2.37940300	-4.01972900
C	0.94349500	-2.57428800	-0.74043800	C	2.69422800	-2.98489100	-4.77708000
C	1.49336700	-2.37668700	-4.51312200	C	1.53384300	-3.41783600	-4.15041200
C	3.09416700	-2.73155600	-2.75939500	C	1.34641900	-3.26654400	-2.77186100
C	2.44684400	-2.74994700	-5.45887400	C	-5.58503000	-1.08336900	2.03315400
H	1.34501100	-3.48464900	-0.31299900	C	-4.42161800	-0.26683900	1.50646700
C	4.04743400	-3.10482600	-3.70219300	C	-4.49155200	1.10698500	1.79326500
C	3.73056600	-3.11590300	-5.06041500	C	-3.77987600	2.19215600	1.24150100
H	0.50045200	-2.10199800	-4.85325900	C	-4.40401400	3.54702000	1.51821300
H	3.35955400	-2.73369300	-1.70674200	C	-3.69449500	-2.19505000	0.34268300
H	2.18049900	-2.75762200	-6.51275900	C	-4.49637300	-2.43054500	-0.80302000
H	5.04233600	-3.39379800	-3.37281100	C	-4.70026800	-3.74666600	-1.22851200
H	4.47268200	-3.41140200	-5.79696200	C	-4.13706100	-4.82334900	-0.55415800
C	-0.61447300	-1.65053400	-2.64325600	C	-3.35168700	-4.58461200	0.56624200
H	-0.59387700	-0.79891300	-3.33521700	C	-3.11688900	-3.28677700	1.03407800
H	-1.05020600	-2.50262000	-3.17566000	C	-2.10509000	3.24807500	-0.09098900
H	-1.29503300	-1.39674200	-1.82609700	C	-2.30404100	3.42833100	-1.48380500
				C	-1.72681800	4.53438700	-2.11202200
				C	-0.96456400	5.45439300	-1.40264900
				C	-0.77867000	5.27464700	-0.04020300
				C	-1.33844300	4.18701700	0.64091800
				H	3.46832300	-1.50976800	4.41914900
				H	4.06597000	-3.08474000	3.85546700
				H	2.40774200	-2.92335000	4.42060400
				H	3.07836300	-4.17088200	2.11778100

TS-1_1a2a

Mg	1.29512100	-0.70651300	0.23210100
Mg	-1.67456100	0.20038500	0.33915100
N	2.32375600	-0.91211700	2.08967600
N	2.20368300	-2.42670500	-0.60105500
N	-3.46421900	-0.84918000	0.77605500
N	-2.65692400	2.08042400	0.53180700

H	2.05747400	-5.31468100	-0.55408900	H	3.38050500	1.34638000	-0.56453000
H	3.55417000	-5.33922900	0.38912500	C	5.25055300	-0.29999000	-2.55618500
H	3.53657900	-4.69111500	-1.26521300	H	5.79036000	-0.55857100	-3.47392700
H	4.74683600	2.58375900	3.85081700	H	4.46569000	0.41510500	-2.81584300
H	1.00275500	1.66608200	5.69460600	H	5.96783400	0.20377500	-1.89861900
H	4.60177600	-2.04600900	-4.50889600	C	5.80237700	-2.54331800	-1.56027100
H	0.75367700	-3.89233600	-4.74053800	H	5.44605600	-3.39239900	-0.97096000
H	-6.37281400	-1.15583000	1.27593100	H	6.23101900	-2.93543700	-2.48994000
H	-6.01879000	-0.60587000	2.91459300	H	6.60952800	-2.06172100	-0.99656100
H	-5.29171100	-2.10348100	2.28443900	C	-1.15083100	-2.94996000	-2.63085900
H	-5.33492200	1.39488800	2.41193500	H	-1.03393700	-1.89314600	-2.37004900
H	-4.10875700	3.89520600	2.51410700	H	-1.26787400	-3.01539200	-3.71881000
H	-5.49393400	3.47377700	1.51001100	H	-2.07249000	-3.31268900	-2.16695600
H	-4.09297600	4.30253800	0.79597700	C	-0.19086500	-5.26188900	-2.43910900
H	-5.31438000	-3.93025900	-2.10668000	H	-0.37168900	-5.44096700	-3.50487600
H	-2.91965700	-5.42579300	1.10252300	H	0.66051400	-5.88297300	-2.14426600
H	-1.86962500	4.67755600	-3.17814000	H	-1.07481200	-5.60848900	-1.89374700
H	-0.18504800	5.99562300	0.51615500	C	0.14123600	-1.09218500	5.50571900
C	4.76718600	0.66894300	1.94792900	H	1.01440500	-1.72022300	5.70041200
C	0.23507600	-0.37989100	4.14751900	H	0.06594600	-0.37119200	6.32738400
H	0.24191200	-1.14105700	3.36012500	H	-0.75100200	-1.72664100	5.54535000
H	4.32199800	0.06790400	1.14781900	C	-1.00596200	0.49724100	3.93758600
C	4.67703000	-1.53934500	-1.85773600	H	-1.08661800	1.27050700	4.70984900
H	4.25647600	-1.21858900	-0.89920500	H	-0.96771700	1.00784700	2.96927400
C	0.05272500	-3.77218600	-2.15386900	H	-1.92212700	-0.10164400	3.97364700
H	0.12904100	-3.64498100	-1.06897700	C	5.89359300	-0.16915400	2.57375100
C	-1.09673300	4.08014200	2.14033600	H	6.35544800	0.36555600	3.41179700
H	-1.67427300	3.22982200	2.51609600	H	5.52458700	-1.12662800	2.94969100
C	-3.18067500	2.47773100	-2.28634000	H	6.67570300	-0.37745400	1.83507900
H	-3.09868800	1.48507200	-1.82470600	C	5.35134300	1.94261300	1.32283600
C	-2.29287700	-3.10865100	2.30036500	H	4.56965900	2.60455100	0.93746300
H	-2.15493000	-2.03252200	2.45187100	H	5.94399800	2.51679200	2.04348800
C	-5.13637500	-1.30214800	-1.60129400	H	6.02037900	1.68531900	0.49473300
H	-4.94707700	-0.36479600	-1.06968500	C	-1.56719800	5.33790000	2.88918700
C	1.11439900	1.56337800	-0.69474000	H	-0.94591600	6.20525400	2.64083200
H	0.59136200	2.31773400	-0.12194800	H	-2.60212900	5.59765600	2.64980200
C	1.55953300	1.48228600	-2.14350500	H	-1.49427800	5.18555200	3.97171000
C	2.38232500	1.13931400	-0.92711800	C	0.38097500	3.81640200	2.45748100

H	0.72953100	2.86985200	2.03485200	C	2.72233900	5.08348900	-2.64775100
H	1.01735700	4.61579800	2.06198400	H	2.57413600	3.74054300	-0.98533800
H	0.54390000	3.76501700	3.53791500	C	1.98880200	4.22899200	-4.77048300
C	-4.65865600	2.89151600	-2.19943000	H	1.26923400	2.21416800	-4.78557900
H	-5.02138300	2.88675800	-1.16855100	C	2.51721300	5.27259000	-4.01400100
H	-4.79749400	3.90123000	-2.60235600	H	3.13612400	5.88625400	-2.04268200
H	-5.28743100	2.20753400	-2.78048900	H	1.82690100	4.35727400	-5.83776400
C	-2.76009100	2.34542000	-3.75358700	H	2.77070200	6.21931900	-4.48324800
H	-2.99582000	3.24824100	-4.32791600	TS-1_1a2b			
H	-1.68726000	2.15762500	-3.85253600	Mg	0.21013600	1.60079900	0.03808500
H	-3.29879500	1.51770000	-4.22511500	Mg	1.34320700	-1.27370500	0.36065400
C	-4.50175000	-1.18223100	-2.99453300	N	0.58222900	2.98867100	1.61368400
H	-3.42568800	-0.99661800	-2.93145500	N	0.48841100	3.05627100	-1.47317000
H	-4.64389300	-2.10062500	-3.57492400	N	3.28792800	-2.06865700	0.08628000
H	-4.95877100	-0.36048600	-3.55709200	N	0.70526000	-3.01909100	1.39821400
C	-6.65813400	-1.46672600	-1.73115100	C	1.90023900	4.91411500	2.47000400
H	-6.91927000	-2.34506500	-2.33165600	C	1.34318800	4.05322400	1.34962200
H	-7.14291200	-1.58032600	-0.75692100	C	1.72202100	4.48584400	0.06315800
H	-7.09488100	-0.59186600	-2.22502200	C	1.27430600	4.10517400	-1.21503600
C	-0.90467600	-3.74655100	2.17759300	C	1.76289300	4.98479800	-2.34932300
H	-0.96716500	-4.83069100	2.03272100	C	0.16378300	2.78509400	2.96951300
H	-0.34605100	-3.32815600	1.33566600	C	-1.08881000	3.30302400	3.38688600
H	-0.31865300	-3.57293300	3.08600200	C	-1.48679000	3.12731500	4.71550200
C	-3.02300500	-3.66668800	3.53257000	C	-0.68292900	2.45901100	5.63086000
H	-3.99437200	-3.18787900	3.68636000	C	0.53653300	1.94431700	5.21233700
H	-3.19637700	-4.74421600	3.43454100	C	0.98014800	2.08853900	3.89315000
H	-2.42534800	-3.50922200	4.43732200	C	-0.07977000	2.95980600	-2.78658800
H	2.82411000	-3.11983500	-5.84762800	C	-1.35595800	3.53134700	-3.02229600
H	3.05748000	3.03629100	5.59553700	C	-1.92106500	3.41691500	-4.29559100
H	-4.31269800	-5.83962400	-0.89645000	C	-1.26635400	2.74618300	-5.32242400
H	-0.51263200	6.29939800	-1.91322600	C	-0.01982400	2.18562300	-5.08049600
C	1.03438200	0.39991300	-3.06077500	C	0.59731100	2.28580900	-3.82847700
H	0.10439600	0.70044000	-3.55670500	C	5.23225700	-3.35943300	0.91120100
H	1.76382500	0.13221000	-3.83222500	C	3.76571200	-2.97845300	0.94308400
H	0.81971300	-0.50772200	-2.49497900	C	2.99113300	-3.69450700	1.87104200
C	1.86973800	2.80376200	-2.79606900	C	1.59127300	-3.82239800	1.98670200
C	2.40399300	3.86795100	-2.04995600	C	1.14544400	-4.98208100	2.85731500

C	4.15281800	-1.64831000	-0.97571600	C	-2.10549000	4.29545800	-1.94019100
C	4.26712000	-2.45067100	-2.13944500	H	-1.66106000	4.00796700	-0.98182000
C	5.09910200	-2.02297000	-3.17848700	C	1.96788000	1.65516900	-3.64093500
C	5.81351200	-0.83388800	-3.09422500	H	2.32009100	1.91373100	-2.63699300
C	5.69532900	-0.05276800	-1.95194700	C	-0.84799100	-2.42025700	3.89810100
C	4.87750500	-0.43610900	-0.88300400	H	0.23479500	-2.35010200	3.75517500
C	-0.69064000	-3.33563800	1.48427500	C	-0.52052400	-4.33209500	-0.87149000
C	-1.31951900	-3.92724700	0.35896300	H	0.31997100	-3.63190300	-0.96393800
C	-2.68998900	-4.19275800	0.41182300	C	4.84158200	0.44564300	0.35604000
C	-3.44396800	-3.88764200	1.53838200	H	4.10565200	0.01428600	1.04315800
C	-2.82128100	-3.31375300	2.63669900	C	3.50520000	-3.75841000	-2.31058800
C	-1.44994500	-3.03154600	2.64019900	H	2.98813300	-3.97151800	-1.37026400
H	1.31973100	4.84062500	3.38948600	C	-1.66587200	0.04179000	0.35562300
H	1.94793900	5.96089500	2.16179200	H	-1.61937000	-0.64009800	1.19410200
H	2.92415200	4.59636900	2.69710500	C	-2.50463700	0.08910600	-0.91011900
H	2.39040700	5.33957500	0.06508700	C	-2.21365700	1.23636100	0.02464700
H	2.58569900	4.48631400	-2.87334300	H	-2.76189200	2.03989600	0.49743400
H	2.13179600	5.94131000	-1.97542000	C	-3.59844400	3.94702100	-1.88964400
H	0.98273200	5.16970500	-3.08992600	H	-4.13583900	4.31434800	-2.77098600
H	-2.43915500	3.53499600	5.04274400	H	-3.75898800	2.86787900	-1.82231500
H	1.16769600	1.42178100	5.92714500	H	-4.06480900	4.41724300	-1.01670400
H	-2.89376600	3.86187600	-4.48646000	C	-1.92602500	5.81382200	-2.09963900
H	0.49482100	1.66219800	-5.88249300	H	-0.87563400	6.10965300	-2.03429300
H	5.41315900	-4.11692800	0.14143700	H	-2.31120700	6.15206900	-3.06863900
H	5.53942000	-3.78251000	1.87003900	H	-2.47277900	6.35082600	-1.31614500
H	5.87144400	-2.50805500	0.67275800	C	1.89316200	0.12560300	-3.72286900
H	3.55451600	-4.38403500	2.49067300	H	1.22617300	-0.27705100	-2.95362800
H	1.18441900	-4.69016700	3.91253400	H	1.51479700	-0.19999500	-4.69877000
H	1.81784700	-5.83380100	2.73138700	H	2.88283800	-0.31632600	-3.57664800
H	0.12550000	-5.29868400	2.63682400	C	2.99809700	2.18034300	-4.65226900
H	5.18833800	-2.63589900	-4.07199400	H	2.75118500	1.86967200	-5.67358400
H	6.26174500	0.87230100	-1.87858000	H	3.05835900	3.27301700	-4.64950200
H	-3.18066600	-4.64164200	-0.44564200	H	3.99031400	1.78036600	-4.41889800
H	-3.40985900	-3.07816000	3.51977500	C	3.47563200	2.10623900	4.35617900
C	-1.97499400	4.10515600	2.44520900	H	3.49375300	3.19794500	4.30225000
C	2.33500100	1.50577600	3.51987300	H	3.38084400	1.83225000	5.41279400
H	2.51906300	1.74441900	2.46710700	H	4.44435300	1.73133800	4.00805300
H	-1.66029400	3.86481000	1.42401300	C	2.34204400	-0.02199400	3.66053000

H	2.18442200	-0.32897900	4.70061700	H	4.34368200	2.48271900	0.93697200
H	1.54321000	-0.47520300	3.06347800	C	6.19951400	0.46834900	1.07568800
H	3.29787500	-0.44413200	3.33259100	H	6.52316100	-0.53303300	1.37419100
C	-1.77001500	5.61616000	2.63980200	H	6.98055900	0.89116200	0.43396000
H	-2.02698000	5.91427300	3.66285500	H	6.14481800	1.08564400	1.97930100
H	-0.73433900	5.91161400	2.45423400	H	-1.72463900	2.66470300	-6.30449600
H	-2.40842000	6.18351200	1.95331200	H	-1.00477600	2.34226600	6.66220400
C	-3.46349600	3.75931200	2.58275000	H	6.45990100	-0.52150900	-3.90995700
H	-3.63923200	2.68041700	2.52950200	H	-4.51053300	-4.09060600	1.55347300
H	-3.87977000	4.11490000	3.53168500	C	-1.85904900	0.01308100	-2.27608800
H	-4.03901900	4.23934500	1.78404300	H	-1.75070500	-1.02212700	-2.61902300
C	-1.10483100	-3.29093500	5.13912800	H	-2.43416000	0.56507100	-3.02661900
H	-2.16785400	-3.30433800	5.40330100	H	-0.86068900	0.45184800	-2.25130500
H	-0.79241600	-4.32785500	4.98748100	C	-3.87763300	-0.51663900	-0.80153600
H	-0.56064900	-2.89240300	6.00251600	C	-4.58742200	-0.47559300	0.43387100
C	-1.37798100	-1.00235700	4.14774600	C	-4.51034000	-1.09569200	-1.88810500
H	-1.11607100	-0.31671900	3.33695200	C	-5.85394000	-0.98972100	0.55419700
H	-2.46886900	-1.00201400	4.24959500	H	-4.11308400	-0.02472200	1.29967500
H	-0.95779400	-0.58609800	5.06792200	C	-5.81745400	-1.63733300	-1.79920600
C	0.08261800	-5.73500800	-0.69479100	H	-4.01235800	-1.13990200	-2.85184100
H	0.75323800	-5.78293200	0.16677600	C	-6.51188000	-1.58634100	-0.55152700
H	-0.71078800	-6.47659200	-0.54763800	H	-6.37160800	-0.94317000	1.50978600
H	0.65476200	-6.02558600	-1.58306600	C	-6.46440400	-2.22964800	-2.91533100
C	-1.32513100	-4.26896400	-2.17379200	C	-7.81943900	-2.12701900	-0.46638000
H	-2.06532200	-5.07442400	-2.23487200	C	-7.73372800	-2.74779800	-2.80254800
H	-1.85717000	-3.31895200	-2.27593200	H	-5.93733600	-2.26732700	-3.86596600
H	-0.65734500	-4.38331100	-3.03326600	C	-8.41891500	-2.69654600	-1.56629500
C	2.43950400	-3.63618200	-3.40943600	H	-8.34321800	-2.08374300	0.48593800
H	1.72302500	-2.84014100	-3.18723200	H	-8.21599700	-3.19869500	-3.66566100
H	2.89510000	-3.40775700	-4.37936300	H	-9.42153700	-3.10823300	-1.48927700
H	1.88579100	-4.57563100	-3.51618000				
C	4.43514200	-4.94350600	-2.61126300				
H	4.92456800	-4.83566800	-3.58549200				
H	5.22263300	-5.04807300	-1.85890000				
H	3.86486000	-5.87854500	-2.63392600				
C	4.39500800	1.87464000	0.02793800				
H	5.09165600	2.37020700	-0.65714300				
H	3.40488500	1.88473200	-0.43665900				

TS-1_1a2c

Mg	1.38009500	-0.51717400	0.44449100
Mg	-1.71233900	-0.02198800	0.49059900
N	2.39808200	-0.25248400	2.32861200
N	2.61945800	-2.13829700	-0.09443300
N	-3.26486100	-1.33516400	1.10165700
N	-3.02828200	1.66508600	0.58895100

C	3.49524900	-1.30143100	4.30933600	H	2.87036200	-4.94312700	0.22133200
C	2.98176100	-1.31745900	2.87851000	H	4.16327900	-4.72942900	1.41419200
C	3.19583600	-2.55291900	2.23375700	H	4.39710400	-4.24197400	-0.27652400
C	3.12450300	-2.90856900	0.87829800	H	4.14713000	3.82138400	3.57638800
C	3.67909800	-4.28045500	0.54563800	H	0.60891600	2.50432900	5.57882000
C	2.36309900	0.95418200	3.10188200	H	5.36889900	-2.18429000	-3.78268900
C	3.37853200	1.92541300	2.91760100	H	1.80689600	-4.54325400	-3.95737000
C	3.36142400	3.08180200	3.70356100	H	-6.07927900	-2.03805600	1.75000600
C	2.37666000	3.29344900	4.66057200	H	-5.72685100	-1.39557600	3.35443500
C	1.37892400	2.34229300	4.82835200	H	-4.82660300	-2.79521200	2.72180000
C	1.34503400	1.17212000	4.06241300	H	-5.37029500	0.66627000	2.76097400
C	2.92214500	-2.54690700	-1.43640200	H	-4.48414300	3.33338600	2.67482900
C	4.11312900	-2.07156200	-2.04081000	H	-5.91203900	2.66319800	1.88866400
C	4.44593300	-2.52545000	-3.32075900	H	-4.76269700	3.64840100	0.95918000
C	3.62810600	-3.41507400	-4.00825100	H	-4.49190000	-4.93131400	-1.50447100
C	2.45060300	-3.85416200	-3.41698500	H	-1.93722100	-5.69775500	1.83621900
C	2.07920600	-3.44087500	-2.13361000	H	-3.24420600	4.06890200	-3.32852400
C	-5.27287700	-1.83463800	2.46318600	H	-1.19234300	5.86929500	-0.05221900
C	-4.27120600	-0.87686600	1.84995900	C	4.53218500	1.70143200	1.95148000
C	-4.54282700	0.48387100	2.08388700	C	0.23338300	0.16703500	4.32643700
C	-4.06836100	1.63569500	1.42607100	H	0.38106500	-0.67669200	3.64434300
C	-4.85474600	2.89473200	1.74182400	H	4.22364800	0.91130800	1.25861300
C	-3.25114100	-2.73352100	0.78807300	C	5.06336600	-1.12824500	-1.31473400
C	-3.97766900	-3.20442600	-0.33310000	H	4.51508200	-0.71964600	-0.45984000
C	-3.93599600	-4.56706200	-0.64406700	C	0.78562000	-3.96425100	-1.53181500
C	-3.20569700	-5.46448100	0.12516600	H	0.77894600	-3.68774400	-0.47226400
C	-2.49957900	-4.99561900	1.22576600	C	-1.66510100	4.04926500	1.83688500
C	-2.50569000	-3.64154900	1.57784300	H	-2.03776900	3.15767600	2.34996200
C	-2.77959500	2.85661000	-0.17320700	C	-4.11846300	1.81136600	-2.10580400
C	-3.23704700	2.90916700	-1.51823500	H	-3.73700700	0.84921700	-1.73784700
C	-2.91024700	4.02235600	-2.29754100	C	-1.74587800	-3.20987900	2.82306900
C	-2.15980000	5.07417600	-1.78599300	H	-1.82036100	-2.11926800	2.89027500
C	-1.75609000	5.03496700	-0.46129200	C	-4.80416900	-2.28053800	-1.21615300
C	-2.06445500	3.95113200	0.36998000	H	-4.77168200	-1.28019400	-0.77369600
H	3.48467700	-0.31146300	4.76258200	C	0.92910400	1.59739400	-0.68363700
H	4.51479400	-1.69513100	4.34458300	H	0.39642300	2.29525000	-0.05378000
H	2.87817200	-1.96774100	4.92209000	C	1.27892000	1.64879300	-2.15725700
H	3.61252800	-3.31823400	2.87925300	C	0.77405600	0.63346400	-3.14554200

C	-0.59951600	0.50910300	-3.38631900	H	5.58345900	0.26183600	3.22506600
C	1.66057300	-0.09582300	-3.94162200	H	6.60112100	1.01567800	1.98909900
C	-1.07423200	-0.31690900	-4.40421300	C	4.88226800	2.95003300	1.13231200
C	1.18992500	-0.92071000	-4.96319000	H	4.00354000	3.37294500	0.63695600
C	-0.17809300	-1.02906700	-5.20136900	H	5.32302800	3.73654300	1.75458400
H	-1.28962000	1.09404100	-2.78394500	H	5.62066800	2.70314200	0.36191000
H	2.72791100	-0.01322600	-3.76401400	C	-2.30554200	5.28027400	2.50296700
H	-2.14253800	-0.39896600	-4.58216400	H	-1.87523200	6.20920000	2.11323000
H	1.89724400	-1.47899100	-5.56839300	H	-3.38520000	5.32565000	2.33724400
H	-0.54633900	-1.66697400	-6.00052300	H	-2.12470600	5.26543800	3.58358300
C	2.21116600	1.30795200	-1.03083200	C	-0.14599900	4.10330600	2.03733300
H	3.21255700	1.58890300	-0.73209200	H	0.34293000	3.16791300	1.75294100
C	5.51712800	0.04781400	-2.18909600	H	0.30327300	4.91321700	1.45261100
H	6.13615900	-0.28083700	-3.03107700	H	0.09822300	4.27630200	3.08896300
H	4.66659100	0.60274500	-2.59424500	C	-5.57477600	1.93442200	-1.62524400
H	6.12496500	0.74360600	-1.59983900	H	-5.66684600	1.80971200	-0.54541100
C	6.29041000	-1.87375500	-0.76561900	H	-5.98430900	2.91462000	-1.89440800
H	6.00817700	-2.64980100	-0.04940300	H	-6.19790100	1.16871800	-2.10122800
H	6.85338700	-2.35139400	-1.57590200	C	-4.11379100	1.76926900	-3.63828400
H	6.96599200	-1.17909600	-0.25357100	H	-4.65930100	2.61910900	-4.06404200
C	-0.43014000	-3.29906000	-2.18794600	H	-3.10422100	1.77653000	-4.05728300
H	-0.38111000	-2.20926600	-2.10033300	H	-4.62075800	0.86335000	-3.98533300
H	-0.47805300	-3.53804100	-3.25601400	C	-4.20999100	-2.18681800	-2.62842600
H	-1.35575300	-3.64423900	-1.71650600	H	-3.17795800	-1.82495700	-2.60798600
C	0.65935000	-5.49201700	-1.61518100	H	-4.20493600	-3.16498800	-3.12209200
H	0.55286300	-5.83293600	-2.65102400	H	-4.80108600	-1.50563600	-3.25074700
H	1.52927400	-6.00315700	-1.18995200	C	-6.27681800	-2.71106800	-1.28817600
H	-0.23155200	-5.82144000	-1.07098500	H	-6.38935500	-3.67956000	-1.78786100
C	0.26714300	-0.36808100	5.76656000	H	-6.72444500	-2.80115200	-0.29386700
H	1.23794100	-0.80061900	6.02102500	H	-6.86147600	-1.97946500	-1.85660200
H	0.06174400	0.42825200	6.49067700	C	-0.25970900	-3.57256600	2.73704800
H	-0.49696100	-1.14084200	5.90531800	H	-0.10928200	-4.65612900	2.67744600
C	-1.14651800	0.76770800	4.03251500	H	0.20913900	-3.12233700	1.85756300
H	-1.36874800	1.60914200	4.69849700	H	0.27840300	-3.21607300	3.62128200
H	-1.20164500	1.14301000	3.00503000	C	-2.35931000	-3.80393400	4.10114000
H	-1.93792900	0.02306200	4.16634400	H	-3.40789500	-3.51915000	4.22617100
C	5.78036100	1.19549800	2.69242200	H	-2.31211500	-4.89861200	4.09070900
H	6.12177500	1.93442300	3.42649500	H	-1.81128700	-3.45870000	4.98494200

H	3.90870800	-3.76432300	-4.99870700	C	4.17096900	3.40878700	0.82957100
H	2.38913900	4.19159500	5.27224600	C	3.69314200	2.20596200	1.35577900
H	-3.19203600	-6.52128700	-0.12737000	C	2.58584100	-0.54347300	-5.44713600
H	-1.89766200	5.91831400	-2.41678400	C	1.54882600	-0.74641800	-4.36043600
C	1.42835600	3.04544800	-2.72449400	C	0.31051100	-1.25423000	-4.78987300
C	1.86004900	4.10319400	-1.90671000	C	-0.84236900	-1.57193200	-4.05042900
C	1.17231900	3.32941000	-4.07445600	C	-1.98140500	-2.19006800	-4.83518100
C	2.02568600	5.38871800	-2.41445600	C	3.18960100	-0.01019400	-2.84086200
H	2.07013100	3.91845000	-0.85795800	C	3.49384700	1.36332200	-2.85306900
C	1.34220800	4.61493900	-4.58411500	C	4.81852300	1.76375100	-2.65608600
H	0.84150700	2.53504400	-4.73477000	C	5.84554500	0.84551800	-2.43157700
C	1.76901300	5.65325600	-3.75879400	C	5.50863500	-0.50916200	-2.37548700
H	2.36127200	6.18584300	-1.75585600	C	4.20015100	-0.95512500	-2.57254100
H	1.14099600	4.80272500	-5.63576300	C	-2.22013300	-1.74974100	-2.14078500
H	1.90420900	6.65467700	-4.15842700	C	-3.28391200	-0.82621600	-2.10448300
				C	-4.47942600	-1.19853600	-1.48523000
				C	-4.65016800	-2.45569700	-0.90055000

TS-1_1b2b

Mg	0.80866300	-0.21330600	1.52141100	C	-3.57639000	-3.34680400	-0.93957200
Mg	0.52893100	-0.64937600	-1.48314600	C	-2.36204300	-3.01872200	-1.54894000
N	0.83803800	-1.80289000	2.87396200	H	0.32009400	-3.24912600	5.16544400
N	2.04575200	0.99648800	2.70037600	H	1.75172000	-2.62219000	6.00882200
N	1.85473100	-0.45254700	-3.09257200	H	1.91954200	-3.72034800	4.62743800
N	-0.97545900	-1.38040600	-2.73636200	H	2.43660500	-0.65962400	5.58367600
C	1.34189100	-2.88224400	5.03166000	H	4.33689200	1.60150700	4.17601800
C	1.38539100	-1.69644700	4.08777100	H	3.56475200	1.12591700	5.69927900
C	2.05889700	-0.56123900	4.57308000	H	2.99867900	2.54564200	4.79742200
C	2.42733000	0.63539700	3.92514100	H	-2.44375300	-5.01977300	2.54862600
C	3.37857100	1.52547100	4.70131600	H	1.44994500	-5.96066300	1.03086100
C	0.35194600	-3.08920100	2.48916200	H	1.93554100	5.56822400	2.15954500
C	-0.98668800	-3.45677800	2.72155500	H	5.05398300	3.38384100	0.19420600
C	-1.41075600	-4.73726100	2.35254500	H	2.93246200	0.49441900	-5.46918600
C	-0.55342500	-5.66166800	1.75509700	H	2.18134400	-0.79666200	-6.42832500
C	0.76238000	-5.26335200	1.50706500	H	3.47250000	-1.15950200	-5.26688000
C	1.23074200	-3.99655700	1.86133100	H	0.24082400	-1.45148900	-5.85285300
C	2.55575000	2.22750500	2.18473900	H	-2.21781800	-3.18700400	-4.44876200
C	1.91647500	3.44927600	2.47817500	H	-1.72831700	-2.27918400	-5.89274400
C	2.43064600	4.62628400	1.92836600	H	-2.89777800	-1.59966000	-4.74381300
C	3.55399500	4.63134700	1.09914100	H	5.05141900	2.82664500	-2.68519100

H	6.28752600	-1.24428300	-2.17934500	H	7.80591100	0.69780700	-1.52675900
H	-5.29401400	-0.47840000	-1.45114800	H	7.82818600	1.19602200	-3.21757200
H	-3.68123100	-4.32933700	-0.48338100	H	7.33563000	2.34498000	-1.97279800
C	-1.43396900	0.25588600	0.73590900	C	-3.13325900	0.54245400	-2.71127000
H	-1.96807400	-0.58312200	0.30469900	H	-2.26788600	1.06761600	-2.29310100
C	-1.69295500	1.75673100	0.74865400	H	-2.97537300	0.49745800	-3.79505000
C	-1.36649200	0.89279100	1.93630100	H	-4.01838500	1.15366200	-2.52177200
H	-1.71880700	0.75642400	2.95090400	C	-1.22837000	-4.00790800	-1.57383000
C	-0.66713300	2.71632100	0.17840700	H	-0.83034600	-4.14734200	-2.58444900
H	-0.80636400	2.86789600	-0.89958600	H	-0.39317400	-3.67855300	-0.94359300
H	-0.72287000	3.69645100	0.66356600	H	-1.55212400	-4.97956600	-1.19407300
H	0.34618500	2.33527500	0.33136300	C	-5.96228800	-2.84512000	-0.27089600
C	-3.12986200	2.17948400	0.60645000	H	-6.46219700	-1.98171500	0.17878800
C	-4.17311300	1.37150900	1.14617600	H	-6.65078400	-3.26604200	-1.01445800
C	-3.48923800	3.36612100	-0.00949400	H	-5.82512500	-3.60084200	0.50847400
C	-5.49068600	1.74681000	1.06332500	C	-1.95066900	-2.50143200	3.37236300
H	-3.91566200	0.43929000	1.63858700	H	-2.91073400	-2.98842100	3.56403900
C	-4.84020200	3.78361100	-0.11446100	H	-1.56884800	-2.11706500	4.32411500
H	-2.72890300	4.01780700	-0.42900600	H	-2.13744900	-1.63012000	2.73598600
C	-5.87095100	2.95964900	0.43346000	C	2.65898800	-3.60868400	1.59006900
H	-6.26482300	1.11209200	1.48903700	H	2.71222100	-2.70592900	0.96840100
C	-5.20520500	5.00091200	-0.74705600	H	3.20556400	-3.38025100	2.51197000
C	-7.22031500	3.38092600	0.33001300	H	3.19094400	-4.41148000	1.07203200
C	-6.52372300	5.38330600	-0.83427800	C	-1.01975700	-7.05324000	1.41382500
H	-4.42151000	5.62939000	-1.16386900	H	-0.73618500	-7.77019100	2.19458200
C	-7.54205200	4.56623000	-0.29051500	H	-2.10821000	-7.09868900	1.31219200
H	-7.99997700	2.74986700	0.75064700	H	-0.57802500	-7.40776900	0.47692600
H	-6.78798000	6.31766800	-1.32205700	C	0.70938400	3.49713400	3.37597700
H	-8.57994100	4.87909900	-0.36457000	H	-0.02661000	2.74158900	3.08572000
C	3.87802500	-2.42438600	-2.51403000	H	0.96763700	3.29860500	4.42340900
H	3.11120100	-2.63399700	-1.75876100	H	0.23468300	4.48163600	3.33736100
H	3.48427800	-2.79880600	-3.46573000	C	4.39316600	0.90882000	1.05922300
H	4.76716400	-3.00920700	-2.26327700	H	4.68176400	0.38284700	1.97582000
C	2.41412300	2.38520500	-3.08714600	H	3.74512700	0.22657500	0.49424200
H	1.89054800	2.22223100	-4.03553600	H	5.28883800	1.07552500	0.45783900
H	1.65404400	2.34491200	-2.29771900	C	4.06728700	5.91307700	0.49612000
H	2.82867500	3.39661300	-3.09594600	H	3.55310300	6.14574100	-0.44504600
C	7.27524500	1.29524000	-2.27504900	H	3.91073500	6.76335400	1.16738100

H	5.13723800	5.85137600	0.27488600	C	2.82850700	3.11656200	-2.03855400
TS-1_1b2c							
Mg	-0.58935400	-1.02852700	0.74311100	C	4.03259200	2.69253400	-2.60805200
Mg	-0.13389400	1.92818600	0.16341800	C	5.03935500	2.08996900	-1.85216800
N	-0.38583700	-1.65420500	2.75283900	C	4.81448300	1.92317400	-0.48422200
N	-2.35550700	-2.12439800	0.49824100	C	3.62916600	2.33510200	0.12860700
N	-1.54322000	3.44737800	0.50994800	H	-0.94744200	-3.17479100	5.14726900
N	1.39254300	3.34291100	-0.06401000	H	-2.34853600	-2.13502900	5.42682000
C	-1.36678800	-2.18144500	4.95160400	H	-0.70249500	-1.45929200	5.43290200
C	-1.47498600	-1.94318800	3.45929300	H	-3.55281600	-2.25508600	3.62972000
C	-2.76194800	-2.10052200	2.90501100	H	-5.07944500	-2.25496500	0.58757400
C	-3.14303400	-2.30513900	1.56354200	H	-5.12673400	-2.75807900	2.29288100
C	-4.55595100	-2.81854400	1.36472500	H	-4.54620000	-3.86397200	1.03813400
C	0.88646700	-1.71802300	3.39183600	H	3.42698300	-3.89572700	4.00508100
C	1.59507800	-2.93531900	3.43891700	H	3.19187000	0.28815700	4.88956700
C	2.88277100	-2.95263300	3.98490400	H	-2.97937300	-5.51871700	-2.53177800
C	3.48466500	-1.80818100	4.50662800	H	-4.55627200	-1.65897000	-3.51685800
C	2.75314900	-0.61814200	4.47510300	H	-2.96191500	5.88070700	0.38129300
C	1.46890200	-0.55145100	3.93194500	H	0.20390300	6.23337600	1.13841800
C	-2.84097500	-2.62545000	-0.74913500	H	3.36525500	5.06422800	0.76593900
C	-2.62857200	-3.97837900	-1.08213400	H	2.29495200	6.48256500	0.74443200
C	-3.14075100	-4.47042000	-2.28509500	H	2.79456700	5.69925100	-0.76394200
C	-3.85761800	-3.66194300	-3.17028000	H	-5.55687100	3.20466200	-1.70897300
C	-4.02106000	-2.31724000	-2.83460800	H	-5.46108400	1.91457500	2.37484800
C	-3.51998200	-1.78054900	-1.64542100	H	4.18468800	2.83635800	-3.67641400
C	-2.29038500	5.68568800	1.22403000	H	5.58484400	1.45759300	0.12770100
C	-1.20951300	4.69854200	0.83224100	C	1.68729300	-0.93116000	-0.02147300
C	0.10474300	5.20319700	0.81755200	H	2.31777400	-0.30011200	0.59043100
C	1.28798400	4.61148500	0.34133300	C	1.88294200	-1.58835700	-1.37184500
C	2.49980200	5.51891000	0.27521000	C	0.98303500	-1.26758300	-2.53336800
C	-2.93538700	3.13137600	0.45523200	C	1.09778900	-0.03639100	-3.19425200
C	-3.64670500	3.33252800	-0.74481500	C	0.07244700	-2.20799600	-3.01719300
C	-5.01005100	3.03352700	-0.78301400	C	0.31506300	0.24474400	-4.31177800
C	-5.68849500	2.52430500	0.32681600	C	-0.71227800	-1.92921600	-4.13745700
C	-4.95654900	2.31191400	1.49580900	C	-0.59277600	-0.70333100	-4.78728900
C	-3.59149200	2.60192300	1.58190500	H	1.82254800	0.69007600	-2.83565800
C	2.62731300	2.93786100	-0.65615000	H	-0.02185800	-3.16431500	-2.51053500

H	0.41729400	1.20192200	-4.81699500	H	5.43249800	-0.95035800	4.89378200
H	-1.41911600	-2.67175300	-4.49315900	H	4.80989600	-1.94532300	6.20926000
H	-1.20216600	-0.48587900	-5.66064400	C	3.43822500	2.16050600	1.61091400
C	1.35934100	-2.24623800	-0.12406700	H	3.35096500	3.12348900	2.12786200
H	1.56559900	-3.15822700	0.42142600	H	2.51952500	1.60913100	1.84109200
C	3.31236500	-1.92270500	-1.72823500	H	4.27641700	1.61587800	2.05303700
C	4.25904600	-2.16411300	-0.71748700	C	1.76656600	3.75588200	-2.89384100
C	3.73216500	-2.05192300	-3.06056800	H	0.82968300	3.18787700	-2.85878700
C	5.57223200	-2.50675000	-1.02724300	H	1.52276500	4.77119900	-2.56245300
H	3.96290900	-2.09395200	0.32498300	H	2.08913100	3.81132700	-3.93721100
C	5.04463400	-2.40320800	-3.37037100	C	6.31246000	1.60482000	-2.49284500
H	3.02166200	-1.88193000	-3.86263200	H	6.26243100	0.52826400	-2.69358600
C	5.97436800	-2.63024500	-2.35693700	H	6.49950600	2.11129100	-3.44445300
H	6.28270400	-2.68557400	-0.22409700	H	7.17754700	1.77536600	-1.84380600
H	5.33879200	-2.50405600	-4.41203400	C	-2.84362800	2.35857100	2.86417000
H	6.99669900	-2.90758000	-2.59932900	H	-3.52242000	2.02955700	3.65555400
C	-1.85555300	-4.88325400	-0.16101300	H	-2.08382800	1.57887900	2.73209700
H	-0.83974000	-4.50279300	-0.00604800	H	-2.31879100	3.25439900	3.21312200
H	-2.31588400	-4.95719200	0.83040200	C	-2.94993800	3.86055200	-1.97055400
H	-1.78232700	-5.89252600	-0.57565200	H	-2.46993600	4.82859000	-1.79118700
C	-3.71662900	-0.32646500	-1.32637900	H	-2.15740600	3.17812700	-2.30044000
H	-4.29487900	-0.17252100	-0.40930500	H	-3.65424100	3.97951500	-2.79841100
H	-2.75622500	0.17957600	-1.16502500	C	-7.15502700	2.18790300	0.25169300
H	-4.23309400	0.18836300	-2.14006700	H	-7.31529900	1.20377500	-0.20608100
C	-4.45222700	-4.22893400	-4.43354800	H	-7.61140100	2.16309900	1.24564300
H	-3.84190400	-5.04382200	-4.83552300	H	-7.70346900	2.91748700	-0.35284400
H	-5.45526500	-4.63589100	-4.25298700				
H	-4.54915800	-3.46451000	-5.21064100				
C	0.70114000	0.74110400	3.96019700				
H	1.32740200	1.56670700	4.30875200	Int-2			
H	0.31350300	0.99311300	2.96429800	Mg	1.91210500	-0.57893100	-1.22795900
H	-0.17226300	0.68057500	4.62023400	Mg	-2.08178500	0.35125500	0.98170400
C	0.97641800	-4.21820600	2.94944300	N	1.95504800	-2.47881900	-2.01504000
H	0.42717900	-4.72418800	3.75408500	N	3.96050600	-0.41606400	-1.18873900
H	0.25895200	-4.03985100	2.14550400	N	-2.15303100	-0.45486000	2.87348500
H	1.74127900	-4.91734600	2.59756400	N	-4.12837100	0.45155200	0.81078800
C	4.86129000	-1.85726000	5.11676900	C	2.93637900	-4.27177900	-3.38649400
H	5.43246000	-2.71427700	4.74787100	C	3.04409900	-2.97715100	-2.60874300
			C	4.31528900	-2.37496400	-2.57597500	
			C	4.75577300	-1.22460700	-1.88990700	

C	6.23400400	-0.91323800	-1.98270100	H	-2.20950100	-3.48896600	-3.67540600
C	0.75263000	-3.24640200	-2.02966400	H	5.90948100	1.44874200	2.53022700
C	0.54601600	-4.24027800	-1.05136100	H	5.11337100	4.01419000	-0.80755700
C	-0.65304600	-4.95634900	-1.05706600	H	-4.23437800	-1.36511800	5.35816200
C	-1.65757000	-4.71217300	-1.99677400	H	-2.64152900	-0.62101000	5.60164300
C	-1.43819800	-3.70543700	-2.93842300	H	-2.74879300	-2.23352400	4.92466400
C	-0.25388200	-2.96350200	-2.97214800	H	-5.39162600	-0.60481500	3.72085300
C	4.53921500	0.68309000	-0.48330800	H	-6.67796900	1.38191500	1.35795000
C	5.01411400	0.49887200	0.82930200	H	-7.02651400	0.04005300	2.46809700
C	5.53603000	1.59625200	1.51819000	H	-6.82025200	-0.24680300	0.72787300
C	5.58715900	2.87070900	0.95050800	H	1.31573300	-3.33016200	3.77396100
C	5.09315600	3.02888900	-0.34582500	H	1.50742200	0.61302500	5.43786000
C	4.56286900	1.96105800	-1.07385700	H	-5.73340400	-0.12393900	-3.45676700
C	-3.23557400	-1.25287700	4.93394500	H	-5.27670500	3.88431100	-2.01591000
C	-3.29437800	-0.66723900	3.53876300	C	0.44169600	0.91634100	-1.23213800
C	-4.57821700	-0.38648000	3.03917900	C	-0.85644100	1.23273500	-0.47462300
C	-4.97354800	0.13237600	1.78869900	C	0.38183000	2.10591200	-0.27305200
C	-6.45946600	0.33295000	1.58319600	C	-0.27428300	3.79897200	-2.05245700
C	-0.91908600	-0.78314600	3.51147900	C	0.38646800	3.49106600	-0.84629800
C	-0.34938000	-2.05591200	3.32041400	C	1.05360600	4.55136900	-0.20826800
C	0.88359300	-2.34078200	3.91475100	C	1.05985000	5.84213800	-0.73978900
C	1.56818800	-1.40090600	4.68736900	C	0.39907500	6.12077500	-1.93153800
C	0.98803400	-0.14042700	4.84831800	C	-0.26935200	5.08260500	-2.58449100
C	-0.24206400	0.18845800	4.27532000	H	-0.80690600	3.01476600	-2.58409900
C	-4.64721700	0.95106900	-0.42272900	H	-0.79347300	5.27532200	-3.51787600
C	-4.99349300	0.05626000	-1.45267200	H	0.40211900	7.12502600	-2.34673800
C	-5.45755600	0.57122400	-2.66547500	H	1.58841800	6.63282700	-0.21184900
C	-5.57267400	1.94370800	-2.89255800	H	1.58491500	4.37137500	0.72045500
C	-5.20380300	2.80928200	-1.86106800	H	-1.57068700	1.74704900	-1.13314600
C	-4.73525300	2.34072100	-0.63170500	H	0.37676700	1.28070100	-2.26955200
H	2.65869100	-5.10527800	-2.73366700	C	-1.05601600	-3.09724700	2.49350300
H	3.87922900	-4.51761700	-3.87736300	H	-2.09145700	-3.24524300	2.81672400
H	2.15168400	-4.20101300	-4.14667000	H	-1.09896300	-2.82071100	1.43294500
H	5.08507800	-2.90037700	-3.12858500	H	-0.54030700	-4.05884900	2.55764800
H	6.39319100	0.09815600	-2.36998600	C	-0.83327000	1.55876700	4.47204000
H	6.74911200	-1.62367800	-2.63104400	H	-0.98539300	2.07163400	3.51556700
H	6.70294600	-0.94168600	-0.99396400	H	-1.81229000	1.51853300	4.96217100
H	-0.80523800	-5.72758400	-0.30372900	H	-0.17573500	2.18280700	5.08290700

C	2.87515900	-1.74201900	5.35431600	H	6.62262000	4.76522800	1.06499700
H	3.37618900	-2.57535600	4.85316000	H	5.32232700	4.58309500	2.24195000
H	3.55937200	-0.88777000	5.35562200	C	1.12077600	1.94502400	1.04187400
H	2.72200700	-2.03497800	6.40054300	H	2.19177300	2.16858600	0.95234000
C	-4.30876900	3.30895300	0.43943100	H	0.71218100	2.59009700	1.83174300
H	-3.22023600	3.28472800	0.57880300	H	1.02396500	0.90983300	1.38895300
H	-4.57647000	4.33337100	0.16759200				
H	-4.76280900	3.08232900	1.40949800				
C	-4.84768200	-1.43072200	-1.26498500	Mg	2.57590500	0.05216000	-0.27264600
H	-5.35200200	-1.78981100	-0.36198000	Mg	-2.54414900	0.13069400	-0.18574400
H	-5.26169700	-1.97104100	-2.12079100	N	3.96044500	-0.96073900	-1.43274100
H	-3.79355400	-1.71925800	-1.17109900	N	3.91815300	1.55142500	0.18663400
C	-6.04588600	2.47594800	-4.22001800	N	-3.66923300	1.80137400	-0.70757500
H	-6.69119800	1.75676900	-4.73351000	N	-4.18425000	-1.14147800	-0.22058900
H	-6.60687600	3.40818100	-4.10142100	C	6.05326800	-1.25585700	-2.69308600
H	-5.20067800	2.68935000	-4.88622800	C	5.15906900	-0.47344400	-1.75728200
C	1.59201000	-4.51717900	-0.00371900	C	5.67330300	0.75026700	-1.28642500
H	2.55411100	-4.80525900	-0.44043800	C	5.12539800	1.66934800	-0.37419800
H	1.78753800	-3.63042300	0.61037600	C	5.99321500	2.85618700	-0.01882600
H	1.27131500	-5.32379900	0.66114700	C	3.57322700	-2.24466600	-1.93690600
C	-0.06605200	-1.87529500	-3.99520800	C	3.81496200	-3.40422500	-1.16435100
H	-0.06087500	-0.88567400	-3.52140500	C	3.34349400	-4.63291000	-1.63785400
H	0.88088200	-1.97875000	-4.53533400	C	2.65452000	-4.73024600	-2.84039300
H	-0.87819600	-1.88436400	-4.72715100	C	2.43351600	-3.58527800	-3.59731100
C	-2.92298000	-5.52953700	-2.00853300	C	2.88657200	-2.33437300	-3.16973400
H	-3.23389200	-5.80338500	-0.99544100	C	3.49824300	2.53076000	1.14203500
H	-3.74737700	-4.98561700	-2.47873000	C	3.77119300	2.34046300	2.51531500
H	-2.78720400	-6.46323000	-2.56869900	C	3.24017100	3.25396200	3.43240200
C	4.94482500	-0.85155600	1.49202100	C	2.47204400	4.33404000	3.01488100
H	5.44576600	-1.63042700	0.90744600	C	2.23680100	4.52793900	1.65728400
H	5.40795100	-0.82196300	2.48194500	C	2.74522500	3.64393400	0.70215300
H	3.90625300	-1.17937100	1.62049100	C	-5.73928700	2.97654900	-1.38863200
C	4.00759100	2.18340200	-2.45515400	C	-4.98496900	1.73116100	-0.96359500
H	2.91323100	2.10339200	-2.45251600	C	-5.76332100	0.56367700	-0.90066600
H	4.25632200	3.18392800	-2.81801900	C	-5.41253600	-0.75795400	-0.56086400
H	4.38710900	1.45239400	-3.17659100	C	-6.53722600	-1.76924000	-0.58012100
C	6.12637800	4.04581900	1.72372800	C	-3.04365600	3.07937800	-0.86812700
H	6.84816900	3.72934800	2.48281600	C	-2.76821200	3.86873300	0.27459000

C	-2.19829000	5.13307200	0.08886500	C	2.48648400	3.86609000	-0.78078300
C	-1.88688800	5.60837000	-1.18021800	H	3.27722900	3.34237600	-1.32906500
C	-2.12269300	4.80678000	-2.29071200	C	-3.27084100	-3.07712900	-2.22665200
C	-2.69777600	3.53941900	-2.16157200	H	-3.60630000	-2.04291900	-2.36235800
C	-3.97530400	-2.50341100	0.17453000	C	-4.71064400	-1.89282400	2.55654100
C	-4.19163300	-2.88084700	1.52073000	H	-5.11436800	-1.02904500	2.01820800
C	-3.89095700	-4.19068000	1.90313500	C	-2.91204900	2.67644200	-3.39837100
C	-3.40198100	-5.11779000	0.98971000	H	-3.64170400	1.90206800	-3.14251400
C	-3.21078300	-4.74028100	-0.33330200	C	-3.11174600	3.38239500	1.67750000
C	-3.49185500	-3.44019400	-0.76575000	H	-2.99655600	2.29017800	1.67757800
H	6.22285300	-2.26831900	-2.31630000	C	-0.74783500	-0.79818300	0.43424000
H	7.01781500	-0.76370000	-2.82554000	H	-1.12374900	-1.83196100	0.46685000
H	5.58077100	-1.36713800	-3.67441000	C	0.04500000	-0.51448100	1.71306000
H	6.65887700	1.00536500	-1.65697400	C	0.06228100	-1.52913100	2.81623700
H	5.46434300	3.79699000	-0.20046400	C	0.78691800	-0.82708300	0.41006900
H	6.91967700	2.85647200	-0.59489500	C	0.15458800	-1.14629900	4.16621000
H	6.24642100	2.84424700	1.04590300	C	-0.01329100	-2.91184300	2.55763200
H	3.52097000	-5.53013500	-1.04997500	C	0.17282700	-2.08661800	5.19780600
H	1.89757300	-3.66397300	-4.53960800	H	1.10928900	-1.88086500	0.42709500
H	3.43351100	3.11463100	4.49307900	C	0.00417200	-3.85053700	3.58244900
H	1.65095200	5.38388400	1.33484300	C	0.09811900	-3.44694900	4.91646400
H	-5.43063000	3.85574700	-0.81939300	H	0.21234000	-0.09381300	4.42378300
H	-6.81472000	2.83530700	-1.26812100	H	-0.09774900	-3.26103200	1.53215100
H	-5.54723400	3.20017000	-2.44343000	H	0.24578000	-1.74586900	6.22818200
H	-6.80845100	0.70422000	-1.14952000	H	-0.06043100	-4.90785900	3.33692100
H	-6.25540500	-2.65643200	-1.15369300	H	0.11211600	-4.18115200	5.71752000
H	-7.44595800	-1.34305500	-1.00793400	H	2.06648100	5.03030800	3.74398600
H	-6.76216900	-2.11460900	0.43422100	H	2.29439700	-5.69455800	-3.18865900
H	-1.99658000	5.75825600	0.95311900	H	-3.17330100	-6.13110500	1.30870000
H	-1.85925500	5.17496700	-3.27836300	H	-1.45301200	6.59723600	-1.30183600
H	-4.03678100	-4.48865300	2.93766600	C	-3.47006200	3.45506500	-4.59655500
H	-2.83452100	-5.46776800	-1.04842800	H	-3.72692900	2.76499800	-5.40722400
C	4.57588800	-3.35819800	0.15388400	H	-4.37093300	4.01880100	-4.33378400
C	2.61033600	-1.10053000	-4.01594400	H	-2.74061300	4.16619100	-4.99915700
H	3.22480900	-0.28545700	-3.61935500	C	-1.61241500	1.95789800	-3.78869700
H	4.87588100	-2.31903600	0.32520300	H	-0.83807200	2.68011700	-4.07051100
C	4.61870400	1.17837500	3.01483300	H	-1.21793000	1.35955600	-2.96120700
H	5.04395100	0.68045200	2.13727500	H	-1.77739100	1.28988700	-4.64146300

C	-4.57368300	3.67694900	2.04927600	H	2.50022600	5.42897500	-2.28351400
H	-4.77481800	4.75335300	2.00244900	H	1.71339200	5.91778000	-0.78606000
H	-5.27541600	3.16875500	1.38414300	C	5.85653000	-4.20547800	0.10301400
H	-4.78171500	3.34098300	3.07123200	H	6.41787200	-4.10540300	1.03850800
C	-2.17940300	3.93802800	2.75943700	H	5.62729900	-5.26833600	-0.03164700
H	-2.35885700	5.00375600	2.94185300	H	6.51489000	-3.90370400	-0.71768300
H	-2.36056600	3.41920500	3.70628500	C	3.69772900	-3.79190800	1.33593100
H	-1.12531300	3.80822400	2.49933100	H	3.37315200	-4.83293100	1.22902200
C	-1.78392500	-3.14032900	-2.60239000	H	4.25416700	-3.71525800	2.27652800
H	-1.38951800	-4.15646600	-2.49302800	H	2.79894200	-3.17581100	1.42631500
H	-1.63964400	-2.84017300	-3.64648900	C	2.99596800	-1.28798600	-5.48918700
H	-1.17977100	-2.48390000	-1.96900500	H	2.36606300	-2.03521600	-5.98384500
C	-4.10529700	-3.95510400	-3.17076400	H	2.87324300	-0.34686900	-6.03630700
H	-3.97697800	-3.62989700	-4.20924300	H	4.03684300	-1.60924900	-5.59837000
H	-3.80112800	-5.00607800	-3.11515800	C	1.14169400	-0.67123900	-3.89248400
H	-5.17263100	-3.90740500	-2.93241400	H	0.96116000	0.25997800	-4.44078800
C	-3.57054200	-1.38337600	3.44906100	H	0.47744300	-1.43885200	-4.30392300
H	-2.76794500	-0.93143700	2.85897700	H	0.85212100	-0.51988600	-2.84660900
H	-3.93979300	-0.63598200	4.16100500	C	0.05771500	0.93438700	2.15939800
H	-3.11694600	-2.20045300	4.01921600	H	-0.80987500	1.17471900	2.78946200
C	-5.84858600	-2.46884700	3.41000400	H	0.95846600	1.20523700	2.72382500
H	-5.50099600	-3.27781400	4.06135500	H	0.01923600	1.58117300	1.27804100
H	-6.26564000	-1.69000500	4.05761400				
H	-6.66096900	-2.86666800	2.79268400				
C	3.77244600	0.14246400	3.76779600				
H	3.30804000	0.58291500	4.65701700	Mg	2.44160400	-0.57869200	-0.07577400
H	2.96732300	-0.26080600	3.14683300	Mg	-2.41204900	-0.61794500	-0.33588800
H	4.39345600	-0.69713500	4.09921100	N	3.45578200	-2.30498200	0.44289500
C	5.78942300	1.65087700	3.88913800	N	4.02766600	0.21289600	-1.17036900
H	6.43327500	0.80429100	4.15109500	N	-3.26799400	-1.11211500	-2.14967900
H	6.40517100	2.39812300	3.37814500	N	-4.04374800	-1.23674800	0.77246100
H	5.43995100	2.09715100	4.82654300	C	5.23436200	-3.99072100	0.16333200
C	1.14769500	3.25118600	-1.21049100	C	4.60109600	-2.65432200	-0.15996300
H	1.08265500	2.18342000	-0.96532200	C	5.30983700	-1.84764200	-1.06392500
H	0.30959700	3.74457900	-0.70924800	C	5.11546900	-0.50288700	-1.44855000
H	1.00087100	3.35519000	-2.29054700	C	6.27267300	0.09644900	-2.22192700
C	2.55092500	5.34148100	-1.19294400	C	3.00013600	-3.12783100	1.52598100
H	3.47964100	5.81438800	-0.85757100	C	3.46445700	-2.86073400	2.83728400
				C	3.01847700	-3.66604300	3.88926500

Int-2_1a2b

Mg	2.44160400	-0.57869200	-0.07577400
Mg	-2.41204900	-0.61794500	-0.33588800
N	3.45578200	-2.30498200	0.44289500
N	4.02766600	0.21289600	-1.17036900
N	-3.26799400	-1.11211500	-2.14967900
N	-4.04374800	-1.23674800	0.77246100
C	5.23436200	-3.99072100	0.16333200
C	4.60109600	-2.65432200	-0.15996300
C	5.30983700	-1.84764200	-1.06392500
C	5.11546900	-0.50288700	-1.44855000
C	6.27267300	0.09644900	-2.22192700
C	3.00013600	-3.12783100	1.52598100
C	3.46445700	-2.86073400	2.83728400
C	3.01847700	-3.66604300	3.88926500

C	2.13713100	-4.71789300	3.67333200	H	-5.65284000	-3.10328200	-3.45676500
C	1.67177900	-4.96059400	2.38718400	H	-3.99709900	-2.97744100	-4.08310700
C	2.08097500	-4.17775100	1.30274300	H	-5.83012200	-3.11534500	-1.33726800
C	3.96352600	1.59899200	-1.53317200	H	-5.69095200	-3.09400600	2.00009400
C	4.15113700	2.57242800	-0.52100300	H	-6.76440200	-3.20926300	0.58859200
C	4.01197700	3.92323800	-0.85124700	H	-6.67581400	-1.71868100	1.54818800
C	3.69552400	4.32294000	-2.14383900	H	-3.25132200	2.13725300	-5.41222200
C	3.52137500	3.36204500	-3.13075900	H	-0.48228100	-1.09159900	-5.83471800
C	3.65045600	1.99659700	-2.85492800	H	-5.41858500	1.78752700	3.95964600
C	-4.79310900	-2.43985900	-3.55905100	H	-3.32119900	-1.68452900	5.31054200
C	-4.31184800	-1.95237600	-2.20957500	C	4.42110500	-1.71665100	3.14359100
C	-5.03339200	-2.42119800	-1.09847700	C	1.49856900	-4.46534600	-0.07171600
C	-4.97955600	-2.03213400	0.25796100	H	2.01415400	-3.81548300	-0.78735200
C	-6.09277500	-2.55043200	1.14070600	H	4.69726400	-1.25074900	2.19236200
C	-2.78067800	-0.55647200	-3.37874400	C	4.56656700	2.19042700	0.89242200
C	-3.32909800	0.66004400	-3.85389500	H	4.32286100	1.13043100	1.03617500
C	-2.83125800	1.20579600	-5.04088400	C	3.45031100	1.00642200	-3.99374500
C	-1.81671100	0.58265100	-5.75614100	H	3.62295100	-0.00037400	-3.59896100
C	-1.27846600	-0.60495300	-5.27738900	C	-2.84728900	-2.85785700	2.93951600
C	-1.74003000	-1.19136600	-4.09486900	H	-2.93169600	-3.09851000	1.87403200
C	-4.17700900	-0.80668300	2.13518000	C	-5.38082100	1.31299400	1.31280100
C	-4.82135500	0.42185600	2.41196200	H	-5.22466100	0.79898100	0.35834400
C	-4.92368100	0.84477300	3.74055700	C	-1.09328200	-2.48075900	-3.61241900
C	-4.40030200	0.09011000	4.78239800	H	-1.67532900	-2.84300700	-2.75808500
C	-3.74779600	-1.10253200	4.49750000	C	-4.44703600	1.39155000	-3.12350200
C	-3.61959500	-1.57077600	3.18608700	H	-4.68500800	0.81768600	-2.22212900
H	5.52903100	-4.03831600	1.21606500	C	-0.80793800	0.26548700	0.69551200
H	6.11746700	-4.16864300	-0.45198200	H	-1.25573500	0.37554600	1.69503800
H	4.52442800	-4.80752300	0.00599500	C	-0.02276900	1.52912800	0.34456300
H	6.22328200	-2.29021100	-1.44584900	C	0.72456100	0.27556500	0.80331400
H	6.26026700	-0.27047800	-3.25403400	H	1.01773000	0.39133800	1.85920400
H	7.22258000	-0.21538400	-1.78043200	C	3.83474700	2.98588500	1.97856300
H	6.23347200	1.18561900	-2.25004900	H	4.12749000	4.04122900	1.97934700
H	3.37323000	-3.46547400	4.89719900	H	2.74990300	2.93855100	1.85388700
H	0.97347600	-5.77668100	2.21807300	H	4.08385900	2.58590300	2.96693300
H	4.15378900	4.67531900	-0.08102300	C	6.08975100	2.31788000	1.05703200
H	3.27778200	3.67555300	-4.14279400	H	6.62816700	1.69707600	0.33463700
H	-5.07293000	-1.60097600	-4.20252800	H	6.40788700	3.35590000	0.90787900

H	6.39795300	2.01274700	2.06333200	H	-4.75797200	3.21913600	2.18354400
C	2.01603900	1.05426300	-4.53672100	H	-3.55241400	2.50462100	1.11551100
H	1.27811300	0.85043800	-3.75795000	H	-5.00043300	3.27058700	0.43407700
H	1.78441300	2.03841100	-4.95816600	C	-4.00799700	2.79530400	-2.68344700
H	1.88304800	0.31588700	-5.33513500	H	-3.13063900	2.75708100	-2.03110200
C	4.44569600	1.24345500	-5.14100000	H	-3.75300800	3.42363600	-3.54374700
H	4.25801500	2.20288500	-5.63533200	H	-4.81404100	3.29647000	-2.13712700
H	5.48196000	1.25231800	-4.79259800	C	-5.72716400	1.47318600	-3.96881300
H	4.34765500	0.45992600	-5.90074800	H	-5.56584600	2.05471800	-4.88326600
C	1.71566400	-5.91709200	-0.52078200	H	-6.08323100	0.48188600	-4.26508200
H	2.77402300	-6.19520500	-0.50441600	H	-6.52832800	1.96142900	-3.40325400
H	1.17914000	-6.62358600	0.12177100	C	0.33999400	-2.21688500	-3.12757300
H	1.34658200	-6.06026300	-1.54241300	H	0.95287300	-1.79371500	-3.92980900
C	0.00367200	-4.11203400	-0.10022200	H	0.34590400	-1.50735600	-2.29151200
H	-0.55381800	-4.71592000	0.62385000	H	0.81742200	-3.14378300	-2.79414700
H	-0.15594100	-3.05819700	0.15330000	C	-1.09768100	-3.58361800	-4.68064500
H	-0.42511100	-4.30342700	-1.08978300	H	-2.10430800	-3.77479500	-5.06501600
C	5.71746100	-2.20011900	3.80957000	H	-0.46369700	-3.32267300	-5.53484600
H	5.52468700	-2.64758200	4.79079600	H	-0.71272500	-4.52040700	-4.26316900
H	6.23258700	-2.94881900	3.19978600	H	3.58843800	5.37808300	-2.38005900
H	6.40450800	-1.36036600	3.96073200	H	1.80964300	-5.33930400	4.50232200
C	3.73883200	-0.64642800	4.00864100	H	-1.44664600	1.02020700	-6.67919400
H	2.83923000	-0.25269300	3.52567900	H	-4.49088400	0.43456800	5.80899000
H	3.43935000	-1.05348000	4.98074900	C	0.07491300	1.87130200	-1.12794900
H	4.41952300	0.19141600	4.19532700	H	-0.78284700	2.46267300	-1.47575600
C	-3.41136700	-4.04774700	3.72952800	H	0.98663400	2.43106000	-1.37062800
H	-3.30275900	-3.90135000	4.80968600	H	0.08517500	0.94370000	-1.70955200
H	-4.47433300	-4.21196500	3.52544200	C	-0.09937500	2.70085500	1.27057900
H	-2.87333500	-4.96587700	3.46932700	C	-0.22891500	2.51864800	2.68299900
C	-1.35894300	-2.65822600	3.26088200	C	-0.04719700	4.00786900	0.80977600
H	-0.92394600	-1.85535100	2.65856200	C	-0.30071000	3.57719100	3.55081700
H	-1.21932000	-2.39747000	4.31602400	H	-0.27523000	1.50992400	3.08342300
H	-0.78844800	-3.57190000	3.06821500	C	-0.11958000	5.12811000	1.67828200
C	-6.89081100	1.54567800	1.46478000	H	0.05938200	4.20715700	-0.25216400
H	-7.44700400	0.60295300	1.47803900	C	-0.25009700	4.91769700	3.08460400
H	-7.12302600	2.08029900	2.39233700	H	-0.40092700	3.39712200	4.61920500
H	-7.27124200	2.14915700	0.63324500	C	-0.06578700	6.46170400	1.19584000
C	-4.62778900	2.65063100	1.25650600	C	-0.32229400	6.03667100	3.94919600

C	-0.13801900	7.53171700	2.05933500	C	-1.21497500	4.18641800	3.23455300
H	0.03350400	6.62586000	0.12497900	C	-1.57654400	5.26852500	2.44192300
C	-0.26772700	7.31948900	3.45055000	C	-2.46518000	5.07520100	1.39069200
H	-0.42207200	5.86577600	5.01908600	C	-3.01401100	3.81689500	1.12249500
H	-0.09582700	8.54652800	1.67201200	C	-4.25596400	-1.90824600	-0.97321100
H	-0.32421600	8.17076000	4.12369500	C	-4.27182200	-3.30928300	-0.76397400
Int-2_1a2c							
Mg	2.54065800	0.35652000	-0.52812500	C	-4.24642200	-2.27043100	-3.36861200
Mg	-2.35256200	-0.04424900	0.54482100	C	-4.25309700	-1.38462900	-2.28720600
N	2.95966000	1.79703600	-1.96077900	H	3.85340700	3.10132000	-4.20301000
N	4.54590100	0.10705900	-0.01894000	H	5.46136000	3.42462200	-3.51717600
N	-3.24171700	1.43869700	1.69753100	H	4.02378600	4.25242800	-2.89459700
N	-4.18737100	-0.99687100	0.13265800	H	6.29061600	2.09399700	-2.07269500
C	4.40370900	3.30005100	-3.28040200	H	7.65577200	1.15472700	-0.67955500
C	4.19779800	2.19934800	-2.26147800	H	7.25742700	-0.54286100	-0.95463000
C	5.36854500	1.68252300	-1.67965500	H	7.14831800	0.11455600	0.67167100
C	5.54093600	0.71607100	-0.67296500	H	-0.12876300	2.11643800	-5.37172800
C	6.98211600	0.34922200	-0.38077500	H	-0.14980700	5.16360500	-2.37133100
C	1.87357900	2.43806500	-2.64048800	H	5.70004800	-4.12226700	1.41643700
C	1.34286000	1.87585600	-3.82212400	H	5.26600000	-1.06563100	4.37317900
C	0.28216100	2.53360800	-4.45578700	H	-4.22174300	2.14244800	4.20055500
C	-0.24966700	3.70916800	-3.94303600	H	-5.90538700	1.83400600	3.73365700
C	0.27144500	4.24531400	-2.76882400	H	-4.99290600	3.17624200	3.01652200
C	1.33031300	3.62794700	-2.10014600	H	-6.26607300	0.19252200	2.45196100
C	4.89522800	-0.84211200	0.99547000	H	-6.57443300	-2.02059900	-0.35474700
C	5.18690600	-2.18157700	0.64715800	H	-7.34446100	-0.55120300	0.27410200
C	5.48577900	-3.08756200	1.67004400	H	-7.00804200	-1.89136300	1.36279900
C	5.52079500	-2.69025100	3.00040700	H	-0.51485100	4.33465100	4.05279700
C	5.23632600	-1.36943400	3.33101600	H	-2.74883000	5.92067800	0.76840900
C	4.90786900	-0.42827800	2.35019400	H	-4.26745000	-5.22616900	-1.72985700
C	-4.92638800	2.14164100	3.36341700	H	-4.25007600	-1.87221900	-4.38023400
C	-4.44164600	1.21529200	2.26699900	C	1.89188700	0.59339000	-4.43088700
C	-5.32672900	0.19207700	1.90961700	C	1.87252700	4.20079600	-0.79905800
C	-5.28208400	-0.72125600	0.83016600	H	2.92693800	3.91248000	-0.72712800
C	-6.62271800	-1.34359400	0.49690100	H	2.66488300	0.21397800	-3.75397400
C	-2.65354400	2.72325900	1.94860300	C	5.16962100	-2.66525600	-0.79627700
C	-1.73968900	2.90941300	3.00996200	H	5.11730200	-1.78202100	-1.44142300

C	4.59940100	1.01140800	2.74343600	H	-1.06746900	4.20904600	-4.45499300
H	3.92283900	1.41579500	1.97932300	H	-4.23792400	-4.32044600	-4.02668800
C	-4.31019600	0.11051300	-2.56349100	H	-1.16661500	6.25532200	2.63976900
H	-4.24115200	0.62926600	-1.60052300	C	-5.28585500	4.47315900	0.20475200
C	-4.31734000	-3.94591700	0.61946000	H	-5.98434200	4.32804400	-0.62686200
H	-4.30243700	-3.13991500	1.36114800	H	-5.79314500	4.16473400	1.12348200
C	-3.99592400	3.67323200	-0.03248200	H	-5.08079200	5.54688300	0.28186900
H	-4.27253600	2.61649100	-0.09801800	C	-3.35939300	4.07515700	-1.36948400
C	-1.29841800	1.75919500	3.89798200	H	-3.09298200	5.13813500	-1.38219800
H	-1.93223900	0.89729600	3.66413500	H	-2.44938800	3.50395500	-1.57346700
C	-0.68990600	-0.92146900	-0.44187500	H	-4.06150900	3.90545000	-2.19346800
H	-1.16307900	-1.31249300	-1.35425800	C	-1.45740800	2.05984600	5.39470400
C	0.16568700	-2.01577300	0.20428000	H	-0.78484400	2.86043600	5.72189100
C	0.24022100	-2.02691500	1.71046900	H	-2.47828400	2.36451700	5.64673900
C	-0.93035400	-2.16061900	2.47203800	H	-1.21455700	1.16963000	5.98444900
C	1.46022300	-2.02011700	2.39599100	C	0.15032300	1.36899700	3.58317800
C	-0.89250100	-2.28203700	3.86118600	H	0.82968800	2.20383200	3.78834200
C	1.50973600	-2.15237000	3.78459400	H	0.46047200	0.51426600	4.19019300
C	0.33423300	-2.28160700	4.52452000	H	0.26947200	1.08786600	2.53227600
H	-1.88941900	-2.23895300	1.95901000	C	-3.14354300	0.58758300	-3.43710500
H	2.38482500	-1.94161900	1.83083000	H	-3.16745200	0.12130400	-4.42812600
H	-1.81748200	-2.39646300	4.42093200	H	-3.18902300	1.67164100	-3.58247200
H	2.47491500	-2.16496800	4.28326600	H	-2.17784300	0.35023300	-2.98146300
H	0.37393600	-2.38890600	5.60533500	C	-5.65883500	0.50335000	-3.18582800
C	0.20585600	-3.40131300	-0.39646200	H	-5.71653200	1.58761600	-3.33351100
C	0.83551500	-0.89334200	-0.59110800	H	-5.79691700	0.02612800	-4.16244600
C	0.56516600	-4.52901400	0.36272200	H	-6.49586500	0.20139200	-2.54868800
C	-0.08824300	-3.62239100	-1.75478500	C	-3.10007000	-4.84411500	0.87629800
C	0.62961700	-5.80305200	-0.20306600	H	-2.15847500	-4.31554700	0.71943900
H	1.09673900	-1.33329000	-1.57182900	H	-3.11591200	-5.22239100	1.90470200
C	-0.02411700	-4.89061500	-2.32095900	H	-3.09849200	-5.71090600	0.20687200
C	0.33627600	-5.99645100	-1.54931000	C	-5.60635000	-4.75733400	0.83282500
H	0.80009700	-4.41260200	1.41547100	H	-5.64525600	-5.61593900	0.15338100
H	-0.38137400	-2.78674400	-2.38336500	H	-5.64445500	-5.14762800	1.85600500
H	0.91176600	-6.64770400	0.42123000	H	-6.50752900	-4.16238800	0.66369100
H	-0.26477000	-5.01589500	-3.37393300	C	3.92451000	-3.51647500	-1.07894000
H	0.38432400	-6.98805300	-1.99130000	H	3.91503900	-4.42066300	-0.46135800
H	5.76653500	-3.40722200	3.77911800	H	3.00011900	-2.97258900	-0.86689700

H	3.89878000	-3.82960600	-2.12844800	C	2.14717400	-3.69382400	-2.95496900
C	6.44253800	-3.43646000	-1.17397300	C	3.52483500	-3.44440300	-2.81611700
H	6.44276100	-3.66168300	-2.24583200	C	4.20229800	-2.53977400	-1.97304400
H	7.35043400	-2.86895200	-0.94544900	C	5.71426800	-2.59926900	-2.00214700
H	6.50915800	-4.39244600	-0.64348300	C	-0.16737700	-3.43989900	-2.46548900
C	3.89271000	1.13047600	4.09770800	C	-0.67439700	-4.46331500	-1.63949300
H	3.02292800	0.47145300	4.15988600	C	-2.01399000	-4.83684000	-1.77014400
H	4.56370400	0.89154200	4.93046200	C	-2.86885200	-4.22163500	-2.68768900
H	3.55235200	2.15981700	4.25076800	C	-2.34776900	-3.19463900	-3.47671800
C	5.85851600	1.89325400	2.73665800	C	-1.01387900	-2.78805800	-3.38231400
H	6.31176100	1.95438400	1.74486600	C	4.39675400	-0.83124400	-0.32687900
H	5.61176300	2.91315800	3.05261000	C	4.75110000	-1.28938800	0.95665200
H	6.60964000	1.49916800	3.43073300	C	5.49363600	-0.45066900	1.79078300
C	2.55217400	0.83769200	-5.79640300	C	5.88128600	0.83158600	1.39641600
H	2.95798800	-0.09762000	-6.19757300	C	5.50132900	1.26739200	0.12568200
H	1.82854700	1.22390100	-6.52297800	C	4.76020600	0.46327500	-0.74396900
H	3.37398100	1.55708700	-5.73230100	C	-3.80536400	-1.45586200	4.71363500
C	0.80529700	-0.48376500	-4.55284300	C	-3.65803000	-0.67475000	3.42488200
H	0.03209100	-0.19263100	-5.27239600	C	-4.80226200	0.01273700	2.98382800
H	1.23890500	-1.42821000	-4.89952500	C	-5.00340900	0.79632800	1.82846700
H	0.31734700	-0.66317700	-3.59111500	C	-6.37420000	1.41663700	1.66637800
C	1.81487700	5.72985900	-0.72081700	C	-1.40229200	-1.42573200	3.35997400
H	0.78627000	6.09862800	-0.64767300	C	-1.19166700	-2.76161000	2.96930200
H	2.34347000	6.07888600	0.17248500	C	-0.10389100	-3.45858000	3.50320800
H	2.28052300	6.19798500	-1.59425600	C	0.78163200	-2.86914000	4.40766100
C	1.14552900	3.57927600	0.40174500	C	0.55929600	-1.53753900	4.76585100
H	1.59258900	3.90457800	1.34691600	C	-0.51503900	-0.80260000	4.25989300
H	0.08977200	3.86577900	0.41407500	C	-4.39708800	1.81155300	-0.23804300
H	1.17206900	2.48250000	0.37468200	C	-4.93123500	1.20291500	-1.38931800
				C	-5.19949700	1.99549500	-2.50798600
				C	-4.93901700	3.36676700	-2.52456500
				C	-4.39047900	3.94120900	-1.37624800
				C	-4.10646200	3.18926700	-0.23423600

Int-2_1b2b

Mg	1.57842300	-1.29602600	-1.26271100	H	1.24670400	-5.61702800	-3.38247700
Mg	-2.13701500	0.33894900	1.03939900	H	2.63683900	-5.21932400	-4.40852700
N	1.18710800	-3.01664500	-2.31710000	H	1.06191800	-4.43819100	-4.66602000
N	3.59870600	-1.65479700	-1.17900900	H	4.16688600	-4.07249100	-3.42212800
N	-2.47962700	-0.68224500	2.79053400	H	6.13525500	-1.62103000	-2.25545500
N	-4.07203700	1.01577100	0.90279000				
C	1.76054700	-4.80552600	-3.90733900				

H	6.06868700	-3.33318700	-2.72747100	C	-5.19085400	-0.27992400	-1.42870100
H	6.11492800	-2.86116900	-1.01775200	H	-5.80828700	-0.61878000	-0.59037500
H	-2.39949900	-5.63243400	-1.13466600	H	-5.69758800	-0.55968900	-2.35641100
H	-2.99587900	-2.69266500	-4.19292700	H	-4.25490400	-0.84992600	-1.37906300
H	5.77317400	-0.81099100	2.77947300	C	-5.20773700	4.19536000	-3.75361600
H	5.78300500	2.26626100	-0.20168300	H	-5.99568900	3.75337200	-4.37087800
H	-4.80953900	-1.35116100	5.12690800	H	-5.51459900	5.21285100	-3.49210300
H	-3.08222100	-1.11983400	5.46327200	H	-4.31086700	4.27884200	-4.38002600
H	-3.60582400	-2.51977000	4.54892500	C	0.20626400	-5.13467600	-0.61873100
H	-5.66646900	-0.07618000	3.63126300	H	1.09055600	-5.59685500	-1.07003900
H	-6.29775800	2.50714300	1.60498100	H	0.57927700	-4.41748200	0.12172600
H	-7.02876500	1.15870300	2.50025900	H	-0.34341400	-5.91466500	-0.08482300
H	-6.84660800	1.08858800	0.73519800	C	-0.49739300	-1.66565000	-4.24228400
H	0.04884700	-4.49529300	3.20774600	H	-0.26587100	-0.77985000	-3.63777300
H	1.24195900	-1.05261200	5.46138700	H	0.42040800	-1.94283400	-4.77134500
H	-5.62142000	1.52333000	-3.39369700	H	-1.24256300	-1.36977600	-4.98563800
H	-4.17034700	5.00721900	-1.36669900	C	-4.29816800	-4.67264300	-2.83977500
C	0.52155300	0.50682800	-1.07807800	H	-4.71088900	-5.02676900	-1.89005100
C	-0.68220900	1.04536900	-0.29709500	H	-4.93754100	-3.86332500	-3.20453100
C	0.72665100	1.54620800	0.02605500	H	-4.37935000	-5.49939600	-3.55665700
H	-1.22407600	1.79873700	-0.88693200	C	4.32312700	-2.65184100	1.43437500
H	0.59153000	0.99587400	-2.06306100	H	4.64269600	-3.45156300	0.75786900
C	-2.12417300	-3.43241200	1.99571500	H	4.73548500	-2.86275000	2.42472000
H	-3.17171000	-3.33964500	2.29986200	H	3.23125600	-2.72406300	1.50687600
H	-2.05286500	-2.99657000	0.99164900	C	4.34225700	0.98505000	-2.09261100
H	-1.89058700	-4.49627400	1.90490000	H	3.26063700	1.16724800	-2.12235000
C	-0.72003000	0.63067000	4.67174300	H	4.83505000	1.93558700	-2.31189900
H	-0.69463200	1.30437800	3.80782100	H	4.57695000	0.28261000	-2.89915000
H	-1.68978300	0.78495500	5.15762400	C	6.65570700	1.72925200	2.32590800
H	0.06016600	0.95181500	5.36676000	H	7.28889200	1.15167200	3.00647200
C	1.92106700	-3.65237600	5.00564400	H	7.29753300	2.42100500	1.77208500
H	2.22206300	-4.48135200	4.35835500	H	5.98270800	2.33631300	2.94421300
H	2.79774000	-3.01941300	5.17410400	C	1.35027300	1.04927100	1.31548500
H	1.64075400	-4.08174100	5.97569500	H	2.44589500	1.01023400	1.26312800
C	-3.47714100	3.83990400	0.96881600	H	1.08180200	1.67858100	2.17507300
H	-2.44104100	3.50224300	1.10054600	H	0.98927300	0.03675400	1.52941500
H	-3.45015500	4.92670600	0.85477200	C	1.96641600	3.71335200	0.38657200
H	-4.01162100	3.60603500	1.89523100	C	1.09780400	2.93954400	-0.36805400

C	2.32820800	5.03583200	0.01969400	C	-5.94773100	-2.19405400	0.03059500
C	0.56863800	3.53562500	-1.55533600	C	-5.20348500	-1.34975800	-0.79753200
C	1.78548200	5.60655100	-1.17152800	C	5.82805200	1.03320200	2.58647600
C	0.89650100	4.80931600	-1.94052000	C	4.94932600	0.22695300	1.65214400
H	-0.11825900	2.96260000	-2.17174800	C	5.58727200	-0.82617700	0.97344400
H	0.47221700	5.22760500	-2.85114600	C	5.07327600	-1.76396300	0.05569900
C	2.14840700	6.92553500	-1.53623500	C	6.06325600	-2.75818800	-0.51247800
C	3.21835300	5.81922700	0.79954700	C	3.19003300	1.68498400	2.26907600
C	3.01534800	7.66095900	-0.75831300	C	3.28846200	2.97062600	1.70537600
C	3.55446300	7.09986600	0.42134000	C	2.83058000	4.06749000	2.44134700
H	3.63338200	5.38863500	1.70840800	C	2.27583600	3.92621200	3.71387800
H	4.23753900	7.68522200	1.03162900	C	2.16842600	2.63689900	4.23961100
H	3.28669400	8.67252000	-1.04829600	C	2.60856700	1.51257700	3.53992700
H	1.72935800	7.35103700	-2.44578900	C	3.39748000	-2.83343900	-1.24520300
H	2.40474300	3.31137600	1.29495900	C	3.39574100	-2.55738700	-2.62487000
Int-2_1b2c							
Mg	-2.05412900	0.65483900	-1.04314000	C	2.51079300	-4.79026900	-3.07010500
Mg	2.32934800	-0.57612600	0.42423900	C	2.51902100	-5.03709000	-1.69595700
N	-1.73527600	2.12887500	-2.45513300	C	2.94932200	-4.08210000	-0.77209700
N	-4.11014700	0.81399400	-1.16569800	H	-1.77856200	4.48951800	-3.94679100
N	3.65366800	0.54781000	1.53527100	H	-3.28486000	4.03009400	-4.76334200
N	3.79680900	-1.82134800	-0.31908900	H	-1.78532600	3.12431100	-5.04490200
C	-2.38236000	3.64364000	-4.28762100	H	-4.75734300	3.04845900	-3.56973000
C	-2.72342000	2.70393200	-3.14928900	H	-6.63280200	0.62054500	-2.33036200
C	-4.09358900	2.48216700	-2.92743100	H	-6.62825900	2.33216800	-2.80114300
C	-4.74019700	1.61764200	-2.02176300	H	-6.67694900	1.85776700	-1.09083200
C	-6.25363700	1.61406400	-2.07015000	H	1.99212400	4.80912600	-2.18541500
C	-0.39257500	2.46603200	-2.79961400	H	2.20278100	1.33113600	-4.67729300
C	0.21501900	3.61084900	-2.24757100	H	-6.37997200	-0.17365600	2.70664000
C	1.53083000	3.91744900	-2.60624400	H	-6.19286300	-3.19304700	-0.32639800
C	2.26386800	3.12179600	-3.48890100	H	6.84602400	0.64141700	2.60490600
C	1.64967200	1.97314000	-3.99424900	H	5.42780000	1.01632600	3.60526700
C	0.33864000	1.62413900	-3.66104200	H	5.86477800	2.08562500	2.28887400
C	-4.89533200	-0.05243400	-0.34494000	H	6.64420100	-0.93096400	1.18716700
C	-5.31441200	0.37294600	0.92949000	H	5.76883500	-3.78420600	-0.26974700
C	-6.05335800	-0.50737600	1.72325600	H	7.06828800	-2.58277800	-0.12581300
C	-6.38086300	-1.79549800	1.29667500	H	6.09256100	-2.69739700	-1.60500100
				H	2.91774600	5.06178000	2.00614700

H	1.72155400	2.49753800	5.22205300	C	1.82185400	5.12409700	4.50654800
H	2.96437700	-3.32827800	-4.57875300	H	1.71035600	6.00705800	3.87045600
H	2.17684600	-6.00222700	-1.32652000	H	0.86084100	4.93819700	4.99714600
C	-1.02287200	-1.06080300	-0.37705400	H	2.54201600	5.37683200	5.29460500
C	0.36368200	-1.29918100	0.22270000	C	2.91828900	-4.38612500	0.70223600
C	-1.08878500	0.01354900	1.94543300	H	2.14705000	-3.79596900	1.21218300
C	-0.86014800	-1.22980500	1.14486100	H	2.68678200	-5.44032100	0.87592400
H	-2.19332300	-0.92187000	3.53902000	H	3.87029400	-4.16069400	1.19358300
C	-1.81616100	0.01695300	3.14657700	C	3.85500300	-1.22000700	-3.14126000
C	-2.06906200	1.20069900	3.83889000	H	4.85469200	-0.95712400	-2.77942700
C	-1.60671000	2.42337200	3.35413800	H	3.87956700	-1.21500000	-4.23466300
C	-0.87618000	2.44471200	2.16673900	H	3.18424800	-0.41324100	-2.82173000
C	-0.62596400	1.26033700	1.47189600	C	2.00873800	-5.82641900	-4.04138700
H	0.00520800	1.28171100	0.58222800	H	2.45141600	-5.69439500	-5.03333300
H	-0.47193800	3.38087900	1.79272000	H	2.23953300	-6.84071700	-3.70099900
H	-1.80417800	3.34398900	3.89604900	H	0.91970400	-5.76448800	-4.15914900
H	-2.63819800	1.16376500	4.76480900	C	-0.53998600	4.50108300	-1.29676300
C	-2.43043600	-3.20660500	1.42271900	H	-1.31803300	5.08259800	-1.80590500
C	-1.27543200	-2.51618900	1.80689100	H	-1.05058600	3.91913600	-0.52357700
C	-0.50109600	-3.06225300	2.84305000	H	0.13425400	5.20988900	-0.80839600
C	-0.85657700	-4.25834900	3.46156800	C	-0.28222900	0.36987100	-4.21601600
C	-2.00428900	-4.94079200	3.05548600	H	-0.47263800	-0.36170000	-3.42033800
C	-2.78914800	-4.40837000	2.03509600	H	-1.24158500	0.56968800	-4.70476100
H	-3.05732000	-2.79163300	0.63924300	H	0.38030500	-0.10343600	-4.94558600
H	-3.68862400	-4.92751400	1.71302700	C	3.65962000	3.50441500	-3.90747800
H	-2.28228500	-5.87763400	3.53143700	H	4.16220100	4.09628200	-3.13672700
H	-0.23523600	-4.66200700	4.25747800	H	4.27480000	2.62249800	-4.11034900
H	0.39682600	-2.53765700	3.16217700	H	3.64642600	4.10805400	-4.82372300
H	0.61099300	-2.36530700	0.09106700	C	-4.97223600	1.74991100	1.43097500
H	-1.40467800	-1.99046000	-0.82020200	H	-5.28492900	2.53306800	0.73203000
C	3.87652600	3.16924700	0.33370200	H	-5.45401000	1.94256700	2.39323600
H	4.87177300	2.72240200	0.24003200	H	-3.89232000	1.86580700	1.57644800
H	3.25334300	2.71201500	-0.44374100	C	-4.73631500	-1.82509700	-2.14815600
H	3.96212900	4.23439100	0.10125200	H	-3.64120400	-1.85436000	-2.20236100
C	2.45082100	0.13838000	4.13286000	H	-5.10534400	-2.83336700	-2.35483900
H	1.69764600	-0.43932500	3.58290100	H	-5.07281300	-1.16888100	-2.95814600
H	3.38288200	-0.43527700	4.10389800	C	-7.14565200	-2.73759700	2.18890600
H	2.11651300	0.19805500	5.17187000	H	-7.83872000	-2.19828100	2.84200500

H -7.72432900 -3.46139100 1.60674400
H -6.46576800 -3.30654000 2.83505900

TS-2

Mg 0.60347000 -1.28876500 -0.23943000
Mg -0.84559200 1.38208000 -0.51508800
N 0.17715700 -2.80823200 -1.65051500
N 2.64967000 -1.76351500 -0.24797500
N -0.24035300 2.99588100 -1.72173200
N -2.76599300 2.22484900 -0.30763100
C 0.74812600 -4.13326900 -3.65029400
C 1.11090900 -3.19754300 -2.51468100
C 2.47160100 -2.84020800 -2.43039500
C 3.19071400 -2.29293100 -1.35017300
C 4.70009100 -2.38024300 -1.47100700
C -1.12478700 -3.37915700 -1.75895100
C -1.43441800 -4.57137400 -1.07346600
C -2.73413400 -5.08007400 -1.14601300
C -3.73591700 -4.45622000 -1.89002500
C -3.40032600 -3.29021700 -2.58131800
C -2.11817900 -2.73820400 -2.52795900
C 3.54710200 -1.49076200 0.83046200
C 3.86424100 -2.51650700 1.74431300
C 4.76633500 -2.25113100 2.77694100
C 5.36977400 -1.00013500 2.92985800
C 5.01790200 0.00506600 2.02840200
C 4.11127100 -0.21250600 0.98648800
C -0.57293300 4.86182200 -3.29904600
C -1.09333500 3.82445800 -2.32468200
C -2.48488300 3.83378600 -2.10655800
C -3.24560900 3.15455700 -1.14008100
C -4.70595400 3.55235000 -1.05449100
C 1.15168100 3.18577000 -1.98064300
C 1.90082700 4.05230800 -1.16117600
C 3.25536000 4.24712700 -1.44218700
C 3.89420600 3.59647000 -2.49953700
C 3.13567400 2.72195400 -3.27995900
C 1.77757400 2.49901300 -3.03878100

C -3.63368300 1.76458600 0.72794500
C -3.71624600 2.48037800 1.93943800
C -4.54504800 1.99845800 2.95672400
C -5.29812200 0.83146500 2.81025300
C -5.19727300 0.13959700 1.60173800
C -4.38304800 0.58495300 0.55724400
H 0.59014400 -5.14815300 -3.26845000
H 1.54738100 -4.17555300 -4.39247700
H -0.18085000 -3.83703300 -4.14385600
H 3.08396500 -3.18489700 -3.25530800
H 5.17678700 -1.42461800 -1.23633400
H 4.99307500 -2.68508400 -2.47704800
H 5.10392800 -3.11113900 -0.76223200
H -2.96435800 -5.99942300 -0.60940900
H -4.15697900 -2.79372200 -3.18670500
H 5.00957200 -3.04950500 3.47640000
H 5.45973400 0.99439800 2.13455400
H 0.06732700 5.58623100 -2.78451400
H -1.39326500 5.40383700 -3.77239500
H 0.04435000 4.40455900 -4.07778900
H -3.03919800 4.53971800 -2.71354000
H -5.35828800 2.67457500 -1.08156900
H -4.97917300 4.21831600 -1.87463300
H -4.91895300 4.06649800 -0.11156300
H 3.82583500 4.93059500 -0.81522500
H 3.61085200 2.19887800 -4.10822500
H -4.60327500 2.55517100 3.89060500
H -5.77349400 -0.77339300 1.46121500
C -1.27279000 -1.35130300 1.26014400
H -2.19920200 -1.34564000 0.70189700
C -0.91788000 -1.16753800 2.71484200
C -0.00465000 -0.06801900 3.18947600
C -0.50844700 1.22562400 3.39042900
C 1.32679800 -0.32327100 3.51924000
C 0.30316600 2.23790300 3.89671400
C 2.14199700 0.68776000 4.03246100
C 1.63452600 1.97045000 4.22107700
H -1.55071500 1.42943700 3.15888600

H	1.72683100	-1.32300100	3.37385600	C	3.23955700	-3.87941600	1.61507400
H	-0.10477100	3.23444400	4.04745700	H	2.14792500	-3.81250800	1.67606000
H	3.17455600	0.46461700	4.28057900	H	3.47060700	-4.35087800	0.65344400
H	2.26825500	2.75684200	4.62278700	H	3.58671000	-4.54521200	2.41012300
C	-0.44049300	-2.27115600	1.82118700	C	6.38273900	-0.75567900	4.01846200
H	-0.35098900	-3.34911600	1.84554400	H	6.11778200	-1.28266500	4.94078300
C	-2.01642700	-1.49380300	3.72342800	H	7.37872300	-1.10755900	3.72126300
H	-1.57693000	-1.83031300	4.66966700	H	6.47170700	0.30946600	4.25234500
H	-2.63857200	-0.61895300	3.94046500	C	-0.37849900	-5.32915800	-0.31302600
H	-2.66651400	-2.28912800	3.34581700	H	0.12986600	-6.05598200	-0.95997500
C	-2.93172200	3.75043400	2.13704700	H	0.39470600	-4.66272300	0.07478100
H	-1.86673500	3.59996400	1.93191800	H	-0.81633600	-5.89136500	0.51740500
H	-3.26403300	4.54781900	1.46242700	C	-1.79315700	-1.49898300	-3.31614500
H	-3.03619300	4.11709700	3.16195700	H	-1.32057500	-0.73988400	-2.67922900
C	-4.33269300	-0.16970900	-0.74253400	H	-1.08239800	-1.70318400	-4.12565200
H	-4.75328800	0.41726000	-1.56784600	H	-2.69320900	-1.06679600	-3.76185300
H	-3.30526300	-0.41187700	-1.03619500	C	-5.13598000	-5.01113900	-1.93024300
H	-4.89079800	-1.10679600	-0.67759400	H	-5.65455000	-4.72366500	-2.84994100
C	-6.21254600	0.35179700	3.90721900	H	-5.13599800	-6.10403800	-1.87098000
H	-5.86401400	0.67861600	4.89145400	H	-5.73658600	-4.64232600	-1.08914900
H	-7.22951600	0.74244300	3.77593100				
H	-6.28447500	-0.74001500	3.92065300				
C	0.99821100	1.54620700	-3.90344600				
H	1.62865200	1.13094600	-4.69432800	Mg	1.49373900	-0.07491200	0.26362500
H	0.60934700	0.70975100	-3.30985400	Mg	-1.63058400	0.14397800	0.33381900
H	0.13262000	2.02579600	-4.37362500	N	2.59125100	0.96718000	1.77364600
C	5.36195100	3.80423500	-2.76762200	N	2.80717400	-1.72780000	0.28931300
H	5.59754500	3.67717100	-3.82872800	N	-3.01799500	-0.86145100	1.58623300
H	5.68650000	4.80540300	-2.46763300	N	-3.08693700	1.61694500	-0.22141800
H	5.97419100	3.08384200	-2.21068800	C	3.77959000	0.85390700	3.95605500
C	1.25631000	4.76029300	0.00077800	C	3.28200400	0.24502100	2.65672600
H	0.37653000	5.33775600	-0.30206300	C	3.60726800	-1.11793600	2.51057300
H	0.91600800	4.04612900	0.76057200	C	3.49130900	-1.98566500	1.41006200
H	1.96274100	5.44307200	0.48082100	C	4.22443200	-3.30435500	1.55663300
C	3.76133400	0.89864100	0.03926000	C	2.51875100	2.38529700	1.96788200
H	4.05751200	0.67487600	-0.99121200	C	3.51509000	3.21633800	1.39257900
H	2.67977900	1.07771400	0.01016600	C	3.43075300	4.59960700	1.57714300
H	4.24476700	1.83341500	0.33196600	C	2.40031900	5.17384900	2.31143800
				C	1.43314900	4.35405400	2.87642700

TS-2_1a2a

Mg	1.49373900	-0.07491200	0.26362500
Mg	-1.63058400	0.14397800	0.33381900
N	2.59125100	0.96718000	1.77364600
N	2.80717400	-1.72780000	0.28931300
N	-3.01799500	-0.86145100	1.58623300
N	-3.08693700	1.61694500	-0.22141800
C	3.77959000	0.85390700	3.95605500
C	3.28200400	0.24502100	2.65672600
C	3.60726800	-1.11793600	2.51057300
C	3.49130900	-1.98566500	1.41006200
C	4.22443200	-3.30435500	1.55663300
C	2.51875100	2.38529700	1.96788200
C	3.51509000	3.21633800	1.39257900
C	3.43075300	4.59960700	1.57714300
C	2.40031900	5.17384900	2.31143800
C	1.43314900	4.35405400	2.87642700

C	1.46897200	2.96401400	2.72036600	H	-5.38045000	1.42947200	2.20201800
C	2.99171600	-2.64802200	-0.79752800	H	-5.11404200	3.70991600	0.87003700
C	4.00216100	-2.38735300	-1.75565900	H	-6.21306200	2.46593700	0.28531400
C	4.20488200	-3.30615100	-2.78945000	H	-5.08572000	3.25152600	-0.83929400
C	3.43099900	-4.45445100	-2.90124000	H	-4.03631100	-5.32170500	1.04455300
C	2.42500600	-4.68891400	-1.97258800	H	-1.23832900	-4.30103300	4.11046000
C	2.18623600	-3.80505300	-0.91401600	H	-3.24391800	1.87497600	-4.80379300
C	-4.90994600	-0.83881000	3.18332800	H	-2.03226100	5.39003300	-2.69928100
C	-4.06150600	-0.20040400	2.10164500	C	4.70898500	2.64312800	0.64049800
C	-4.51109900	1.05741100	1.66990400	C	0.39953400	2.13032300	3.40954600
C	-4.17741100	1.80488000	0.52093400	H	0.58128200	1.08164100	3.15026100
C	-5.20309200	2.86865400	0.17416700	H	4.44629900	1.62163300	0.34440400
C	-2.88068800	-2.24194200	1.94713100	C	4.88766400	-1.15192300	-1.68180800
C	-3.62064800	-3.22235800	1.23872300	H	4.45695200	-0.49274100	-0.92157900
C	-3.47037800	-4.56819900	1.58671600	C	1.05777300	-4.11255000	0.05704800
C	-2.61698700	-4.96263600	2.60997000	H	1.12101600	-3.39406500	0.88058000
C	-1.89724800	-3.99653200	3.30108700	C	-2.28303600	4.52885000	-0.18722900
C	-2.01279800	-2.63621700	2.99348600	H	-2.51900500	3.89610600	0.67394300
C	-2.94049500	2.35680800	-1.44220700	C	-3.78432900	0.28075000	-2.68911200
C	-3.21082300	1.69034300	-2.66400500	H	-3.48815200	-0.21504300	-1.75614300
C	-3.03392400	2.38005000	-3.86615200	C	-1.23312000	-1.63512600	3.83262300
C	-2.60504700	3.70184800	-3.88532400	H	-1.41941700	-0.64079100	3.41249000
C	-2.35400200	4.35174400	-2.68476200	C	-4.57171400	-2.86873600	0.10304300
C	-2.51751800	3.70993500	-1.45172700	H	-4.61898400	-1.77784800	0.03298000
H	3.79734200	1.94318600	3.93672100	C	0.76336800	1.60109300	-1.30114200
H	4.77939900	0.48505700	4.19760000	H	0.19163800	2.35369400	-0.77758000
H	3.11766100	0.54176300	4.77217300	C	1.11849200	1.48543900	-2.77129600
H	4.14320100	-1.53542600	3.35549900	C	0.74077200	0.31331700	-3.64099700
H	3.51490800	-4.13658900	1.58604100	C	0.30267400	0.50248200	-4.95995700
H	4.81799600	-3.32389500	2.47164400	C	0.86219600	-1.00519800	-3.18850100
H	4.88438900	-3.49105000	0.70588500	C	0.00556400	-0.57994200	-5.78930700
H	4.19530200	5.23954200	1.14556900	C	0.56068300	-2.08979900	-4.00635300
H	0.63391600	4.79908900	3.46416500	C	0.13150900	-1.88284100	-5.31764500
H	4.98670000	-3.11686400	-3.52029500	H	0.19296800	1.50518500	-5.35745600
H	1.81253900	-5.58268500	-2.06265000	H	1.23505400	-1.19453600	-2.18651200
H	-5.64371800	-1.51978200	2.73963100	H	-0.32440600	-0.39677600	-6.80887500
H	-5.45877600	-0.07697900	3.74091100	H	0.68605800	-3.09614600	-3.61987100
H	-4.31196600	-1.43067900	3.87750900	H	-0.09441100	-2.72794800	-5.96223200

C	2.06574900	1.34936300	-1.61474400	C	-3.20037300	5.76346400	-0.13435500
H	3.03445400	1.75695900	-1.35687500	H	-2.92640800	6.49253400	-0.90469800
C	1.16095000	2.82830900	-3.49375600	H	-4.25163900	5.50666100	-0.28598500
H	1.86307500	2.79898100	-4.33542800	H	-3.10763700	6.26479600	0.83553600
H	0.17803600	3.11943900	-3.87807500	C	-0.82525400	4.98782000	-0.04608100
H	1.49253000	3.61170100	-2.80723300	H	-0.12750900	4.15159800	0.03980400
C	4.91240800	-0.38196700	-3.00886400	H	-0.51561600	5.59283500	-0.90519000
H	5.40297000	-0.95546900	-3.80314100	H	-0.70201600	5.60068100	0.85262100
H	3.90093900	-0.13780800	-3.34324000	C	-5.32091200	0.33274800	-2.69704100
H	5.47200800	0.55325300	-2.89378300	H	-5.71362600	0.86595200	-1.82688700
C	6.31639400	-1.50339000	-1.23925900	H	-5.68273200	0.84523400	-3.59578400
H	6.33315900	-1.97456000	-0.25215900	H	-5.74290500	-0.67846000	-2.69327200
H	6.78985800	-2.19296300	-1.94759200	C	-3.27165900	-0.57385300	-3.85085800
H	6.93642900	-0.60112000	-1.18841400	H	-3.64375100	-0.21573000	-4.81712300
C	-0.30615700	-3.91860900	-0.61768500	H	-2.18025200	-0.58844400	-3.89480200
H	-0.41100400	-2.90113500	-1.00867200	H	-3.62336500	-1.60407500	-3.73886600
H	-0.43181700	-4.61424400	-1.45584900	C	-4.05138800	-3.40100100	-1.23981300
H	-1.11647000	-4.09624700	0.09512400	H	-3.06370400	-2.99614500	-1.47789000
C	1.14730800	-5.52322600	0.65678400	H	-3.96588800	-4.49326100	-1.22643400
H	0.99484700	-6.29588800	-0.10493000	H	-4.73567300	-3.13259800	-2.05222900
H	2.11785700	-5.71386100	1.12586300	C	-5.99773900	-3.38187600	0.35427800
H	0.36956700	-5.65474800	1.41586100	H	-6.03738200	-4.47672900	0.35945000
C	0.46981100	2.26561500	4.93861400	H	-6.39586100	-3.03490500	1.31253400
H	1.45948700	2.01053700	5.32621300	H	-6.67192900	-3.03392500	-0.43594100
H	0.24752500	3.29095600	5.25492800	C	0.27572300	-1.89579200	3.77224600
H	-0.26442500	1.60802300	5.41688400	H	0.53381500	-2.87815900	4.18277700
C	-1.00771500	2.49473600	2.92304800	H	0.64595900	-1.85762300	2.74383400
H	-1.27257500	3.52409200	3.18959200	H	0.82197800	-1.14527300	4.35280500
H	-1.08341400	2.41594300	1.83294500	C	-1.70534500	-1.62546900	5.29542400
H	-1.76278000	1.83712800	3.36670900	H	-2.76972100	-1.38952100	5.38416900
C	5.94744400	2.54945200	1.54700800	H	-1.54159600	-2.59892500	5.77089900
H	6.23921500	3.54266400	1.90741000	H	-1.14831900	-0.87917200	5.87269900
H	5.76772900	1.91668000	2.41894500	H	3.60679900	-5.15835300	-3.71031400
H	6.79597800	2.12850500	0.99611300	H	2.35724800	6.25100800	2.44805000
C	5.06254100	3.43744500	-0.62485200	H	-2.51856300	-6.01308700	2.87016900
H	4.18978100	3.60807400	-1.26242600	H	-2.47789900	4.22442100	-4.82971500
H	5.49066000	4.41652800	-0.38343000				
H	5.81358300	2.89736500	-1.21103800				

TS-2_1a2b

Mg	1.59011800	0.23156300	0.26251900	C	-2.34810800	0.68200300	-4.96831400
Mg	-1.45554400	0.97651800	0.17256800	C	-2.35040400	1.42699200	-3.78373400
N	3.01021000	1.81972200	0.10867800	H	4.63596700	3.91255000	0.34609600
N	2.75329400	-0.82838400	1.66895500	H	5.54300200	3.20794700	1.70245400
N	-2.67805000	1.78711900	1.70472600	H	4.01692800	4.03138100	1.99756700
N	-2.86568900	1.51550400	-1.34675200	H	4.61091800	1.60214300	3.03506800
C	4.54492500	3.37947300	1.29196000	H	3.48166000	-1.07178200	4.39069700
C	3.78431500	2.07107700	1.16519700	H	4.98281200	-0.17218600	4.10856800
C	3.97145000	1.20065600	2.25702300	H	4.71895300	-1.75951500	3.35936900
C	3.59880300	-0.14200500	2.44680500	H	4.80838700	3.13784300	-3.92254700
C	4.23885500	-0.81953900	3.64229100	H	1.67313700	5.53794900	-2.29035400
C	3.08268600	2.71019100	-1.01192000	H	4.12482200	-5.15269500	0.88568900
C	4.02682700	2.45626000	-2.04067000	H	1.07029300	-4.56081300	3.81801600
C	4.08201700	3.32312800	-3.13619100	H	-5.11961400	2.92247500	2.90614500
C	3.23963500	4.42366800	-3.23599600	H	-4.64326900	4.45635700	2.17288200
C	2.32337000	4.66911100	-2.22263300	H	-3.60706500	3.66961200	3.38696800
C	2.22517100	3.83217800	-1.10562100	H	-4.73188000	3.88380300	0.09340600
C	2.67369600	-2.24268900	1.90522600	H	-4.56246600	3.85459400	-2.53045400
C	3.52011900	-3.11116500	1.17292700	H	-5.80698200	2.88856100	-1.74634900
C	3.46922000	-4.48311000	1.43609100	H	-4.80922500	2.17356100	-3.02891400
C	2.60140600	-5.00770900	2.38569000	H	-4.12215100	-0.70991600	5.29709100
C	1.75595700	-4.15180500	3.08000500	H	-0.75819300	1.85499100	5.90949800
C	1.77287000	-2.76968600	2.86016600	H	-3.78569900	-2.18632700	-3.90683800
C	-4.26524800	3.49768200	2.53436600	H	-1.95268200	1.13439100	-5.87429400
C	-3.56803000	2.74534800	1.41823500	C	5.02639300	1.31033900	-1.95451000
C	-3.99205700	3.09060400	0.12547400	C	1.22834200	4.19420100	-0.01517700
C	-3.80371800	2.43084500	-1.10720500	H	1.28149100	3.41440900	0.75239900
C	-4.80125900	2.84721500	-2.17259900	H	4.63969900	0.59638700	-1.21899100
C	-2.58784400	1.37354000	3.07442400	C	4.49896300	-2.59525500	0.12802900
C	-3.51578600	0.42620000	3.57691500	H	4.25484900	-1.54313700	-0.04953100
C	-3.41258000	0.01710600	4.90993900	C	0.80877600	-1.89164100	3.64146200
C	-2.42643200	0.52037700	5.74970400	H	1.07198000	-0.84790400	3.44239300
C	-1.52276900	1.44984200	5.25130100	C	-1.84517000	2.86422600	-3.84551800
C	-1.58295600	1.89285800	3.92519400	H	-1.97685800	3.31161600	-2.85546200
C	-2.87116100	0.82980100	-2.60772800	C	-4.08182000	-1.11601500	-1.45026000
C	-3.39861500	-0.48455600	-2.65468400	H	-3.75367400	-0.56993600	-0.55757700
C	-3.37533600	-1.18180800	-3.86569000	C	-0.59188500	2.95321600	3.47000400
C	-2.85137800	-0.61110900	-5.01895400	H	-0.76374800	3.12392400	2.40179200

C	-4.62045000	-0.17438600	2.71756300	H	7.09798100	0.96216600	-1.37661500
H	-4.59727700	0.32535500	1.74446300	C	5.21673400	0.57467800	-3.28861500
C	0.73713000	-0.11100300	-1.95849600	H	4.26305700	0.28540800	-3.74048100
H	0.31886100	0.81594300	-2.32307700	H	5.75378300	1.19010300	-4.01865600
C	0.82734100	-1.46937000	-2.62954600	H	5.81208500	-0.33196300	-3.13724800
C	1.94349200	-0.74421600	-1.93555900	C	-2.64922500	3.70303000	-4.85463300
H	2.97233200	-0.50290500	-2.16761100	H	-2.46315600	3.37080600	-5.88180000
C	0.84830300	-1.39697600	-4.15250700	H	-3.72623400	3.64123900	-4.68055300
H	1.40432100	-2.24138900	-4.57676800	H	-2.35358100	4.75640600	-4.79449000
H	-0.16072200	-1.40316400	-4.57708400	C	-0.35539900	2.94908400	-4.20475000
H	1.33825600	-0.47510000	-4.47637900	H	0.28483100	2.46815100	-3.46146100
C	4.36154700	-3.33870100	-1.20714800	H	-0.15400800	2.47707200	-5.17252100
H	4.66460600	-4.38811100	-1.12234700	H	-0.03674700	3.99419200	-4.27317100
H	3.33107500	-3.31272000	-1.57043900	C	-5.60527900	-0.93389800	-1.54965400
H	5.00491800	-2.87768700	-1.96512100	H	-5.88302500	0.12161900	-1.62416000
C	5.94962400	-2.65906000	0.63026000	H	-5.99808200	-1.44575600	-2.43561000
H	6.09445400	-2.06055800	1.53438400	H	-6.10428500	-1.35498900	-0.66971500
H	6.24163500	-3.69010400	0.86064000	C	-3.72600600	-2.59169600	-1.25083600
H	6.63845100	-2.28086600	-0.13366900	H	-4.10444400	-3.22059800	-2.06325200
C	-0.63127000	-2.10261400	3.15658400	H	-2.64542900	-2.74086100	-1.19024800
H	-0.71965300	-1.90005700	2.08399600	H	-4.17487500	-2.96435600	-0.32498400
H	-0.95650100	-3.13522300	3.33044100	C	-4.38229900	-1.67227100	2.47898900
H	-1.31748300	-1.43696600	3.68784000	H	-3.42212500	-1.85422000	1.98813100
C	0.88637200	-2.11357400	5.15878900	H	-4.38092400	-2.22808200	3.42325700
H	0.54049500	-3.11485400	5.43848100	H	-5.17325400	-2.09286900	1.84833500
H	1.90516100	-2.00054300	5.54302800	C	-6.01586400	0.04550900	3.32118000
H	0.24507200	-1.39098800	5.67352100	H	-6.13694800	-0.49683400	4.26536500
C	1.56970100	5.53951800	0.64418500	H	-6.21425700	1.10249600	3.52257400
H	2.58750700	5.55244800	1.04254100	H	-6.78851900	-0.31719200	2.63456200
H	1.48744400	6.36329400	-0.07370800	C	0.85813800	2.48962600	3.64415300
H	0.87800800	5.75079700	1.46707700	H	1.10163600	2.30615500	4.69639900
C	-0.20887700	4.22913800	-0.54728900	H	1.04994600	1.56490600	3.09250000
H	-0.34434300	5.02252200	-1.29088100	H	1.55452600	3.24982200	3.27565000
H	-0.47450500	3.28438700	-1.03434100	C	-0.80782300	4.28759700	4.20192900
H	-0.92583500	4.41148300	0.26026200	H	-1.81757100	4.68097800	4.05338400
C	6.39147800	1.79725600	-1.44095900	H	-0.65107700	4.17719800	5.28072900
H	6.81580800	2.54586500	-2.11991300	H	-0.09905700	5.04139200	3.84146300
H	6.31659300	2.24918700	-0.44943900	H	2.58008100	-6.07701100	2.57826100

H	3.30353400	5.08827000	-4.09331000	C	3.38314200	-3.12989300	0.66272200
H	-2.36679800	0.19533000	6.78489600	C	-2.53329700	-2.39546100	-1.64120400
H	-2.84663700	-1.16588800	-5.95347700	C	-3.19799200	-1.79878600	-2.73153700
C	0.22093200	-2.72641500	-2.06662500	C	-4.55380900	-1.48551600	-2.60183100
C	0.30947700	-3.02516200	-0.68155900	C	-5.26751300	-1.73885200	-1.42846600
C	-0.39271600	-3.65774600	-2.88407000	C	-4.57987100	-2.31384700	-0.35792100
C	-0.19201300	-4.18945900	-0.15561000	C	-3.22652100	-2.65060100	-0.44308800
H	0.81944900	-2.33087900	-0.02164700	C	-0.97810500	1.61407400	5.37836300
C	-0.91962500	-4.87609700	-2.38131800	C	-0.19983900	1.61951200	4.07740300
H	-0.48344700	-3.47862900	-3.95031400	C	0.84865300	2.55284400	4.00321200
C	-0.82081400	-5.15387600	-0.98473500	C	1.74179300	2.83192200	2.95511400
H	-0.08626000	-4.38950600	0.90650500	C	2.80608300	3.86741800	3.25959000
C	-1.54125800	-5.83294900	-3.22455600	C	-1.58525800	-0.15431900	3.39687400
C	-1.34257800	-6.37303600	-0.48428200	C	-2.91431200	0.16784500	3.06639800
C	-2.04071300	-7.00803900	-2.71094400	C	-3.93045700	-0.73107100	3.40340100
H	-1.61525600	-5.62303200	-4.28936400	C	-3.66834400	-1.93868400	4.05242100
C	-1.94041500	-7.28186200	-1.32734100	C	-2.33687300	-2.25050900	4.33776900
H	-1.26114900	-6.57882300	0.58051400	C	-1.28944700	-1.38353700	4.01923400
H	-2.51348900	-7.73209300	-3.36922900	C	2.67766300	2.69044400	0.79766900
H	-2.33689800	-8.21358100	-0.93294600	C	2.41756600	3.82718300	0.00662600
				C	3.38224600	4.23939800	-0.91568100
				C	4.58408400	3.54913700	-1.09457900
Mg	0.34899400	-1.48572600	-0.95402400	C	4.81061200	2.42026100	-0.30648400
Mg	0.44776300	0.65557800	1.24862300	C	3.88131600	1.97921000	0.64117100
N	1.87561800	-2.89391800	-1.25091200	H	3.68503600	-4.55932700	-2.51796100
N	-1.14708400	-2.73723200	-1.73154500	H	2.51095900	-5.88234100	-2.66727000
N	-0.53013500	0.76420600	3.10542600	H	3.14243500	-5.40344000	-1.08221500
N	1.71394600	2.24673800	1.75413000	H	0.45739500	-5.43793700	-2.89706200
C	2.81197100	-5.02937600	-2.05722100	H	-2.64114100	-5.08607000	-1.91729600
C	1.66825600	-4.04739300	-1.89097600	H	-1.59983600	-5.73324600	-3.19793400
C	0.42998900	-4.47497500	-2.40183100	H	-2.62245400	-4.31271500	-3.48866600
C	-0.85968100	-3.92348500	-2.27258800	H	6.28569400	-1.55600500	-1.36493000
C	-1.98828500	-4.81553500	-2.75414000	H	4.81093300	-3.31747000	2.25028600
C	3.16560200	-2.70669400	-0.66554600	H	-5.06336400	-1.02368500	-3.44566700
C	4.21802200	-2.12210800	-1.39605900	H	-5.10863200	-2.51479800	0.57178700
C	5.47253500	-1.99554600	-0.78957800	H	-2.04227600	1.79415800	5.19681700
C	5.71696500	-2.42496300	0.51483800	H	-0.60745200	2.38073600	6.06047900
C	4.65102500	-2.98003100	1.22741800	H	-0.91181800	0.64228500	5.87732000

TS-2_1b2b

Mg	0.34899400	-1.48572600	-0.95402400	C	4.81061200	2.42026100	-0.30648400
Mg	0.44776300	0.65557800	1.24862300	C	3.88131600	1.97921000	0.64117100
N	1.87561800	-2.89391800	-1.25091200	H	3.68503600	-4.55932700	-2.51796100
N	-1.14708400	-2.73723200	-1.73154500	H	2.51095900	-5.88234100	-2.66727000
N	-0.53013500	0.76420600	3.10542600	H	3.14243500	-5.40344000	-1.08221500
N	1.71394600	2.24673800	1.75413000	H	0.45739500	-5.43793700	-2.89706200
C	2.81197100	-5.02937600	-2.05722100	H	-2.64114100	-5.08607000	-1.91729600
C	1.66825600	-4.04739300	-1.89097600	H	-1.59983600	-5.73324600	-3.19793400
C	0.42998900	-4.47497500	-2.40183100	H	-2.62245400	-4.31271500	-3.48866600
C	-0.85968100	-3.92348500	-2.27258800	H	6.28569400	-1.55600500	-1.36493000
C	-1.98828500	-4.81553500	-2.75414000	H	4.81093300	-3.31747000	2.25028600
C	3.16560200	-2.70669400	-0.66554600	H	-5.06336400	-1.02368500	-3.44566700
C	4.21802200	-2.12210800	-1.39605900	H	-5.10863200	-2.51479800	0.57178700
C	5.47253500	-1.99554600	-0.78957800	H	-2.04227600	1.79415800	5.19681700
C	5.71696500	-2.42496300	0.51483800	H	-0.60745200	2.38073600	6.06047900
C	4.65102500	-2.98003100	1.22741800	H	-0.91181800	0.64228500	5.87732000

H	0.99664600	3.14467300	4.89841200	H	0.95762600	4.93145200	1.17673200
H	3.80602600	3.44429600	3.11885300	H	1.11724800	5.46444200	-0.50233800
H	2.72186300	4.22577400	4.28663300	C	5.59123800	4.00051900	-2.11990300
H	2.73815300	4.72616000	2.58531000	H	5.32809800	3.64139400	-3.12266900
H	-4.95869200	-0.47074900	3.15826500	H	5.64697600	5.09254800	-2.17357500
H	-2.10368300	-3.19420200	4.82835900	H	6.59223600	3.62313700	-1.89086200
H	3.18757100	5.13016300	-1.51118500	C	0.13125300	-1.74760600	4.35703000
H	5.74237600	1.86895300	-0.41879400	H	0.18802700	-2.75893900	4.76874600
C	4.02420200	-1.67326700	-2.81985100	H	0.77476700	-1.70395500	3.47105800
H	4.94457200	-1.23602900	-3.21661400	H	0.56960900	-1.06040800	5.09000700
H	3.73958400	-2.50409100	-3.47554700	C	-3.23988300	1.46906700	2.38530800
C	2.26994000	-3.76661400	1.44941500	H	-2.75868500	1.54154700	1.40341300
H	1.38884600	-3.11468900	1.49292200	H	-4.31785800	1.57148000	2.23451400
H	1.93482000	-4.70647200	0.99574100	H	-2.89646900	2.33282400	2.96518500
H	2.58690800	-3.98073300	2.47372100	C	-4.78530900	-2.86568500	4.45754800
C	7.08778100	-2.31732600	1.13119100	H	-5.68189100	-2.70366000	3.85175700
H	3.22909100	-0.92684300	-2.90240200	H	-4.49458100	-3.91621100	4.35590100
H	7.03881900	-1.94686100	2.16059800	H	-5.06960700	-2.71044300	5.50593100
H	7.58647900	-3.29385300	1.16492400	C	1.25880200	0.57702700	-1.74913600
H	7.73185300	-1.64174300	0.56079200	H	2.24595000	0.68285600	-1.31260500
C	-2.47123500	-1.49885200	-4.01485100	C	0.48865700	1.51247900	-2.66834500
H	-2.16810100	-2.41238500	-4.54035200	C	0.71621300	0.04609500	-2.88483800
H	-3.10454500	-0.91988400	-4.69214100	H	1.03712700	-0.58574400	-3.70494800
H	-1.55644200	-0.92802600	-3.82448200	C	1.35718300	2.45083200	-3.49685000
C	-2.52422800	-3.29361600	0.72027400	H	0.84591600	2.74012900	-4.42255600
H	-3.21586000	-3.46912300	1.54640000	H	1.61935300	3.36380900	-2.95193200
H	-2.06680200	-4.24918000	0.44085900	H	2.29126600	1.95275400	-3.76828000
H	-1.71777200	-2.65578300	1.10347000	C	-0.86335000	2.06016500	-2.29725100
C	-6.73865300	-1.42726700	-1.33180900	C	-1.19596900	3.38524000	-2.50889200
H	-7.34764000	-2.27404500	-1.67283100	C	-1.85803600	1.21343100	-1.74008600
H	-7.03627100	-1.20973500	-0.30138800	C	-2.47562200	3.90644600	-2.18007300
H	-7.00849200	-0.56611700	-1.95095700	H	-0.47542300	4.06982700	-2.94538400
C	4.17460600	0.77641700	1.49593400	C	-3.10890200	1.67655700	-1.41441200
H	3.49315100	-0.05507500	1.27634900	H	-1.64034900	0.15705100	-1.61693500
H	5.18835600	0.41102400	1.32089200	C	-2.81359100	5.26669700	-2.39828300
H	4.06627300	0.99952000	2.56283500	C	-3.45826600	3.03696100	-1.61705700
C	1.12671900	4.58758200	0.15092300	H	-3.85073700	0.98885000	-1.01800700
H	0.26673000	3.96400300	-0.11596700	C	-4.06284100	5.74487800	-2.07418400

H	-2.06616800	5.92960100	-2.82851800	C	-1.22955100	-1.60611800	-3.95052600
C	-4.73731200	3.55672700	-1.29610800	C	-1.62058600	-0.40571700	-4.54565300
C	-5.03492600	4.88207600	-1.51804900	C	-0.74447900	0.67953600	-4.46110400
H	-4.30697600	6.78968600	-2.24655900	C	0.48820600	0.58734100	-3.81088900
H	-5.48202100	2.88796600	-0.87074100	C	4.92081400	-0.29170900	0.76264500
H	-6.01855200	5.26994500	-1.26739700	C	5.38310000	-1.34330300	1.57649700
Int-3							
Mg	-2.16610400	0.75006200	0.69679000	C	5.55737900	1.29438800	2.47657100
Mg	2.21988300	-0.40079700	-0.53629300	C	5.00802700	1.04166400	1.22100700
N	-2.76723700	2.70306800	0.37219400	H	-4.06798800	5.11229200	0.92510300
N	-4.10254000	0.02788900	0.67525800	H	-5.43959600	4.68822200	-0.11720500
N	2.12576500	-0.74956300	-2.57058300	H	-3.82642300	4.97239900	-0.80429000
N	4.29108100	-0.54395300	-0.49361200	H	-6.09907400	2.65410800	0.08510900
C	-4.37020800	4.54076300	0.04121800	H	-6.66496600	-0.64174200	-0.14517200
C	-4.03755300	3.07406700	0.21750300	H	-7.33008600	0.93028100	0.34423500
C	-5.13258900	2.18767900	0.23412200	H	-6.73995800	-0.22444100	1.55455800
C	-5.17497600	0.80422400	0.48110000	H	-0.02085100	5.63168100	2.60422600
C	-6.55757200	0.19001100	0.55738200	H	0.36858100	5.38343900	-1.65436200
C	-1.76009300	3.71613300	0.40265800	H	-4.66819600	-3.38728600	3.69252000
C	-1.35517700	4.26287600	1.63555800	H	-4.73975200	-4.38153500	-0.47384000
C	-0.33158000	5.21264700	1.64864300	H	2.30693900	-2.16838300	-4.92753000
C	0.30332900	5.63540200	0.47917300	H	3.96326900	-1.61866300	-5.25504600
C	-0.11280000	5.07280000	-0.72848600	H	2.59937800	-0.48717600	-5.32531200
C	-1.13178100	4.11883400	-0.78967200	H	5.27047300	-1.28446800	-3.60138800
C	-4.32694500	-1.34635600	0.99530100	H	6.88860600	0.11587800	-0.91236700
C	-4.39865500	-1.74149800	2.34697500	H	7.02452600	-0.80667500	-2.42623000
C	-4.60760400	-3.08841200	2.64749500	H	6.90680200	-1.63914000	-0.86819300
C	-4.74008400	-4.05828900	1.65036200	H	-1.89002800	-2.46926800	-4.01022300
C	-4.64453100	-3.64387200	0.32121100	H	-1.02371300	1.62602600	-4.92086400
C	-4.43101300	-2.30653300	-0.02743800	H	6.26776700	-1.85886600	3.46087000
C	3.01548500	-1.34580700	-4.78863600	H	5.62773100	2.32582700	2.81798300
C	3.19948000	-1.03611600	-3.31691600	C	-2.00681000	3.83100400	2.92231200
C	4.52458600	-1.05831100	-2.84854500	H	-1.62755300	4.41521400	3.76506200
C	5.04178100	-0.79024400	-1.56467600	H	-3.09564600	3.94571600	2.89271900
C	6.55065600	-0.77896600	-1.44364200	C	-1.54565800	3.52919300	-2.11050600
C	0.86631400	-0.64250300	-3.23463100	H	-1.33197800	2.45539300	-2.16082300
C	-0.00393300	-1.74650800	-3.29116500	H	-2.61955200	3.64013400	-2.29480300

H	-1.01192100	4.01124100	-2.93392400	C	-2.94984700	-0.27473500	-5.24270100
C	1.38242800	6.68589800	0.51846800	H	-3.34576200	-1.25163900	-5.53520400
H	-1.80628500	2.77431200	3.13633800	H	-3.69641500	0.20022700	-4.59432000
H	2.05574400	6.60076000	-0.33972500	H	-2.86967400	0.33995200	-6.14512000
H	0.95584500	7.69677600	0.49885300	C	1.16549400	0.27801000	1.15245900
H	1.98502000	6.60715700	1.42868700	H	1.78021000	0.99034800	1.72028300
C	-4.23872300	-0.73079000	3.45160400	C	0.56873600	-0.76257600	2.08942200
H	-4.92328700	0.11640400	3.33987700	C	0.44559500	-2.16764400	1.55851000
H	-4.41924800	-1.18913800	4.42758000	C	1.61666600	-2.90585400	1.31024400
H	-3.22179700	-0.31816300	3.46540000	C	-0.77912800	-2.80920900	1.35006100
C	-4.31084500	-1.90787700	-1.47361800	C	1.56906100	-4.22931500	0.87367800
H	-4.50255000	-2.76229900	-2.12847700	C	-0.83538100	-4.13282700	0.90871100
H	-5.01103400	-1.11052500	-1.74362300	C	0.33603900	-4.84976600	0.66909000
H	-3.30678600	-1.53296700	-1.70476100	H	2.57920400	-2.43526900	1.50723900
C	-4.95361600	-5.50658100	2.00596600	H	-1.69987800	-2.26907000	1.54936700
H	-5.72056600	-5.62014600	2.77942200	H	2.49231600	-4.77663300	0.69900700
H	-5.26565800	-6.09065100	1.13542900	H	-1.80401500	-4.60017700	0.75437400
H	-4.03425400	-5.96002200	2.39590600	H	0.29005600	-5.88047500	0.32726700
C	4.52030500	2.17991400	0.36438800	C	-0.32336000	0.35078200	1.60123100
H	3.42642700	2.17009600	0.27184600	H	-0.39373200	1.08485300	2.42418400
H	4.79867000	3.14214900	0.80289100	C	0.98244500	-0.75422500	3.55591900
H	4.93013600	2.13420400	-0.64989700	H	0.22172200	-1.22382300	4.19489900
C	5.33908400	-2.78281600	1.13036800	H	1.92422900	-1.29381400	3.71981700
H	5.01013300	-3.43431400	1.94646100	H	1.12419200	0.27624100	3.89930600
H	4.66712400	-2.92593800	0.28152100				
H	6.33264700	-3.13623200	0.82613400				
C	6.56640500	0.56597600	4.67597500				
H	7.14824200	-0.27428700	5.06581100				
H	7.21532800	1.44795500	4.66244500				
H	5.76146400	0.76857500	5.39313300				
C	1.40006500	1.78329200	-3.73212900				
H	0.98749100	2.62435000	-4.29561000				
H	1.53756400	2.11172700	-2.69483100				
H	2.39920500	1.56968800	-4.12566100				
C	0.38100000	-3.06023100	-2.66816800				
H	0.44656100	-2.98881900	-1.57670500				
H	-0.35778400	-3.83208900	-2.89937800				
H	1.35832500	-3.40812300	-3.01883600				

Int-3_1a2a

Mg	-2.53939800	0.23265300	-0.16147200
Mg	2.50630300	0.11070500	-0.28607300
N	-3.65985600	1.68437000	-1.13689100
N	-4.10708900	-1.13208800	-0.09412400
N	3.44928900	-1.23173900	-1.53884600
N	4.21676500	1.28080800	-0.04297700
C	-5.55821100	2.48585600	-2.49294600
C	-4.83726900	1.41440200	-1.70373600
C	-5.51991200	0.19022800	-1.57468000
C	-5.24790900	-0.92766500	-0.76327900
C	-6.37053200	-1.93982500	-0.66932400
C	-3.20801400	3.04496200	-1.14195400

C	-3.65780200	3.92524800	-0.12702400	H	-3.37973400	-5.62143900	0.73931900
C	-3.19162300	5.24261800	-0.12085600	H	5.29813200	-2.82640900	-2.89466500
C	-2.30740800	5.70244200	-1.08908600	H	6.03083900	-1.42455500	-3.69844900
C	-1.86428600	4.82917200	-2.07340000	H	4.36338200	-1.91420900	-4.06072300
C	-2.29103600	3.49757700	-2.11681900	H	6.28702300	0.29531600	-2.46910800
C	-4.02234600	-2.27745600	0.76801100	H	6.95166000	2.28998800	-1.57336700
C	-4.21104800	-2.10299900	2.15982700	H	7.27980000	1.39909200	-0.09073200
C	-4.10173000	-3.21498200	3.00002400	H	6.32814100	2.88428900	-0.01429800
C	-3.80500300	-4.47482400	2.49799900	H	3.11153900	-5.73229500	-0.62976400
C	-3.61573300	-4.63548300	1.13162900	H	0.58771900	-4.14270100	-3.69383500
C	-3.72251700	-3.55861700	0.24679600	H	4.92808300	2.47403300	4.34768400
C	5.10892400	-1.81548100	-3.26566200	H	3.42982500	5.47760500	1.69909700
C	4.59404000	-0.91308900	-2.16493800	C	-4.60345900	3.47446500	0.97810200
C	5.38757400	0.20436100	-1.87053100	C	-1.74251100	2.59007100	-3.20731500
C	5.28238600	1.15034100	-0.82546300	H	-2.18205500	1.59678500	-3.06184300
C	6.52173400	1.99440400	-0.61260000	H	-4.95057700	2.46636400	0.73086200
C	2.89791100	-2.53201900	-1.77998600	C	-4.56984300	-0.75494700	2.76879800
C	3.34584800	-3.62954300	-1.00343900	H	-4.46276100	0.00332700	1.98443600
C	2.77297400	-4.88572000	-1.22206200	C	-3.49180300	-3.80830900	-1.23679800
C	1.78584700	-5.07531800	-2.18184300	H	-3.75195100	-2.89163100	-1.77644400
C	1.35540300	-3.99307200	-2.93915800	C	3.32283200	4.04022700	-0.57886100
C	1.89352500	-2.71503800	-2.75720800	H	3.23100400	3.15812000	-1.22214800
C	4.23284300	2.23939000	1.02279500	C	5.14180900	0.43006300	2.60702300
C	4.64840700	1.83937700	2.31329200	H	5.11107400	-0.13395500	1.66866400
C	4.60924400	2.77430000	3.35255800	C	1.38028700	-1.56719300	-3.61401600
C	4.17830200	4.07689500	3.13724600	H	2.01635200	-0.69746600	-3.41568500
C	3.76744100	4.45807000	1.86562500	C	4.43320300	-3.48961200	0.05421200
C	3.77544100	3.55983500	0.79408900	H	4.76196600	-2.44571400	0.05388800
H	-5.97933600	3.23961800	-1.81946900	C	0.78351300	0.98433400	0.53945000
H	-6.37478000	2.05928100	-3.07804300	H	1.14588000	2.02040100	0.63201200
H	-4.87556500	3.01454200	-3.16215200	C	0.10590400	0.61303000	1.86496700
H	-6.46853600	0.14651200	-2.09694600	C	0.16075700	-0.81999800	2.28884900
H	-6.14717500	-2.82473500	-1.27281200	C	0.27212900	-1.19932200	3.63677200
H	-7.30886800	-1.51445200	-1.02841300	C	0.11385200	-1.85719100	1.33767900
H	-6.50725400	-2.28572100	0.35801700	C	0.32699300	-2.54204600	4.01585500
H	-3.52931300	5.92104700	0.65859900	C	0.16740700	-3.19676100	1.71169400
H	-1.16806000	5.18628300	-2.82811700	C	0.27340800	-3.55011200	3.05833000
H	-4.25243500	-3.08838900	4.06873300	H	0.31640200	-0.43760100	4.40856400

H	0.02569500	-1.59291200	0.28588400	C	-3.86709100	3.39547900	2.32402000
H	0.41158300	-2.79548600	5.07008100	H	-3.00604700	2.72204900	2.27214400
H	0.13157900	-3.96750200	0.94716800	H	-3.49485900	4.38053100	2.62692500
H	0.31362200	-4.59530900	3.35218400	H	-4.53768300	3.03539800	3.11238800
C	-0.74548400	0.97666600	0.64774300	C	4.35957800	4.97807500	-1.21875500
H	-1.08506700	2.01948300	0.77470800	H	4.49522500	5.88075200	-0.61212500
C	0.18219600	1.62979200	2.99005600	H	5.33695500	4.50020300	-1.32534700
H	-0.64788500	1.52910800	3.70300800	H	4.02909200	5.29268600	-2.21506400
H	1.11844900	1.55475300	3.55865500	C	1.95365200	4.73159600	-0.53719600
H	0.13768700	2.64076300	2.57503500	H	1.18432000	4.08642700	-0.10569700
C	-3.63548500	-0.37048700	3.92293900	H	1.98445200	5.65738500	0.04753200
H	-3.75795300	-1.03980500	4.78141400	H	1.63696300	5.00034600	-1.55032200
H	-2.58606600	-0.41246900	3.61861900	C	6.59804000	0.42817600	3.09543000
H	-3.85613200	0.64513100	4.26840800	H	7.26230800	0.93038400	2.38549400
C	-6.03730700	-0.72264800	3.22320900	H	6.69659000	0.94094800	4.05866900
H	-6.72230200	-0.92569600	2.39426000	H	6.95696400	-0.59818200	3.23022400
H	-6.22304100	-1.47251600	4.00043800	C	4.23341300	-0.28958100	3.61376400
H	-6.29196400	0.25904200	3.63815800	H	4.22635400	0.22525200	4.58093500
C	-2.01431900	-4.10778900	-1.51866000	H	3.19849500	-0.34395900	3.26276700
H	-1.36492400	-3.29631400	-1.18130800	H	4.58396600	-1.31274500	3.78692300
H	-1.69354500	-5.02041700	-1.00474200	C	3.90154800	-3.81133400	1.45777700
H	-1.84730400	-4.25581000	-2.59126300	H	3.04311600	-3.18813600	1.72161100
C	-4.36397400	-4.94608600	-1.78986400	H	3.57996000	-4.85634000	1.53069800
H	-4.06866200	-5.91548200	-1.37405200	H	4.68492000	-3.65571100	2.20795500
H	-5.42489500	-4.80483700	-1.56237300	C	5.65917200	-4.36038300	-0.26070200
H	-4.25640300	-5.01329300	-2.87803500	H	5.40701900	-5.42655900	-0.24729000
C	-2.13482500	3.06894700	-4.61296900	H	6.08310100	-4.13334100	-1.24359700
H	-3.22023200	3.14481700	-4.73051900	H	6.44322700	-4.19828900	0.48717400
H	-1.70890600	4.05427900	-4.83239300	C	-0.05862500	-1.19470800	-3.22735000
H	-1.76359800	2.37250800	-5.37316100	H	-0.72638900	-2.05552400	-3.33445300
C	-0.21734600	2.45729000	-3.08802400	H	-0.11312400	-0.84542900	-2.18929900
H	0.27209500	3.43059000	-3.20026300	H	-0.43877000	-0.39496300	-3.87056900
H	0.06628000	2.04555000	-2.11417500	C	1.46772400	-1.87137600	-5.11659300
H	0.17705100	1.80297600	-3.87304800	H	2.47986500	-2.16264200	-5.41427700
C	-5.84416200	4.37058700	1.09827400	H	0.79291300	-2.68450400	-5.40539700
H	-5.58220700	5.38608700	1.41474400	H	1.18457500	-0.98908300	-5.70083300
H	-6.38295400	4.45013900	0.14884500	H	-3.72025400	-5.32625300	3.16762500
H	-6.53558400	3.96443600	1.84463000	H	-1.96232100	6.73265900	-1.07298500

H 1.35745200 -6.06109100 -2.34142900
H 4.16027400 4.79125300 3.95584900

Int-3_1a2b

Mg -2.57612300 -0.45598700 0.23828600
Mg 2.47976600 -0.48442700 0.43963500
N -3.73528900 -2.07596000 0.81778900
N -4.11962900 0.91551500 0.47825500
N 3.42750600 0.50085900 1.98500000
N 4.16272800 -1.61259800 -0.04859200
C -5.67247400 -3.14392200 1.90857200
C -4.92257300 -1.92736600 1.41054500
C -5.58560400 -0.69644100 1.56574800
C -5.27831900 0.57987500 1.05515800
C -6.38359500 1.60579600 1.19762500
C -3.30254100 -3.40631700 0.50476600
C -3.73676100 -4.00689600 -0.70283400
C -3.28798000 -5.29257500 -1.01674300
C -2.43560300 -5.98922200 -0.16892300
C -2.00769800 -5.38827400 1.00740000
C -2.41874100 -4.09898700 1.36224800
C -3.98422000 2.23147500 -0.07988900
C -4.11879200 2.39678600 -1.47946300
C -3.94602300 3.67105800 -2.02743000
C -3.64054700 4.76621300 -1.23049100
C -3.51033000 4.59413700 0.14116000
C -3.68024500 3.34292600 0.74122300
C 5.10771700 0.66860200 3.78063300
C 4.56529500 0.03026100 2.52016900
C 5.33698100 -1.01021700 1.98352600
C 5.22086600 -1.69243100 0.75124000
C 6.43988700 -2.50194100 0.36118700
C 2.89486800 1.72061100 2.51522700
C 3.38589600 2.96004300 2.03508500
C 2.81885000 4.14117300 2.52164100
C 1.80114600 4.12055900 3.46828400
C 1.33457900 2.90028000 3.94048800
C 1.86229800 1.68969800 3.47946400

C 4.16810300 -2.30423400 -1.30436900
C 4.59194700 -1.62678900 -2.47051900
C 4.53883600 -2.29907200 -3.69563500
C 4.08543200 -3.60891900 -3.78301900
C 3.66788300 -4.26405400 -2.63100000
C 3.69095300 -3.63500800 -1.38240300
H -6.06307100 -3.72562500 1.06725600
H -6.51262200 -2.85530100 2.54241600
H -5.01504700 -3.81315300 2.46860700
H -6.54591900 -0.76086800 2.06431300
H -6.21375200 2.23161200 2.07967200
H -7.35171300 1.11655000 1.31780000
H -6.42592000 2.27397100 0.33507800
H -3.61404900 -5.75634200 -1.94436400
H -1.33642200 -5.93030700 1.66880100
H -4.05054000 3.80627200 -3.10023800
H -3.26984500 5.45162700 0.76461800
H 5.43563900 1.69475400 3.58872200
H 5.95517800 0.10485500 4.17347400
H 4.33512600 0.73037100 4.55205500
H 6.23057000 -1.25231900 2.54793200
H 6.85605800 -3.01037400 1.23490300
H 7.21596900 -1.82796000 -0.01938500
H 6.22726800 -3.23524300 -0.41620100
H 3.18589800 5.09582700 2.15326800
H 0.54571900 2.88447000 4.68796400
H 4.86449000 -1.78490000 -4.59652300
H 3.31356500 -5.28929800 -2.70041300
C -4.64913400 -3.28607100 -1.68626400
C -1.88861500 -3.49215900 2.65239900
H -2.31958500 -2.48895600 2.74658100
H -4.98310000 -2.35706700 -1.21365700
C -4.49490000 1.24321800 -2.39848500
H -4.38275300 0.31325800 -1.82842700
C -3.51282700 3.23034500 2.24975400
H -3.79937100 2.21576600 2.54577800
C 3.22957100 -4.41188700 -0.15613100
H 3.19524700 -3.71129200 0.68527700

C	5.11195500	-0.19694800	-2.43656600	H	0.02154300	-2.91166200	3.52608100
H	5.07420700	0.14539100	-1.39671900	C	-5.90305800	-4.10028600	-2.03523800
C	1.31319000	0.38447900	4.03642200	H	-5.65225400	-5.01963800	-2.57551800
H	1.92101900	-0.43036500	3.62797100	H	-6.46508500	-4.38671100	-1.14076400
C	4.50378100	3.04634700	1.00428200	H	-6.56960200	-3.51518300	-2.67822900
H	4.89032100	2.03442400	0.84839300	C	-3.88310900	-2.90867700	-2.96324000
C	0.74981100	-1.05711700	-0.60869600	H	-3.01214800	-2.28485100	-2.73998700
H	1.09466700	-2.04173700	-0.96254700	H	-3.52141700	-3.80233200	-3.48398000
C	0.08964400	-0.35424600	-1.80263800	H	-4.53062100	-2.35863600	-3.65534100
C	-0.77781700	-0.99163000	-0.71579600	C	4.21877100	-5.53066400	0.20905500
H	-1.13513300	-1.96076200	-1.10567500	H	4.29134500	-6.26779700	-0.59865900
C	0.15594300	-1.05795400	-3.14560600	H	5.22451500	-5.14528000	0.39715700
H	-0.66438400	-0.76072700	-3.81338300	H	3.88656800	-6.05712800	1.11086400
H	1.09924900	-0.86274500	-3.67234300	C	1.82243300	-4.99769700	-0.33376300
H	0.08599300	-2.13949700	-2.99855800	H	1.08498000	-4.22392300	-0.56133700
C	-3.58591300	1.14843100	-3.62981900	H	1.79198500	-5.73863100	-1.13995300
H	-3.72758100	1.99928100	-4.30488300	H	1.50609700	-5.50465700	0.58389800
H	-2.53031200	1.12211100	-3.34568600	C	6.57660100	-0.11639200	-2.89251500
H	-3.81449200	0.24167100	-4.19986800	H	7.22032300	-0.77436400	-2.30071900
C	-5.97063500	1.33181500	-2.81799200	H	6.68327300	-0.40859400	-3.94308800
H	-6.63874900	1.32326600	-1.95145600	H	6.95408400	0.90747900	-2.79479200
H	-6.16117300	2.25473800	-3.37733500	C	4.23399600	0.74620700	-3.27081000
H	-6.24176700	0.48738600	-3.46162900	H	4.23633100	0.46018700	-4.32846900
C	-2.04851100	3.43447200	2.65747300	H	3.19399900	0.74113500	-2.93060700
H	-1.38669600	2.72044700	2.16140000	H	4.60347700	1.77515800	-3.20692500
H	-1.70351200	4.44007300	2.39346700	C	3.97937100	3.55607300	-0.34534900
H	-1.92892300	3.31717600	3.74039600	H	3.17296600	2.92717000	-0.73222400
C	-4.40589200	4.21762100	3.01721300	H	3.58074900	4.57253500	-0.25814700
H	-4.08963800	5.25339400	2.85276800	H	4.78482600	3.57817300	-1.08777200
H	-5.45524600	4.14689700	2.71609900	C	5.67442400	3.91727100	1.48383700
H	-4.34718200	4.02706900	4.09453000	H	5.37925800	4.96628200	1.59560500
C	-2.31168200	-4.29660500	3.89050000	H	6.06829700	3.58101000	2.44820300
H	-3.39948400	-4.39066000	3.96460400	H	6.49310900	3.88488200	0.75673300
H	-1.89311100	-5.30892200	3.87132600	C	-0.13807500	0.16037300	3.58781700
H	-1.95462000	-3.80957600	4.80482300	H	-0.77965800	0.98677900	3.90966800
C	-0.36057000	-3.35052100	2.59802900	H	-0.20689200	0.07818200	2.49650000
H	0.12042900	-4.32699700	2.47799800	H	-0.54006000	-0.76135400	4.01964600
H	-0.05381500	-2.71736400	1.75931900	C	1.41686500	0.31510800	5.56708800

H	2.44238800	0.47909100	5.91227300	C	-3.98378800	-2.40100600	-2.90182600
H	0.78246700	1.06653200	6.04968800	C	-3.89281500	-3.75868100	-3.21634300
H	1.09326700	-0.66754000	5.92729600	C	-4.00344100	-4.75426200	-2.24371100
H	-3.49953300	5.74622800	-1.67707600	C	-4.20151000	-4.35451300	-0.92105500
H	-2.10348400	-6.99136100	-0.42600500	C	-4.29737300	-3.00861600	-0.55955900
H	1.37868600	5.05001700	3.84031200	C	-2.48951400	3.23113700	-0.09971500
H	4.05612100	-4.11652100	-4.74333700	C	-1.81818100	3.94608200	-1.11122800
C	0.17859400	1.13522600	-1.85511400	C	-1.02821500	5.03901000	-0.75428200
C	0.13861600	1.89685900	-0.64785000	C	-0.87439100	5.43944500	0.57543200
C	0.31913700	1.83633300	-3.04158700	C	-1.52234000	4.69356800	1.56022400
C	0.23043300	3.26653400	-0.64715200	C	-2.32370600	3.59027400	1.25002900
H	0.02800300	1.36049700	0.29160000	C	2.28587500	-2.47610700	5.00010500
C	0.41690200	3.25256600	-3.08094500	C	2.56985300	-2.15150900	3.54816800
H	0.35956000	1.30440900	-3.98770900	C	3.86039900	-2.46403300	3.08707800
C	0.37142700	3.99126900	-1.85966500	C	4.42831800	-2.31986900	1.80416300
H	0.20318700	3.81306200	0.29187500	C	5.87407900	-2.74609300	1.66197300
C	0.56217200	3.96536700	-4.29935400	C	0.34554500	-1.33100500	3.40876700
C	0.47267700	5.40382700	-1.90099700	C	0.14542800	-0.09983200	4.06337100
C	0.65809600	5.33855200	-4.30993200	C	-1.10080800	0.16612300	4.63822900
H	0.59724400	3.40533600	-5.23132200	C	-2.15440500	-0.74813900	4.58074000
C	0.61328400	6.06721500	-3.09924300	C	-1.93859800	-1.94945800	3.90070600
H	0.43563600	5.95763200	-0.96541100	C	-0.71237100	-2.25623400	3.30593000
H	0.76946600	5.86837300	-5.25246500	C	4.46648300	-1.76745900	-0.50722100
H	0.69029100	7.15108200	-3.11885300	C	5.15715600	-0.58838000	-0.84426300
Int-3_1b2b							
Mg	-2.44117800	0.28730000	-0.81101500	C	5.74698000	-1.55920100	-3.00814200
Mg	1.77374700	-1.36025200	0.75910400	C	5.04491600	-2.71280600	-2.65281000
N	-4.23919900	-0.64226300	-1.21078000	C	4.39775000	-2.83624400	-1.42118000
N	-3.31374300	2.11558300	-0.44904900	H	-6.60055900	-1.20153700	-2.57837800
N	1.59997800	-1.62058200	2.79558400	H	-7.55221400	-0.14211600	-1.51847600
N	3.77557800	-1.85607300	0.74019800	H	-6.80841800	-1.62809100	-0.89188100
C	-6.66885600	-0.78040300	-1.57010100	H	-6.59584900	1.71969900	-1.01061200
C	-5.41234800	-0.01130100	-1.22199800	H	-4.95458800	4.13611200	0.56090500
C	-5.57652800	1.35916000	-0.94110500	H	-6.23550900	3.78180700	-0.61560800
C	-4.62418600	2.33924000	-0.60730100	H	-4.66850800	4.42977400	-1.14171900
C	-5.15923500	3.74657200	-0.44082700	H	-3.72569900	-4.04420900	-4.25356000
C	-4.19870900	-2.02577100	-1.56144600	H	-4.28054900	-5.11164900	-0.14263900
				H	-0.51458200	5.59100200	-1.53900100

H	-1.40839700	4.97908300	2.60481700	H	3.74465500	-4.83647200	-1.87527400
H	1.99033000	-1.58381300	5.55994900	H	3.98364200	-4.54320900	-0.14513800
H	3.15872500	-2.91628200	5.48447000	C	5.21139100	0.57100400	0.11333400
H	1.45085700	-3.18030000	5.07948400	H	4.20776500	0.94451300	0.34347300
H	4.52362800	-2.88209600	3.83492700	H	5.67197300	0.29656000	1.06915000
H	5.97487300	-3.53371500	0.90837500	H	5.78067900	1.40132800	-0.31136600
H	6.27441900	-3.11389000	2.60795600	C	6.41031600	-1.43859300	-4.35550100
H	6.49516900	-1.91220000	1.32040900	H	5.71369500	-1.04975100	-5.10882800
H	-1.24778800	1.11568000	5.14993400	H	7.26530100	-0.75647200	-4.32152400
H	-2.74659700	-2.67588100	3.83524800	H	6.76683600	-2.40874600	-4.71555600
H	6.32665900	0.40109700	-2.34241400	C	-0.52558200	-3.55345300	2.56482500
H	4.99665400	-3.54441900	-3.35389900	H	-1.40225500	-4.19688300	2.67778600
C	-3.83339300	-1.35891400	-3.97827400	H	-0.38083900	-3.37766000	1.49107600
H	-3.74853700	-1.82633000	-4.96299200	H	0.35108400	-4.10542800	2.91963800
H	-4.67917500	-0.66375200	-4.00453700	C	1.25532100	0.91358200	4.15109200
C	-4.48757200	-2.61861600	0.88173300	H	1.70874800	1.09703000	3.17183300
H	-3.61380600	-2.08253600	1.27150200	H	0.88467400	1.86429400	4.54407400
H	-5.34826900	-1.95600500	1.02126600	H	2.06846200	0.57898800	4.80606100
H	-4.63788200	-3.50385300	1.50608300	C	-3.47134800	-0.46377300	5.25493300
C	-3.93475400	-6.21283500	-2.61394400	H	-3.64700200	0.61131800	5.35540700
H	-2.93211100	-0.75366200	-3.82060900	H	-4.30975000	-0.89187200	4.69683300
H	-3.55908700	-6.81942200	-1.78437700	H	-3.50081300	-0.89410500	6.26388100
H	-4.92498300	-6.60355500	-2.88048500	C	0.52627300	-1.46802200	-0.93027700
H	-3.27949300	-6.37696900	-3.47487000	H	0.64548500	-2.43281900	-1.44497500
C	-1.94373200	3.53597900	-2.55459200	C	0.64876900	-0.33210600	-1.96248800
H	-2.98852200	3.43071100	-2.86508400	C	-0.72486500	-0.74786300	-1.43780400
H	-1.46427100	4.26819200	-3.20956600	H	-1.19717500	-1.37161700	-2.21507600
H	-1.45474200	2.57020000	-2.73555600	C	1.00519800	-0.69997600	-3.38894400
C	-2.99112300	2.80483200	2.34797700	H	0.67138300	0.05727600	-4.11279300
H	-2.83581600	3.28736300	3.31698400	H	2.08643200	-0.83581200	-3.52291800
H	-4.06984100	2.70250800	2.19096400	H	0.52142800	-1.64449700	-3.65511700
H	-2.58829100	1.78746400	2.41923600	C	1.25347300	0.93079700	-1.45043300
C	-0.03767800	6.64232900	0.92396900	C	2.13398900	1.70236100	-2.19006800
H	-0.49171200	7.56614300	0.54574200	C	0.96942200	1.36663200	-0.11641200
H	0.07569200	6.75079900	2.00662500	C	2.75909500	2.86148200	-1.66242100
H	0.96261100	6.56991400	0.48399400	H	2.38033200	1.41742300	-3.20839600
C	3.63898500	-4.09164100	-1.08179300	C	1.55668800	2.48585000	0.42739300
H	2.56856900	-3.88726700	-0.95904200	H	0.21347800	0.82491100	0.45265500

C	3.67111100	3.63883400	-2.42395200	C	-1.63221600	-3.60582100	-2.55440800
C	2.47962400	3.26204700	-0.31937800	C	-2.76172700	-4.28980100	-3.29856300
H	1.29189300	2.80745600	1.43131100	C	2.29143000	-2.69169000	-0.58117800
C	4.27773700	4.75034500	-1.88483400	C	3.27043400	-1.89864700	-1.21073800
H	3.88547100	3.33774100	-3.44687700	C	4.49048300	-1.69425800	-0.56392800
C	3.12245900	4.40891300	0.21076100	C	4.76747000	-2.25389200	0.68646800
C	4.00382700	5.14041700	-0.55309800	C	3.78481900	-3.04479800	1.28261800
H	4.97358100	5.33326300	-2.48263800	C	2.54849600	-3.27823600	0.67245300
H	2.91003500	4.69967600	1.23714200	C	-3.17531900	-1.89693700	-2.03985700
H	4.49343200	6.01616500	-0.13579000	C	-3.50294700	-1.06715500	-3.13120800
TS-3				C	-4.80369700	-0.57024700	-3.23649300
Mg	0.23896400	1.78511400	-0.19453600	C	-5.78494300	-0.85236100	-2.28202300
Mg	-0.41367900	-1.38765500	-0.85870500	C	-5.42183400	-1.63853900	-1.18692700
N	1.64516500	3.21030900	-0.81862800	C	-4.13513000	-2.16782900	-1.04666900
N	-1.15590700	3.29889200	0.23626700	H	3.20892600	5.52843400	-0.80611200
N	1.01383900	-2.86529800	-1.19486300	H	2.01734700	6.42113700	-1.76837000
N	-1.86161700	-2.44505400	-1.93155900	H	2.91732200	5.05963900	-2.46835200
C	2.42501500	5.42971500	-1.56488100	H	-0.02516900	6.07909600	-1.24646800
C	1.34414000	4.48431300	-1.07989300	H	-3.16989000	4.98575600	-0.50515400
C	0.06837300	5.05331000	-0.91005600	H	-2.09071000	6.37646400	-0.74682500
C	-1.06981300	4.53085300	-0.27238400	H	-2.43214400	5.76678000	0.87993300
C	-2.25283600	5.47165400	-0.15852600	H	5.92163600	2.40884600	0.65430300
C	2.99664400	2.80263500	-1.03109300	H	5.08584500	1.74936300	-3.49550200
C	3.89944300	2.78388100	0.04958500	H	-3.41790900	3.34119200	4.23562300
C	5.22490700	2.40984100	-0.18235400	H	-5.27337500	1.37460600	0.91105200
C	5.68201600	2.05081400	-1.45226800	H	2.82650800	-4.37110500	-2.64804600
C	4.75787200	2.04115400	-2.49892100	H	1.67900700	-5.70709800	-2.86932300
C	3.42005400	2.40028200	-2.31224500	H	2.33481700	-5.32841900	-1.26535300
C	-2.29272300	2.99982100	1.04559300	H	-0.38117900	-5.19079700	-3.15297800
C	-2.31291200	3.39341100	2.39953500	H	-3.60182700	-4.49447600	-2.62714600
C	-3.41155400	3.04276100	3.18853900	H	-2.43010500	-5.23246300	-3.73657000
C	-4.48938400	2.31555200	2.67998200	H	-3.15484200	-3.65365400	-4.09766000
C	-4.44660100	1.94093800	1.33566400	H	5.24023900	-1.07460500	-1.05088300
C	-3.37191100	2.27473900	0.50655600	H	3.97786300	-3.49616300	2.25381100
C	1.97463100	-4.89503500	-2.20316200	H	-5.05512500	0.05986000	-4.08810200
C	0.82422600	-3.94006600	-1.95945400	H	-6.16400000	-1.86078000	-0.42189500
C	-0.39504100	-4.27197500	-2.57903000	C	3.44682200	3.17430500	1.43123900
				H	4.27792900	3.13415400	2.14062500

H	3.02784300	4.18620400	1.45361200	C	3.01401300	-1.30977200	-2.57097200
H	2.66073500	2.50291000	1.79879000	H	2.12427900	-0.66922700	-2.56494200
C	2.45144800	2.36194700	-3.46386300	H	3.86037700	-0.70187900	-2.89703000
H	1.56896000	1.75973400	-3.21689600	H	2.83493600	-2.08625100	-3.32391400
H	2.07939600	3.35851400	-3.72822000	C	6.08278600	-1.99315800	1.37350800
H	2.91958800	1.93293800	-4.35391100	H	6.92584800	-2.11112300	0.68419400
C	7.13110800	1.71218600	-1.68911800	H	6.12992100	-0.97050900	1.76727300
H	7.25455500	1.05639600	-2.55632500	H	6.23792300	-2.67685200	2.21317400
H	7.72386900	2.61587300	-1.87916100	C	0.51326100	-0.14807500	1.62130700
H	7.57459500	1.21267300	-0.82215800	C	-0.79326700	-0.57470900	1.60761600
C	-1.17230800	4.17638800	2.99616500	H	-1.74751600	-0.14900900	1.33280600
H	-0.20385300	3.74400500	2.72629300	C	-0.10972700	-0.51250300	2.96131300
H	-1.15493800	5.21400200	2.64153900	H	1.45286700	-0.49012400	1.21116400
H	-1.24721800	4.20317900	4.08664100	C	0.24228400	-1.78234400	3.69018800
C	-3.38518000	1.89525400	-0.94768200	C	1.50226100	-1.94187500	4.27972600
H	-4.26998600	1.30608500	-1.19493300	C	-0.71177200	-2.78860600	3.87954200
H	-3.36742500	2.78011800	-1.59525900	C	1.80175700	-3.07567700	5.03411200
H	-2.50601900	1.29669700	-1.22025800	C	-0.41822100	-3.92354300	4.63359100
C	-5.67232400	1.97103500	3.54694100	C	0.84098700	-4.07062900	5.21551600
H	-6.42496800	2.76944200	3.52952800	H	2.25404300	-1.16817300	4.14278500
H	-6.16413800	1.05449800	3.20735500	H	-1.69376900	-2.67437600	3.42600400
H	-5.37654200	1.82798000	4.59081800	H	2.78624900	-3.18189100	5.48315700
C	-3.79040000	-3.03418700	0.13504000	H	-1.17371300	-4.69337800	4.76931400
H	-2.92651800	-2.64007600	0.68339400	H	1.07184300	-4.95367200	5.80542100
H	-4.63241600	-3.10077200	0.82945100	C	-0.44978700	0.61348100	3.92631500
H	-3.52274600	-4.05224600	-0.17042600	H	-1.26502300	0.32015100	4.59850700
C	-2.46581000	-0.71729000	-4.16448400	H	0.41344200	0.87065300	4.55272800
H	-2.88264100	-0.05464400	-4.92779100	H	-0.76820900	1.50520800	3.38439300
H	-1.60901400	-0.20914600	-3.70419900				
H	-2.06447700	-1.60406900	-4.66728800				
C	-7.19291000	-0.34030200	-2.44291500				
H	-7.20882700	0.66519000	-2.87535500				
H	-7.77682100	-0.98736800	-3.10944500				
H	-7.71853500	-0.30318600	-1.48414500				
C	1.52202800	-4.15634900	1.33254400				
H	1.81978000	-4.41131700	2.35156200				
H	0.54720900	-3.66300400	1.38420000				
H	1.37063300	-5.09117700	0.77914400				

TS-3_1a2a

Mg	1.44112200	-0.71349100	0.59233700
Mg	-1.54728900	1.04719100	-0.38935200
N	3.55258100	-0.53718200	0.53871800
N	1.52386000	-2.33693400	1.93918700
N	-1.71628500	3.14504800	-0.59942100
N	-3.64291800	0.78083000	-0.56216500
C	5.86169600	-1.12384100	1.22423500
C	4.36897000	-1.38730000	1.16508700

C	3.95102500	-2.52936500	1.87274300	H	3.54845000	-4.72941600	3.09459700
C	2.67018300	-2.93453200	2.28458800	H	5.35353400	1.67463400	-3.08458200
C	2.66609900	-4.10481200	3.25089700	H	5.14880300	3.78451700	0.62718700
C	4.15030800	0.60704800	-0.08387500	H	-2.38960100	-4.76124100	2.12551200
C	4.48656400	0.56440100	-1.46072100	H	-1.29743100	-2.49912400	5.58343300
C	5.07852000	1.69509700	-2.03436200	H	-1.99612100	5.67264500	-1.48277700
C	5.31828200	2.84673100	-1.29256700	H	-3.08244400	5.73408900	-0.10260700
C	4.96671800	2.88164600	0.05042000	H	-3.75397600	5.54543600	-1.72317500
C	4.39293000	1.77255400	0.67955400	H	-4.92297000	3.77037100	-1.34060900
C	0.33798500	-2.78120500	2.60920700	H	-6.50072600	2.27734700	-1.43103200
C	-0.55959900	-3.64791600	1.94242700	H	-6.35129000	1.70161500	0.22942400
C	-1.69653400	-4.09155100	2.62497300	H	-6.27301300	0.54515300	-1.09320900
C	-1.95669300	-3.69292800	3.93061900	H	0.61522000	6.00414500	2.16670800
C	-1.08294200	-2.82022400	4.56759100	H	2.25545100	5.20663300	-1.69696800
C	0.06834000	-2.34864900	3.93006600	H	-5.47666200	-2.30768300	2.32393400
C	-2.92091100	5.26026500	-1.07694800	H	-5.05374300	-3.43644500	-1.77613200
C	-2.86544900	3.75108700	-0.92258100	C	4.24576100	-0.67888900	-2.30881600
C	-4.10370700	3.10809500	-1.08443800	H	3.38362300	-1.19830000	-1.87401200
C	-4.48738300	1.77888200	-0.82775600	C	4.04463000	1.85118000	2.15913700
C	-5.98719100	1.55375600	-0.79400300	H	3.81183900	0.83696300	2.49897300
C	-0.60589900	3.99838200	-0.30028600	C	-0.28043000	-4.13608500	0.52906000
C	-0.53075200	4.64632200	0.95611600	H	0.30569200	-3.35408100	0.02944900
C	0.54956200	5.49725700	1.20772300	C	0.97785600	-1.37040800	4.66218300
C	1.53877400	5.71048400	0.25591700	H	1.92885900	-1.32783600	4.12255200
C	1.47014800	5.04922600	-0.96475100	C	-3.93470800	-1.15518200	-2.74111000
C	0.41184800	4.18621900	-1.26543500	H	-3.11612500	-0.42648400	-2.68767700
C	-4.21304200	-0.50065300	-0.27096300	C	-4.48316400	0.20333400	2.18231000
C	-4.62250100	-0.80253100	1.04849400	H	-4.25368300	1.17603300	1.73564800
C	-5.16691800	-2.06320300	1.31141200	C	0.34533300	3.49607300	-2.62072700
C	-5.32943400	-3.00283200	0.30192100	H	-0.13345700	2.52118500	-2.45479200
C	-4.92624100	-2.69546900	-0.99294100	C	-1.57399800	4.42273000	2.04330600
C	-4.35467600	-1.45759200	-1.30691200	H	-2.45331000	3.96851600	1.57663500
H	6.41338200	-2.05646000	1.36160600	C	0.78722200	-0.41574300	-2.02042700
H	6.08066100	-0.48313300	2.08642100	C	-0.50847400	-0.80570700	-1.90630400
H	6.23896200	-0.61061400	0.33952200	H	-1.06370100	-1.53426400	-1.33379700
H	4.76009400	-3.13542100	2.26468200	C	0.15932600	-1.01077600	-3.27318700
H	1.77034800	-4.72018200	3.15842300	H	1.38539700	0.47673500	-1.92173300
H	2.69971400	-3.74047700	4.28347300	C	0.58521000	-2.38876600	-3.69955200

C	0.28886900	-2.88358100	-4.97945900	C	5.21065700	2.36574400	3.01487500
C	1.30857900	-3.22821800	-2.83822200	H	6.12584700	1.78959500	2.84552600
C	0.69447900	-4.15690400	-5.37754700	H	5.43808000	3.41620100	2.80326900
C	1.72476400	-4.49633800	-3.23499900	H	4.95826900	2.29748300	4.07869400
C	1.41558700	-4.97223200	-4.50907000	C	2.79406400	2.71030400	2.38338000
H	-0.26100100	-2.26821000	-5.68402600	H	2.95556500	3.73969500	2.04887500
H	1.56645900	-2.86634500	-1.84647500	H	1.93519800	2.32294900	1.82442200
H	0.44813100	-4.50815900	-6.37639100	H	2.52521800	2.73473600	3.44546400
H	2.29889000	-5.11128300	-2.54694300	C	-1.05510400	3.42961000	3.09256600
H	1.73722700	-5.96208600	-4.82070600	H	-0.78434300	2.47388900	2.63204900
H	-2.84088100	-4.05674500	4.44739200	H	-0.16286800	3.82096100	3.59351400
H	5.77649100	3.71314000	-1.76212600	H	-1.81588700	3.23626500	3.85726300
H	2.36519800	6.38421000	0.46624300	C	-2.03152300	5.72232600	2.71932100
H	-5.76703700	-3.97309500	0.52130000	H	-1.23442100	6.17365600	3.32007400
C	-1.54701400	-4.36287800	-0.30061000	H	-2.35813500	6.47037600	1.98984600
H	-2.23351200	-3.51294100	-0.24772800	H	-2.86897700	5.52072300	3.39590000
H	-1.27488000	-4.52752200	-1.34804200	C	-0.53389300	4.25979400	-3.62365900
H	-2.09729900	-5.25096400	0.03050600	H	-0.53165600	3.75305300	-4.59543900
C	0.57741700	-5.41105600	0.52083500	H	-1.57095500	4.33073300	-3.28946200
H	1.56020500	-5.24713700	0.96902000	H	-0.15169800	5.27576200	-3.77555700
H	0.07920300	-6.21399600	1.07637400	C	1.72169500	3.23726800	-3.23966100
H	0.73023300	-5.75738300	-0.50689200	H	2.18966700	4.16490900	-3.58851100
C	1.28535100	-1.79533700	6.10454500	H	2.41171200	2.76284600	-2.53589100
H	0.39826100	-1.73966000	6.74481500	H	1.61942900	2.58753000	-4.11489600
H	1.66545700	-2.82052700	6.15706200	C	-3.41107300	-2.38753400	-3.48706900
H	2.03937400	-1.13145900	6.54105000	H	-2.63422100	-2.91213800	-2.92530500
C	0.38015700	0.04336800	4.63878200	H	-4.21137200	-3.10273200	-3.70828800
H	0.21172300	0.38412300	3.61211300	H	-2.98226600	-2.08712400	-4.44807600
H	-0.58385800	0.06908600	5.15864100	C	-5.06686700	-0.51062400	-3.55769500
H	1.04932000	0.75864300	5.13033900	H	-5.95079800	-1.15874300	-3.57630400
C	5.43072600	-1.65752500	-2.27361700	H	-5.36496400	0.45970500	-3.15584500
H	6.34953100	-1.16990700	-2.62001900	H	-4.74490900	-0.35390600	-4.59342400
H	5.61163500	-2.05180500	-1.27168400	C	-3.31452600	-0.16740700	3.10390900
H	5.23268700	-2.50945200	-2.93326800	H	-3.47504900	-1.14262700	3.57365300
C	3.90119800	-0.35799700	-3.76813400	H	-2.37076600	-0.23017100	2.55119300
H	3.12199600	0.40512500	-3.84674300	H	-3.19472700	0.57833800	3.89793700
H	4.77610300	-0.00497000	-4.32621300	C	-5.77664300	0.36482500	2.99307400
H	3.53993400	-1.26131800	-4.26850500	H	-6.63377300	0.59358300	2.35176400

H	-6.01938300	-0.54203800	3.55755600
H	-5.66890700	1.17807200	3.71908500
C	-0.26175800	-0.07662000	-4.39480400
H	0.51790100	0.01475100	-5.16097400
H	-1.17691500	-0.41947600	-4.89245800
H	-0.46463400	0.92058900	-3.99827800

TS-3_1a2b

Mg	-0.35261600	-1.30667400	1.04506800
Mg	1.50159200	1.14017200	-0.85741400
N	-0.95338700	-3.33717500	0.97484300
N	-0.95262700	-1.10873900	3.05853800
N	3.10458500	0.69941900	-2.16418000
N	1.90152300	3.21783500	-0.93055200
C	-1.83206400	-5.44264800	1.94439000
C	-1.56684300	-3.94980200	1.98971700
C	-1.95133500	-3.32611400	3.19103000
C	-1.62495600	-2.06309500	3.71283400
C	-2.03646700	-1.85828500	5.15917100
C	-0.58253100	-4.14503700	-0.14954200
C	-1.44720600	-4.23194300	-1.26991800
C	-1.05995900	-5.03936500	-2.34516500
C	0.14816400	-5.72817700	-2.34024900
C	0.99451400	-5.61861100	-1.24477200
C	0.64698400	-4.84374600	-0.13396200
C	-0.55506500	0.03734600	3.82058400
C	-1.28198000	1.24492200	3.70021300
C	-0.89287000	2.34278800	4.47395900
C	0.18817000	2.26648100	5.34382700
C	0.91242400	1.08406300	5.43506200
C	0.56372700	-0.04247600	4.68449100
C	4.92720000	1.27530400	-3.74518200
C	3.79638100	1.65045900	-2.80447100
C	3.61481600	3.03385200	-2.64285800
C	2.82853200	3.75504900	-1.72524900
C	3.16550100	5.23123600	-1.63448300
C	3.56779100	-0.64601000	-2.32810400
C	4.70321700	-1.09493100	-1.61162800

C	5.15096700	-2.40332800	-1.81685000
C	4.50398800	-3.25881200	-2.69984000
C	3.37401400	-2.81765400	-3.37838800
C	2.88426800	-1.51919200	-3.20721000
C	1.23501700	4.09320400	-0.01309400
C	1.82070800	4.36892700	1.24416400
C	1.14711700	5.21791600	2.12762500
C	-0.06314800	5.80447900	1.78196000
C	-0.62995200	5.52868300	0.54241000
C	-0.01030100	4.66824200	-0.37035600
H	-2.67336800	-5.70524300	2.58951800
H	-0.95142900	-5.97706400	2.31947000
H	-2.02461200	-5.81023700	0.93627900
H	-2.49316500	-3.96787100	3.87659100
H	-2.27694100	-0.81784000	5.38150400
H	-1.21880100	-2.14787300	5.82829300
H	-2.89719100	-2.48536000	5.40191100
H	-1.71602900	-5.12711500	-3.20582700
H	1.94113900	-6.15231600	-1.24526300
H	-1.44627100	3.27320000	4.39421100
H	1.76612700	1.03312000	6.10551400
H	4.73645700	0.34174200	-4.27627500
H	5.85706100	1.13910800	-3.18239400
H	5.09673900	2.07258100	-4.47215000
H	4.27498500	3.64633700	-3.24654000
H	3.56817300	5.59410000	-2.58281100
H	3.93952600	5.37837000	-0.87228000
H	2.31193900	5.84585400	-1.34785700
H	6.02469400	-2.75742400	-1.27636500
H	2.86260800	-3.49639100	-4.05330300
H	1.58518500	5.42919500	3.09946900
H	-1.57827900	5.98793900	0.28074200
C	-2.78146600	-3.49631800	-1.31465400
H	-2.66666300	-2.59253300	-0.70416200
C	1.59734500	-4.77176900	1.05284100
H	1.05598500	-4.30681200	1.88294100
C	-2.49488200	1.34677000	2.78805400
H	-2.33657800	0.63749100	1.96534000

C	1.40781800	-1.30535100	4.79688100	H	0.84612700	-1.73590700	6.87237400
H	0.83399000	-2.13201000	4.36700100	H	2.23597800	-2.66013500	6.27712400
C	-0.66069700	4.39764200	-1.72254300	C	2.69357000	-1.16894600	3.96956500
H	-0.32878600	3.40222300	-2.04331100	H	2.46655600	-0.96079600	2.91881800
C	3.15644500	3.76791100	1.65838100	H	3.31369300	-0.34685300	4.34346600
H	3.60644200	3.31570900	0.76881200	H	3.28709200	-2.08909600	4.01455400
C	1.66160100	-1.05172900	-3.98408700	C	-3.93020200	-4.31419000	-0.70258300
H	1.13991200	-0.32764200	-3.34363200	H	-4.04229100	-5.27538300	-1.21783100
C	5.42919800	-0.20586700	-0.61030900	H	-3.77578600	-4.51315500	0.35975900
H	5.11709200	0.82729100	-0.79072000	H	-4.87382300	-3.76680500	-0.80251500
C	-1.25150400	-0.37685900	-1.36746400	C	-3.17837600	-3.05047500	-2.72706600
C	-1.07176100	0.94284900	-1.10404900	H	-2.35923700	-2.53961400	-3.24066300
H	-1.17800300	1.59293400	-0.24767800	H	-3.49078800	-3.89687800	-3.34956200
C	-2.15113800	0.58399200	-2.13577800	H	-4.02457700	-2.35938000	-2.67174300
H	-0.69458900	-1.22448600	-1.73515400	C	2.05999700	-6.15703900	1.52575000
C	-3.60285900	0.65624700	-1.75808100	H	1.21452900	-6.82332700	1.72437100
C	-4.55061000	1.20715200	-2.60324200	H	2.69980200	-6.64765600	0.78420700
C	-4.05635100	0.13709200	-0.51222800	H	2.64472000	-6.06621100	2.44764400
C	-5.92618100	1.26730500	-2.26167600	C	2.80573700	-3.88217900	0.73511400
C	-5.38114100	0.16809800	-0.15249100	H	3.38421500	-4.28422000	-0.10232800
C	-6.35921900	0.73699000	-1.00812900	H	2.49686000	-2.86946600	0.45359700
H	-4.25746900	1.60730600	-3.56917300	H	3.47016800	-3.80533100	1.60316300
H	-3.33044800	-0.31811500	0.15536500	C	5.01431800	-0.56029700	0.82454100
H	-5.69625600	-0.25460900	0.79868200	H	3.93119300	-0.46981100	0.95666700
H	0.46872000	3.12805500	5.94396900	H	5.29288300	-1.59134800	1.06857800
H	0.42748600	-6.34647800	-3.18923800	H	5.50261500	0.10280700	1.54755900
H	4.87402600	-4.26896200	-2.85409100	C	6.95650600	-0.25640000	-0.75164100
H	-0.56630200	6.47308700	2.47536700	H	7.36234000	-1.23125500	-0.46021000
C	-2.68019500	2.73511100	2.17005100	H	7.27963000	-0.05865400	-1.77870800
H	-1.75565900	3.11728400	1.72783200	H	7.42028900	0.49245200	-0.10060100
H	-3.44801300	2.69075200	1.39107400	C	2.03820300	-0.31218400	-5.27764000
H	-3.01854900	3.46873600	2.91051700	H	1.13553900	-0.01937900	-5.82588500
C	-3.78769200	0.92179800	3.50187400	H	2.61401900	0.59409700	-5.07923400
H	-3.75561400	-0.12234500	3.82183600	H	2.63211500	-0.95966300	-5.93289000
H	-3.96113400	1.54442200	4.38716300	C	0.67775600	-2.17986800	-4.30622200
H	-4.64640600	1.04242600	2.83279800	H	1.07086900	-2.85203900	-5.07744600
C	1.74248100	-1.68275500	6.24621100	H	0.43937400	-2.78735000	-3.42836100
H	2.42596400	-0.96270200	6.70916200	H	-0.25370200	-1.75978500	-4.69938300

C	-2.19214900	4.37848200	-1.65996500	C	4.38839500	2.87636900	0.00449700
H	-2.56573600	3.72093000	-0.87108000	C	3.20576300	3.54682400	-0.35033500
H	-2.60742600	5.37861700	-1.49228700	C	3.38057800	5.03278700	-0.60428200
H	-2.60032500	4.02242100	-2.61082900	C	4.20404700	-0.81406900	0.23954100
C	-0.20899600	5.39841800	-2.79886700	C	4.30511300	-1.42672400	1.51411600
H	-0.43880300	6.42634400	-2.49509500	C	4.77174200	-2.74350600	1.58477400
H	0.86239300	5.33446400	-2.99888400	C	5.11216600	-3.45547000	0.44002200
H	-0.73293200	5.20302300	-3.74132800	C	4.99529500	-2.84879200	-0.80377200
C	2.96080400	2.65289100	2.69336400	C	4.55718000	-1.52681400	-0.92939000
H	2.49768500	3.03779000	3.60709000	C	0.97881200	3.77915100	-1.08934100
H	2.30772100	1.86021400	2.31279400	C	-0.03724900	4.29615700	-0.25233000
H	3.92221200	2.20120400	2.96297800	C	-1.01974300	5.11374000	-0.81997800
C	4.14033100	4.82210200	2.18531300	C	-1.01576500	5.41386500	-2.17665300
H	4.27034200	5.64791000	1.47870400	C	-0.02877500	4.87777800	-2.99525500
H	3.80582600	5.25112400	3.13610400	C	0.97683900	4.05588000	-2.47810400
H	5.12177900	4.36883000	2.36249100	C	-2.95870300	-4.78190400	-1.98193300
C	-1.83749100	0.87416800	-3.59282500	C	-2.85599900	-3.36282200	-1.45490800
H	-2.39703000	0.21458900	-4.26747400	C	-4.09456300	-2.75694000	-1.18578700
H	-2.08048900	1.90876000	-3.86387600	C	-4.43099100	-1.40805400	-0.96547100
H	-0.77222900	0.73076900	-3.78558600	C	-5.92409900	-1.13804000	-1.00053700
C	-6.89360600	1.83594800	-3.13063400	C	-0.53076500	-3.48714400	-1.83961100
H	-6.56604900	2.24009700	-4.08578600	C	-0.24540000	-3.49065100	-3.22606100
C	-8.22222400	1.87904400	-2.77618700	C	0.85246100	-4.22525500	-3.68342500
H	-8.95115200	2.31868700	-3.45164700	C	1.65725800	-4.94367100	-2.80737300
C	-7.73467700	0.79358800	-0.67091000	C	1.37952500	-4.91870800	-1.44614000
H	-8.05704400	0.38673200	0.28488300	C	0.29513700	-4.19688100	-0.93680400
C	-8.64831100	1.35273200	-1.53463700	C	-4.02145900	0.92462800	-0.68344100
H	-9.70043400	1.39149700	-1.26613100	C	-3.85735900	1.74599700	-1.82869500
				C	-4.25667600	3.08305400	-1.76447500
				C	-4.81232400	3.61704900	-0.60772300
				C	-4.98582600	2.80294900	0.50268100
				C	-4.60645600	1.45521700	0.49301600

TS-3_1a2c

Mg	1.67133700	0.91629300	-0.17124600	H	6.71663400	1.98387300	0.58696500
Mg	-1.45552800	-0.79571500	-0.61864200	H	6.49616300	0.99871300	-0.85897400
N	3.73781500	0.53776500	0.13713300	H	6.35172800	0.24753100	0.72434900
N	2.01487200	2.96450700	-0.52939600	H	5.25988500	3.51641500	0.08449900
N	-1.66568200	-2.76281200	-1.34785900	H	2.48610900	5.60566900	-0.35621800
N	-3.55233500	-0.42754100	-0.75215600	H	3.59305400	5.21313300	-1.66373700
C	6.13875200	1.15854400	0.16507700				
C	4.66162400	1.50185400	0.12573900				

H	4.22513400	5.41917000	-0.02937000	C	-1.06897700	0.91351500	5.27559100
H	4.86547700	-3.22227600	2.55505600	C	0.90842100	1.57026300	4.08410900
H	5.25953200	-3.40772100	-1.69754500	C	-0.82522100	1.90239300	6.22584700
H	-1.80282900	5.52091600	-0.18840400	C	1.16340000	2.55265600	5.03959700
H	-0.03850600	5.10267600	-4.05837000	C	0.29492500	2.72579800	6.11617900
H	-2.08844300	-5.38933600	-1.73276300	H	-1.93651100	0.26919500	5.38273900
H	-3.03756500	-4.76579700	-3.07478100	H	1.58377200	1.44667700	3.24071300
H	-3.85861700	-5.26681200	-1.59669200	H	-1.51316400	2.02700600	7.05818000
H	-4.94963100	-3.41383100	-1.30512900	H	2.04494000	3.18087700	4.94196200
H	-6.37869300	-1.45637800	-0.05625900	H	0.48923600	3.49210100	6.86155300
H	-6.39544700	-1.72012300	-1.79634100	C	-1.11477800	-1.60085000	3.66279200
H	-6.15645800	-0.08344900	-1.14866300	C	-0.60243100	-2.23732600	4.80398000
H	1.07787200	-4.23799300	-4.74667600	C	-2.20940100	-2.18729300	3.01987400
H	2.01518400	-5.47410000	-0.76288500	C	-1.16898300	-3.41606300	5.28291700
H	-4.13229700	3.71777200	-2.63596500	C	-2.78541800	-3.36306400	3.49979000
H	-5.43499500	3.21701600	1.40188100	C	-2.26643800	-3.98393100	4.63469600
C	3.95582300	-0.67627800	2.79331000	H	0.24177200	-1.79469100	5.32530300
H	3.23701400	0.10258400	2.51430800	H	-2.61630100	-1.70697600	2.13252300
C	4.48160400	-0.89320100	-2.31119200	H	-0.75309200	-3.89175500	6.16741200
H	4.31421700	0.17998300	-2.17341700	H	-3.64140100	-3.79086000	2.98485000
C	-0.04738100	4.01942200	1.24403500	H	-2.71259600	-4.90019500	5.01169100
H	0.42728500	3.04114900	1.39767200	H	-1.78435300	6.05741400	-2.59620000
C	2.01628000	3.46056700	-3.41952800	H	5.46753900	-4.47941100	0.51913500
H	2.85247700	3.10120200	-2.81226100	H	2.49939200	-5.51861000	-3.18358700
C	-4.89329900	0.62143700	1.73565200	H	-5.11682100	4.65974000	-0.57648100
H	-4.57179300	-0.40514600	1.53270500	C	-1.45650600	3.94801800	1.84069900
C	-3.33984500	1.17460200	-3.14181200	H	-2.12424200	3.31322700	1.25021200
H	-2.67323800	0.33720400	-2.89888700	H	-1.40706500	3.55070500	2.85914400
C	-0.00186700	-4.23459000	0.55464600	H	-1.92021900	4.93915700	1.90454100
H	-0.62883100	-3.36613800	0.78778600	C	0.79059000	5.04611600	2.02192700
C	-1.08723100	-2.70975200	-4.22632800	H	1.84251900	5.02279500	1.72735100
H	-2.00336300	-2.39439900	-3.71738400	H	0.41130700	6.06053800	1.85216800
C	0.42415700	-0.41851300	1.93074300	H	0.73802900	4.83941900	3.09588700
C	-0.80673900	0.10377600	1.70759000	C	2.58047800	4.47696600	-4.42113200
H	-1.20677600	1.06067100	1.40928600	H	1.82814300	4.79191500	-5.15240600
C	-0.48462900	-0.33108900	3.14911800	H	2.95389700	5.37762500	-3.92335000
H	1.04822900	-1.23023300	1.59322700	H	3.40877800	4.03248200	-4.98338500
C	-0.20359000	0.72611300	4.18646500	C	1.44089900	2.24476700	-4.15998100

H	1.06995500	1.49126900	-3.45688700	H	-4.33764700	0.48091100	3.82983600
H	0.60302100	2.53852200	-4.80148600	C	-6.39611500	0.59479600	2.06489400
H	2.20325500	1.77615700	-4.79261300	H	-6.74573400	1.58243200	2.38528400
C	5.17510500	0.02705900	3.41192200	H	-7.00520100	0.29473600	1.20859000
H	5.96789300	-0.69613400	3.63597700	H	-6.59316400	-0.10300300	2.88632700
H	5.59071500	0.79182900	2.75290500	C	-2.53463200	2.17350500	-3.97571800
H	4.89270100	0.51635100	4.35076400	H	-3.17064300	2.96039400	-4.39691900
C	3.29392600	-1.56141800	3.85603400	H	-1.74817700	2.65347700	-3.38782500
H	2.46251300	-2.14325000	3.45018300	H	-2.06655400	1.65751000	-4.82050100
H	4.00705200	-2.26228300	4.30464200	C	-4.49408900	0.59856300	-3.97815100
H	2.90508900	-0.93516000	4.66527900	H	-5.02561800	-0.19497000	-3.44732700
C	5.78572900	-1.05627000	-3.10491200	H	-5.21866700	1.38329000	-4.22419800
H	6.65313400	-0.69681600	-2.54229800	H	-4.11727700	0.18063900	-4.91858200
H	5.97326000	-2.10321700	-3.36699800				
H	5.73140400	-0.49244500	-4.04261600				
C	3.29523600	-1.44708600	-3.10943100				
H	3.39370800	-2.52516700	-3.26931400	Mg	1.64985400	-1.34144200	-0.44594600
H	2.34772500	-1.28691000	-2.58408600	Mg	-0.61493700	0.06922200	1.49084300
H	3.22687300	-0.96192400	-4.08965300	N	3.74014300	-1.50319400	-0.51504200
C	-0.35507300	-1.43822700	-4.67822300	N	1.44074900	-3.15339500	-1.49515200
H	-0.10920900	-0.79754900	-3.82482000	N	-0.38417900	1.91954200	2.41836500
H	0.58323600	-1.68555300	-5.18691500	N	-1.99624300	-0.56103500	2.92386100
H	-0.97288600	-0.85883700	-5.37369200	C	5.90270500	-2.65146200	-0.82510900
C	-1.50096400	-3.54795700	-5.44386000	C	4.38737100	-2.62395400	-0.84304400
H	-0.64111000	-3.80894400	-6.07042900	C	3.76140700	-3.81822600	-1.24510100
H	-1.98895500	-4.48224900	-5.14907800	C	2.41837700	-4.05916900	-1.58166300
H	-2.19936700	-2.98444200	-6.07205700	C	2.10562700	-5.45197000	-2.09144400
C	-0.80408100	-5.48544100	0.94718800	C	4.53529900	-0.37840600	-0.14028300
H	-0.98766500	-5.49305600	2.02643200	C	4.85465600	0.60326600	-1.09795700
H	-1.77408000	-5.52511800	0.44570600	C	5.66022200	1.68000600	-0.72054400
H	-0.25152100	-6.39604800	0.68728500	C	6.15551100	1.81536900	0.57827000
C	1.26042500	-4.14530700	1.41779900	C	5.79144000	0.84931000	1.51853300
H	1.84816500	-5.06933900	1.37867800	C	4.98204200	-0.24111100	1.18796700
H	1.92027900	-3.33249400	1.10028500	C	0.18221600	-3.48443300	-2.08111500
H	0.98172900	-3.98530300	2.46428100	C	-0.00826400	-3.33278300	-3.46992100
C	-4.12125400	1.11770100	2.96527800	C	-1.26505900	-3.61163600	-4.01378700
H	-3.04219500	1.10587600	2.80576500	C	-2.33796800	-4.03362600	-3.22705700
H	-4.41006300	2.14148100	3.22743700	C	-2.11962200	-4.18968500	-1.85656800
				C	-0.87909300	-3.92765400	-1.26886900

C	-0.62754800	3.59611000	4.20438100	H	-5.20061600	-3.45244700	1.34157400
C	-0.95631300	2.25865100	3.57349900	C	4.34815100	0.48655600	-2.51076100
C	-1.86752500	1.45168400	4.27996300	H	4.70972400	1.31548000	-3.12533900
C	-2.36273900	0.17090700	3.98104500	H	4.66381900	-0.45051000	-2.98232900
C	-3.38438000	-0.38263200	4.95420400	H	3.25159700	0.49893100	-2.54405900
C	0.47981800	2.86836500	1.79147500	C	4.59961100	-1.25323400	2.23448200
C	1.86931500	2.80487800	2.01424400	H	3.51226100	-1.38971300	2.27202300
C	2.70162600	3.70211400	1.34278400	H	5.02678000	-2.24234200	2.03270200
C	2.19650500	4.66026200	0.45941300	H	4.93900400	-0.93841200	3.22498000
C	0.81563900	4.71100600	0.26764100	C	7.07472700	2.95171100	0.94490600
C	-0.05749700	3.83429700	0.91930700	H	7.01238500	3.19198700	2.01063200
C	-2.57514100	-1.85999100	2.79847400	H	8.12111700	2.70060600	0.73009200
C	-1.96995700	-2.96321600	3.43347900	H	6.83861000	3.85873600	0.37986700
C	-2.57087800	-4.21913200	3.32520200	C	1.11942100	-2.88832800	-4.36505100
C	-3.74206300	-4.42006000	2.58948600	H	1.68154600	-2.06016100	-3.92323400
C	-4.29627300	-3.31944400	1.93312200	H	1.84450100	-3.69217700	-4.54220200
C	-3.73604000	-2.04151100	2.02353700	H	0.74042800	-2.56972200	-5.33992800
H	6.30251200	-1.92846900	-1.54435000	C	-0.66927000	-4.15875500	0.20156800
H	6.28067400	-3.64107100	-1.08644800	H	-1.59507700	-4.46961800	0.68883500
H	6.30546000	-2.36789900	0.15112400	H	0.09239500	-4.92618500	0.38475700
H	4.42930400	-4.65799200	-1.39629600	H	-0.32042800	-3.25044300	0.70993200
H	1.24605500	-5.87493300	-1.56287600	C	-3.69381400	-4.28724400	-3.83250500
H	2.96072100	-6.11725400	-1.96010000	H	-4.30820900	-3.37815400	-3.82713600
H	1.84155400	-5.44087200	-3.15333600	H	-3.61328700	-4.61723000	-4.87278500
H	5.91491800	2.42931400	-1.46826100	H	-4.24368500	-5.05322600	-3.27701100
H	6.15061600	0.94149200	2.54244500	C	-4.37828300	-0.87428900	1.32309500
H	-1.40786200	-3.48890300	-5.08618700	H	-3.67103200	-0.37153600	0.65266300
H	-2.93374300	-4.53133700	-1.22014600	H	-5.23769000	-1.19929700	0.73023100
H	0.44905100	3.68764500	4.37969900	H	-4.72449000	-0.11363300	2.03229200
H	-1.14673000	3.72169500	5.15581200	C	-0.69279700	-2.79212000	4.21150300
H	-0.90424600	4.42454000	3.54562200	H	-0.35119300	-3.74832200	4.61704100
H	-2.25427800	1.89020200	5.19205900	H	0.10425400	-2.38858100	3.57430700
H	-4.32019900	-0.62425300	4.44013000	H	-0.80513500	-2.09071400	5.04562700
H	-3.59963900	0.33386000	5.74836600	C	-4.39460200	-5.77673000	2.52561100
H	-3.03495200	-1.31396700	5.41067900	H	-3.65158100	-6.58010800	2.49938900
H	3.77448200	3.64268000	1.51187200	H	-5.02992200	-5.95324500	3.40261600
H	0.39678900	5.45240600	-0.41001000	H	-5.02935500	-5.87552100	1.64002000
H	-2.10617000	-5.06589100	3.82772000	C	-1.54261700	3.93827800	0.70966800

H	-1.77697300	4.63768500	-0.09542200
H	-1.97965200	2.97011800	0.44986000
H	-2.05838100	4.28187000	1.61443400
C	2.43998800	1.80881400	2.98652200
H	2.17345200	0.78272700	2.70694800
H	3.52947700	1.87437900	3.01495700
H	2.05682200	1.96580200	4.00168200
C	3.12159100	5.59771200	-0.27223700
H	3.85743500	6.04481800	0.40498300
H	3.68237200	5.07238600	-1.05482400
H	2.56947000	6.41125900	-0.75157000
C	0.06275500	0.68566200	-1.21810200
C	-1.13534600	0.02852900	-1.06344600
H	-1.45531100	-1.00237100	-1.01589800
C	-0.99134600	0.89899800	-2.29647200
H	0.62274300	1.43803000	-0.68039800
C	-0.76089400	0.25443500	-3.65539300
H	-1.71336600	0.05366600	-4.16007400
H	-0.17436200	0.90923900	-4.31186500
H	-0.23250400	-0.69364600	-3.54736900
C	-1.77589500	2.17833500	-2.41237700
C	-3.11273200	2.23405300	-2.07893300
C	-1.16365500	3.33825400	-2.96012300
C	-3.88334800	3.40960400	-2.26773100
H	-3.59305400	1.35284900	-1.65752700
C	-1.87741500	4.49636300	-3.15571600
H	-0.10877300	3.30077200	-3.22079300
C	-5.26071100	3.47515500	-1.93145300
C	-3.25475400	4.56928400	-2.82124600
H	-1.39239700	5.37616700	-3.57320500
C	-5.98238900	4.62880800	-2.13186100
H	-5.73830900	2.59310700	-1.51116700
C	-4.02578000	5.74407200	-3.01421400
C	-5.35942800	5.77509000	-2.67850100
H	-7.03641300	4.66386300	-1.86982700
H	-3.54353200	6.62337700	-3.43537400
H	-5.93958000	6.68085500	-2.83239200

TS-3_1b2c

Mg	0.69881700	1.38552300	-0.71485000
Mg	-0.78767700	-1.54801200	-0.48587400
N	2.32381500	2.31892500	-1.64293100
N	-0.49660700	3.10196200	-0.85242900
N	0.39684600	-3.27164200	-0.40323200
N	-2.46153200	-2.63848300	-1.11203600
C	3.57570400	4.22526600	-2.58770000
C	2.33169100	3.61759200	-1.96939400
C	1.24703600	4.49566100	-1.81186200
C	-0.06466600	4.25751200	-1.35805000
C	-1.02273300	5.42376700	-1.48780400
C	3.47483000	1.56277900	-2.02770600
C	4.55332400	1.39275800	-1.13988900
C	5.68792700	0.70316800	-1.57691700
C	5.78002300	0.16091300	-2.85999800
C	4.67803500	0.30329800	-3.70666200
C	3.52714100	0.99160800	-3.31509200
C	-1.87186100	3.02006300	-0.46511800
C	-2.30682300	3.48968100	0.78889400
C	-3.65647100	3.34155200	1.13330200
C	-4.58596400	2.76641600	0.27232400
C	-4.13419000	2.32692000	-0.97687100
C	-2.79939000	2.44173900	-1.36059000
C	0.95994200	-5.64019600	-0.78248900
C	-0.02355500	-4.48794500	-0.75045500
C	-1.34453300	-4.80064600	-1.12045200
C	-2.46127100	-3.96568600	-1.28774700
C	-3.73746100	-4.66385300	-1.71573100
C	1.77022600	-3.12794100	-0.03539300
C	2.71307700	-2.71954000	-0.99892500
C	4.04261300	-2.54458900	-0.61010200
C	4.46479000	-2.76358200	0.70379100
C	3.51207700	-3.17044200	1.63804900
C	2.17058800	-3.36426500	1.29473200
C	-3.67905200	-1.95930400	-1.42473800
C	-3.92152200	-1.53363500	-2.74505100
C	-5.14438100	-0.92824700	-3.04730400

C	-6.13161600	-0.72896000	-2.07969400	H	-0.33562900	4.03751600	1.49723300
C	-5.84780800	-1.12023500	-0.76927900	H	-1.57175800	5.27446400	1.74402700
C	-4.63657800	-1.72285900	-0.42062000	H	-1.53855700	3.84694800	2.77304400
H	4.45387300	4.05288400	-1.95812400	C	-2.36654800	2.00759000	-2.73523500
H	3.45589200	5.29982600	-2.73382700	H	-3.20823100	1.58774300	-3.29088600
H	3.79758100	3.76684300	-3.55688600	H	-1.95198100	2.84273800	-3.31188800
H	1.43255500	5.50968900	-2.14518500	H	-1.58352500	1.24060500	-2.68442100
H	-1.93729600	5.11904400	-2.00554500	C	-6.03300600	2.62400200	0.66389100
H	-0.56573300	6.24745400	-2.03843600	H	-6.22763900	3.06827500	1.64419000
H	-1.32845600	5.79468500	-0.50503600	H	-6.69349200	3.11246100	-0.06176400
H	6.52886300	0.59787700	-0.89342300	H	-6.32745700	1.56956900	0.70810400
H	4.71682100	-0.12304900	-4.70791100	C	-4.36730800	-2.13382000	1.00152800
H	-3.98391700	3.70327200	2.10684100	H	-3.46750500	-1.64051600	1.38820200
H	-4.83828400	1.87458500	-1.67094800	H	-5.20448400	-1.86714100	1.65220700
H	1.76887400	-5.43332800	-1.49084200	H	-4.19448800	-3.21201500	1.09250400
H	0.46918000	-6.56833200	-1.07950200	C	-2.88941600	-1.74688200	-3.81972400
H	1.43422000	-5.79212400	0.19090100	H	-3.21700300	-1.31275400	-4.76830500
H	-1.52225700	-5.84792600	-1.33316900	H	-1.93186300	-1.28702000	-3.54769000
H	-4.55172100	-4.45771100	-1.01412800	H	-2.68371800	-2.81008300	-3.98818800
H	-3.59272500	-5.74371600	-1.77317100	C	-7.46936400	-0.13839500	-2.44343500
H	-4.07656800	-4.30667500	-2.69325600	H	-7.39487300	0.51994800	-3.31433700
H	4.76320600	-2.21700500	-1.35548800	H	-8.19463700	-0.92345400	-2.69197000
H	3.81571900	-3.34756600	2.66829800	H	-7.89200300	0.44160500	-1.61739200
H	-5.33413500	-0.61673800	-4.07334400	C	1.18610000	-3.84589900	2.32367100
H	-6.59587800	-0.96512800	0.00649900	H	1.59816700	-3.76316200	3.33142900
C	4.49643600	1.95028900	0.25619800	H	0.25657300	-3.27268400	2.29543800
H	5.45548800	1.82799900	0.76674400	H	0.91111600	-4.89552700	2.16076600
H	4.23663100	3.01389800	0.26531400	C	2.30353400	-2.51052800	-2.43195600
H	3.73494600	1.43225700	0.85113600	H	1.51037000	-1.75719600	-2.51369500
C	2.36545700	1.13160700	-4.26192700	H	3.14978300	-2.16841300	-3.03153800
H	1.44695200	0.71960500	-3.82632600	H	1.90957300	-3.43016300	-2.88055200
H	2.15065400	2.17960800	-4.49908600	C	5.91101500	-2.59366600	1.08963100
H	2.56060600	0.60559400	-5.20041700	H	6.50093500	-3.47996400	0.82391000
C	7.03552100	-0.52843400	-3.32823900	H	6.36192300	-1.73927600	0.57556800
H	6.81192900	-1.34185200	-4.02557600	H	6.02292800	-2.43876800	2.16685300
H	7.70071900	0.17080400	-3.85037700	C	0.77450500	0.11107900	1.49602300
H	7.60046400	-0.94833800	-2.49061900	C	-0.58881500	0.23894000	1.61099800
C	-1.38482100	4.19267900	1.74737800	H	-1.35684700	0.90085700	1.23513300

C	0.21221200	0.35322800	2.90180700	C	5.07316100	-0.52676500	2.06274600
H	1.44963400	-0.68819800	1.22206100	C	5.36444100	-1.75186500	2.66610700
C	0.47074900	1.68994200	3.55233900	C	5.38727100	-2.94697000	1.94376800
C	-0.26635900	2.08537200	4.67901100	C	5.09165500	-2.89105700	0.58081200
C	1.47177300	2.54800700	3.08793300	C	4.79193400	-1.68886700	-0.06487700
C	-0.01442200	3.30146900	5.30943800	C	1.66956000	3.95659100	-0.91119900
C	1.73521600	3.76196300	3.72119900	C	1.38691600	4.88150300	0.11461400
C	0.98969600	4.14620500	4.83410000	C	0.26766400	5.70602000	-0.01049400
H	-1.03510600	1.42374600	5.06945200	C	-0.58352900	5.63853800	-1.11636200
H	2.05202100	2.24949300	2.21788500	C	-0.29608500	4.69627600	-2.10426100
H	-0.60025800	3.58842000	6.17908500	C	0.81108400	3.84724500	-2.01998600
H	2.52657300	4.40566700	3.34562700	C	-3.54003600	-3.77917700	-3.36415300
H	1.19115200	5.09185700	5.33002800	C	-3.56365200	-2.66127300	-2.34304000
C	0.10585300	-0.76937300	3.90362500	C	-4.78109200	-1.96437200	-2.21501500
C	1.16032200	-1.02780500	4.79085700	C	-5.14748700	-0.93808000	-1.32289700
C	-1.05642700	-1.53857600	4.01507000	C	-6.57659800	-0.44664000	-1.41477200
C	1.05752800	-2.03190000	5.75036300	C	-1.31180400	-3.22249400	-1.83437700
C	-1.16733300	-2.54089700	4.97885400	C	-0.30827900	-2.82134700	-2.73475800
C	-0.10857800	-2.79301300	5.84933300	C	0.81574800	-3.63559100	-2.90088600
H	2.06315100	-0.42537500	4.73024600	C	0.97941400	-4.82427000	-2.18907100
H	-1.88151200	-1.34049900	3.33450800	C	-0.01929600	-5.18551800	-1.28155000
H	1.88768400	-2.21866700	6.42702800	C	-1.15909000	-4.40475200	-1.08284400
H	-2.08340900	-3.12155800	5.05159800	C	-4.82624900	0.59943600	0.46699300
H	-0.19114500	-3.57311200	6.60134500	C	-4.65491900	1.96636100	0.17619200
Int-4							
Mg	2.44345800	1.18315500	-0.06392900	C	-5.09673600	2.91466300	1.10166900
Mg	-2.29752400	-0.77604800	-0.38207900	C	-5.69570700	2.55002000	2.30877800
N	4.44644300	0.73699000	0.05490100	C	-5.84087900	1.18807000	2.57974500
N	2.78648100	3.07621900	-0.78707200	C	-5.41687900	0.20375400	1.68357300
N	-2.46037600	-2.39666500	-1.63932000	H	7.16780400	0.90608400	0.64319500
N	-4.32211000	-0.38523700	-0.43352400	H	7.51518000	1.75447100	-0.87602800
C	6.84470400	1.04128600	-0.39411300	H	6.95755100	0.06735400	-0.88097800
C	5.40684900	1.51023000	-0.45216800	H	6.06574900	3.25111900	-1.44474500
C	5.18009100	2.76346600	-1.05499100	H	3.44560700	4.92372600	-2.72050900
C	3.98725000	3.49865400	-1.19179600	H	5.13326200	5.04603500	-2.17879800
C	4.10969700	4.85525600	-1.85280500	H	3.80763600	5.65589600	-1.17037100
C	4.80147000	-0.49551300	0.68097800	H	5.57351900	-1.77144400	3.73433600
				H	5.08890800	-3.81104300	-0.00122700
				H	0.05381100	6.42003600	0.78313400

H	-0.95206500	4.61477200	-2.96917300	H	-5.99336200	-1.37587700	3.02675500
H	-2.73264800	-3.62857900	-4.08785300	H	-6.24661000	-1.77055100	1.32259000
H	-4.48697700	-3.84379500	-3.90224700	C	-3.99626200	2.40071600	-1.10581500
H	-3.34693100	-4.74384200	-2.88403000	H	-4.05315200	3.48610000	-1.22318500
H	-5.56794300	-2.29164700	-2.88423600	H	-2.93474300	2.12429200	-1.12093900
H	-7.11376000	-0.61657700	-0.47646400	H	-4.46022500	1.93742600	-1.98311500
H	-7.11764600	-0.94819000	-2.21867700	C	-6.19045500	3.59231000	3.27740100
H	-6.60262900	0.63322800	-1.59345900	H	-5.59173900	4.50662700	3.22235700
H	1.58209200	-3.33000500	-3.61123900	H	-7.23041100	3.87159100	3.06574700
H	0.09072300	-6.10339300	-0.70633500	H	-6.15613000	3.22892800	4.30900100
H	-4.96296700	3.97022900	0.87123600	C	-2.19411100	-4.81293200	-0.06856800
H	-6.29436500	0.87798000	3.51980000	H	-1.97015800	-5.80368000	0.33607800
C	5.02897400	0.73478700	2.88340100	H	-2.21990100	-4.11169300	0.77379100
H	5.29717400	0.53223600	3.92368400	H	-3.20397400	-4.83815200	-0.49056300
H	5.70959100	1.50315800	2.50119400	C	-0.43706100	-1.53050700	-3.49846900
H	4.02597200	1.17845900	2.87898500	H	-0.40657200	-0.67053100	-2.81708700
C	4.43987200	-1.67664200	-1.52858800	H	0.38188400	-1.41750200	-4.21450200
H	3.38096100	-1.43008600	-1.67772800	H	-1.38131200	-1.46759800	-4.04981900
H	5.02162800	-0.93751300	-2.08886700	C	2.20452200	-5.68216000	-2.36982700
H	4.61218400	-2.65802400	-1.97841600	H	2.74380100	-5.42232300	-3.28548100
C	5.73930400	-4.25035800	2.61192200	H	2.90144100	-5.56224300	-1.53123800
H	5.30242000	-5.10262000	2.08292200	H	1.94600700	-6.74505700	-2.42273400
H	6.82547900	-4.40442800	2.63691300	C	0.77463700	-0.02761100	0.30019900
H	5.38500600	-4.27844900	3.64703400	C	-0.71468100	0.43213600	0.27732300
C	2.26738300	4.97408100	1.33297100	H	-0.82133200	1.51720200	0.15613600
H	2.32293100	4.01529400	1.86107600	C	-0.02254700	0.08836900	1.58167600
H	3.29822200	5.24713700	1.08152700	H	0.88683400	-1.07089000	-0.01835600
H	1.88373000	5.72031200	2.03370700	C	-0.45154100	-1.16413100	2.30207700
C	1.07074000	2.82252300	-3.09174700	C	0.40632300	-2.26306700	2.44145000
H	0.37491500	2.94550900	-3.92619100	C	-1.72300900	-1.24586900	2.89579300
H	2.09044200	2.88598700	-3.48598700	C	0.01098500	-3.40325700	3.14188600
H	0.94129300	1.80438300	-2.70266800	C	-2.12046700	-2.38164900	3.60221700
C	-1.76332700	6.56700100	-1.24018300	C	-1.25313200	-3.46804000	3.72616700
H	-1.446662400	7.57784100	-1.52565100	H	1.39405100	-2.21678500	1.99106400
H	-2.46862300	6.21891600	-2.00028700	H	-2.39698000	-0.39373700	2.81734800
H	-2.30494200	6.65565800	-0.29261700	H	0.69487200	-4.24375400	3.23202900
C	-5.57912900	-1.25444600	2.02199100	H	-3.10528000	-2.41635000	4.06159900
H	-4.62136600	-1.78407200	1.98112100	H	-1.56044200	-4.35478400	4.27441100

C	0.31225000	1.21872000	2.54474600
H	-0.54089100	1.48330600	3.18325300
H	1.14841100	0.95940300	3.20981300
H	0.57816700	2.12331000	1.98166000

Int-4_1a2a

Mg	2.67034300	0.41377900	-0.24390300
N	-4.13317600	0.82973600	0.58586100
N	-3.38964400	-2.05326800	-0.13516700
Mg	-2.39463500	-0.31840800	0.42371300
N	3.39818700	2.19440800	-1.01481400
N	4.30701900	-0.65729400	-0.90276500
C	-6.53767000	0.99972600	1.16786100
C	-5.28804400	0.20826300	0.83499000
C	-5.48204800	-1.18694200	0.76380400
C	-4.67823000	-2.19574000	0.19804600
C	-5.38943000	-3.50209600	-0.08389900
C	-4.15143100	2.25395000	0.42529500
C	-3.63221800	3.09190700	1.44438300
C	-3.65722200	4.47586400	1.24935700
C	-4.16129700	5.03926100	0.08280500
C	-4.64445000	4.21037700	-0.91885200
C	-4.65289800	2.81909800	-0.77250800
C	-2.77334100	-3.12836400	-0.86235700
C	-2.14938300	-4.19884500	-0.17833600
C	-1.60158700	-5.24598100	-0.92700000
C	-1.64475500	-5.24996000	-2.31520600
C	-2.22397300	-4.17589800	-2.97848000
C	-2.78867800	-3.10575700	-2.27776800
C	4.75978500	3.55151700	-2.56714600
C	4.43839300	2.25579300	-1.85095700
C	5.27636000	1.16861200	-2.16587600
C	5.24532900	-0.16279800	-1.71185400
C	6.36331500	-1.06256800	-2.18836800
C	2.66472000	3.38870800	-0.72389800
C	1.61057500	3.79908900	-1.57102300
C	0.86926500	4.93107900	-1.21827900
C	1.16009400	5.65394500	-0.06864400

C	2.19892200	5.24153900	0.75874000
C	2.96126100	4.10791600	0.46101700
C	4.38853700	-2.02193600	-0.47873800
C	3.73532700	-3.02922300	-1.22538100
C	3.71649100	-4.33157000	-0.71760200
C	4.33578700	-4.64782100	0.48588100
C	5.00220200	-3.65566200	1.19547300
C	5.04782900	-2.33767700	0.73157300
H	-6.30987900	1.97288700	1.60434700
H	-7.16678200	0.43334500	1.85924700
H	-7.12749100	1.17382900	0.26178300
H	-6.47966100	-1.51002100	1.03888900
H	-5.53871500	-3.62327300	-1.16207800
H	-6.36714000	-3.52843700	0.39950900
H	-4.80476100	-4.36340600	0.24330200
H	-3.26910500	5.12846100	2.02419000
H	-5.02480700	4.64890200	-1.83799700
H	-1.13178200	-6.07593400	-0.40533400
H	-2.24362900	-4.16715500	-4.06555600
H	4.56878300	4.42642300	-1.94328400
H	4.12465500	3.64800200	-3.45536300
H	5.79949300	3.56790500	-2.89972600
H	6.08328400	1.39978400	-2.85138400
H	6.93290300	-1.45197600	-1.33854500
H	7.04723800	-0.53102400	-2.85164600
H	5.96434400	-1.93311200	-2.71804400
H	0.04857100	5.24978700	-1.85527800
H	2.41466800	5.80733700	1.65989800
H	3.20525200	-5.11166100	-1.27562800
H	5.49659200	-3.90855600	2.13007100
C	-3.06662300	2.51411400	2.73454200
H	-2.48919200	1.62477900	2.45173400
C	-5.16422800	1.97405400	-1.93195900
H	-5.22995600	0.93520000	-1.59511600
C	-2.02487400	-4.24884000	1.33704100
H	-2.48985400	-3.34502800	1.74349800
C	-3.38491600	-1.95149800	-3.07054300
H	-3.76816000	-1.21846300	-2.35298600

C	5.78914900	-1.27903200	1.53619400	H	-5.35779000	-2.85898700	-3.35800000
H	5.85886100	-0.38149600	0.91301900	H	-4.99439000	-1.53655300	-4.47640600
C	3.05301000	-2.72527600	-2.55151600	C	-2.30956400	-1.25993100	-3.92175600
H	3.35776000	-1.71749900	-2.85333100	H	-1.47968400	-0.90458000	-3.30290800
C	4.09125700	3.67683200	1.38937100	H	-1.89310900	-1.94409600	-4.66917600
H	4.17845500	2.58594000	1.30271500	H	-2.72945200	-0.40161000	-4.45640600
C	1.24931800	3.02918300	-2.83325800	C	-4.16715000	2.07224600	3.71145700
H	2.06054000	2.32179200	-3.03427700	H	-4.80073000	2.92231500	3.98994200
C	-0.46210100	0.42875500	0.80900400	H	-4.80726600	1.29609900	3.28690400
C	0.91737200	-0.29419500	0.70086500	H	-3.72163700	1.67197200	4.62895800
C	0.39276200	0.20254000	2.03750700	C	-2.09469700	3.45341000	3.45429500
H	-0.39324500	1.48073800	0.50107000	H	-1.31255000	3.82248400	2.78467100
C	-0.00653600	-0.78653600	3.10407200	H	-2.60892900	4.31653000	3.89310100
H	0.79231500	-1.37976000	0.60789000	H	-1.61153300	2.91844900	4.27780900
C	0.97698300	-1.54527900	3.75855000	C	-6.56220800	2.39834800	-2.40576500
C	-1.32555400	-0.92924200	3.55169400	H	-7.28239000	2.42784100	-1.58265500
C	0.65948900	-2.39905300	4.81107600	H	-6.54933500	3.39282000	-2.86494200
C	-1.65721800	-1.78968200	4.60074100	H	-6.93710800	1.69759100	-3.15969700
C	-0.66331300	-2.52699500	5.23967900	C	-4.17597300	2.01609700	-3.10646800
H	2.00789800	-1.46401400	3.42527300	H	-4.06054100	3.03751000	-3.48604200
H	-2.10877200	-0.32290100	3.10058200	H	-3.18539700	1.66097600	-2.80826900
H	1.44552000	-2.97260000	5.29652800	H	-4.52905000	1.39056100	-3.93407600
H	-2.69165600	-1.87048400	4.92586700	C	-0.03292300	2.20868700	-2.63031900
H	-0.91392700	-3.19194100	6.06196300	H	0.06436600	1.50444300	-1.79720600
H	-1.22180900	-6.07906100	-2.87623700	H	-0.88180400	2.86471500	-2.40872000
H	-4.16903600	6.11844300	-0.04481500	H	-0.27279400	1.64039600	-3.53632900
H	0.57534600	6.53340700	0.18671900	C	1.11700100	3.93859600	-4.06260700
H	4.30522000	-5.66532400	0.86602200	H	0.25696900	4.61168300	-3.97901700
C	-0.54935600	-4.24319800	1.75828600	H	2.00773900	4.55819100	-4.20755700
H	-0.01732500	-3.38505400	1.34058000	H	0.97041700	3.33649100	-4.96589200
H	-0.46324200	-4.18912400	2.84694500	C	5.44396200	4.26946800	0.96222700
H	-0.03705800	-5.15151200	1.42116500	H	6.23130300	3.96753700	1.66213500
C	-2.73854700	-5.46051500	1.95574500	H	5.74169800	3.93639500	-0.03431500
H	-3.80655100	-5.48362700	1.71889800	H	5.40119600	5.36463200	0.95700600
H	-2.30146500	-6.40247000	1.60580500	C	3.83090500	4.00560200	2.86400400
H	-2.63984600	-5.43649800	3.04625700	H	3.89808100	5.08179300	3.05913400
C	-4.56292200	-2.39504100	-3.94978400	H	2.84678100	3.66174800	3.19298200
H	-4.24676600	-3.12146400	-4.70653500	H	4.58709000	3.52170000	3.49099400

C	5.01229100	-0.89689700	2.80382400	C	-2.75713200	4.25920400	0.63198000
H	4.00897900	-0.53062500	2.56155000	C	-3.49709700	-1.48926000	-2.27677500
H	4.89486400	-1.75981000	3.46886600	C	-3.92104500	-2.74900500	-1.79271100
H	5.53418700	-0.11126800	3.36176100	C	-3.40794000	-3.90209400	-2.39360100
C	7.22087000	-1.70494900	1.88890900	C	-2.51798200	-3.82923300	-3.45912900
H	7.23499900	-2.55774000	2.57620600	C	-2.14384500	-2.58639200	-3.95522300
H	7.78834500	-1.99007700	0.99728400	C	-2.62644600	-1.40358500	-3.38673800
H	7.75246900	-0.88228900	2.37951500	C	6.23031100	2.91265500	-0.50826900
C	1.52462100	-2.72183700	-2.40920500	C	5.35648300	1.68963900	-0.31068900
H	1.15102900	-3.70259400	-2.09774200	C	6.03292400	0.46006900	-0.39209100
H	1.18968400	-1.99505100	-1.66233400	C	5.54935800	-0.86212100	-0.35769700
H	1.04846900	-2.47332300	-3.36413100	C	6.59025800	-1.93598200	-0.59927200
C	3.48883400	-3.68578600	-3.66693900	C	3.50608000	3.16185500	-0.11492300
H	4.57794500	-3.71496900	-3.77619700	C	3.21817300	3.81342800	-1.33738500
H	3.14779000	-4.70948100	-3.47862700	C	2.68987900	5.10683400	-1.30066400
H	3.06064600	-3.37215000	-4.62522500	C	2.45176800	5.75486600	-0.09451400
C	1.09508000	1.40690600	2.64988200	C	2.72603800	5.10141500	1.10101100
H	0.45325300	1.93672200	3.36431100	C	3.24704900	3.80354500	1.12016400
H	2.00706000	1.11612600	3.18949900	C	3.91842600	-2.58181600	-0.16144000
H	1.36841700	2.12071700	1.86368200	C	3.67182500	-3.26670400	-1.37346000
				C	3.30679100	-4.61550400	-1.31940500
				C	3.19298400	-5.28395300	-0.10683100
				C	3.42192800	-4.59668600	1.08002700

Int-4_1a2b

Mg	2.73954400	0.20697600	-0.05725200	C	3.77534500	-3.24410300	1.08196600
N	-3.86230500	2.09470800	0.24136900	H	-5.76461600	3.82058400	1.00944800
N	-3.89631700	-0.29005500	-1.60070900	H	-6.92251800	3.34041900	-0.25419000
Mg	-2.57452900	0.53296700	-0.23617500	H	-5.53599200	4.35990100	-0.64832500
N	4.03784800	1.83118000	-0.12563800	H	-6.56231600	1.73436900	-1.69984700
N	4.26996700	-1.19345400	-0.17843400	H	-5.34967000	-0.46767100	-3.92742500
C	-5.86751800	3.51561400	-0.03343000	H	-6.81182200	0.23097800	-3.19940600
C	-5.04150500	2.28551900	-0.35166900	H	-6.23242700	-1.37330900	-2.71419500
C	-5.59225000	1.42891900	-1.32541600	H	-2.99358000	3.69596500	4.47089400
C	-5.06981500	0.26678000	-1.91854000	H	-1.75966400	6.09048000	1.15520100
C	-5.91987300	-0.36440900	-2.99919200	H	-3.71084500	-4.87569800	-2.01753400
C	-3.37436100	3.09322300	1.14185600	H	-1.46567200	-2.53054600	-4.80312700
C	-3.45255300	2.87065400	2.53796300	H	5.91242900	3.75381100	0.10984000
C	-2.93537500	3.84478900	3.39730500	H	6.17468900	3.24664700	-1.55060300
C	-2.33677700	4.99997800	2.90674300	H	7.27462800	2.68185700	-0.28952300

H	7.10296500	0.54396500	-0.54345200	H	-2.12774600	-4.73850000	-3.90847500
H	6.38755100	-2.84410100	-0.02929400	H	-1.93797500	5.74153300	3.59374000
H	7.58987500	-1.57231700	-0.35326500	H	2.05143100	6.76514700	-0.08573100
H	6.59017900	-2.21784900	-1.65851100	H	2.92069600	-6.33569900	-0.08409300
H	2.46456400	5.61696800	-2.23323400	C	-4.21204300	-3.32713500	0.64564100
H	2.53042600	5.60986000	2.04028600	H	-3.40766300	-2.64340200	0.93127300
H	3.11306700	-5.15157800	-2.24490800	H	-4.92510700	-3.37554500	1.47628000
H	3.31385900	-5.12043100	2.02480400	H	-3.76559500	-4.31979300	0.52940600
C	-4.09178600	1.60724900	3.10123800	C	-6.07680800	-3.81764100	-0.97624700
H	-3.83840000	0.78627400	2.41637600	H	-6.57840100	-3.53593900	-1.90800900
C	-2.59866000	4.49601100	-0.86384400	H	-5.74345600	-4.85557500	-1.08225000
H	-3.27344500	3.81046300	-1.38577500	H	-6.82036300	-3.79657100	-0.17211800
C	-4.90976500	-2.87713900	-0.64256400	C	-2.53542400	0.02686400	-5.47870000
H	-5.33165000	-1.88433000	-0.45600300	H	-1.93934500	-0.68363800	-6.06177700
C	-2.21833100	-0.06321300	-3.97907000	H	-3.59048200	-0.18174000	-5.68296800
H	-2.80833200	0.71022200	-3.47562200	H	-2.30998500	1.03046300	-5.85599300
C	4.02049100	-2.52457800	2.40198700	C	-0.73727400	0.24031900	-3.72064700
H	3.85557700	-1.45519100	2.21986800	H	-0.49953500	0.22701400	-2.65129600
C	3.76284900	-2.57216500	-2.72469200	H	-0.09573800	-0.49994200	-4.21101700
H	4.24987700	-1.60386500	-2.56861600	H	-0.47232300	1.22643300	-4.11715500
C	3.55375000	3.13005000	2.45178000	C	-5.62545400	1.69737900	3.14394800
H	3.51414700	2.04718000	2.28238800	H	-5.94501400	2.54547600	3.76028700
C	3.44010700	3.12926900	-2.67904700	H	-6.05569200	1.81758600	2.14767900
H	4.09688800	2.26998900	-2.51012800	H	-6.04937600	0.78605100	3.58064800
C	-0.57551800	0.52441100	0.45398900	C	-3.56470300	1.22490200	4.48822500
C	0.68293200	-0.28757700	0.05342100	H	-2.47106500	1.22904300	4.52690400
C	0.09042500	-0.42439900	1.44375200	H	-3.92984800	1.90720200	5.26422300
H	-0.32896500	1.56084600	0.72624700	H	-3.91372600	0.22243000	4.75591000
C	-0.57230100	-1.69871400	1.88972200	C	-2.97844000	5.92095700	-1.28830700
H	0.41154600	-1.13596000	-0.58510100	H	-3.97784400	6.19804500	-0.93744900
C	-0.29640200	-2.92511700	1.31459700	H	-2.27405400	6.66434800	-0.89974200
C	-1.44828900	-1.68067600	3.01612600	H	-2.96613900	6.00564700	-2.38035200
C	-0.85136200	-4.13480000	1.81192600	C	-1.17076500	4.16168300	-1.31944100
C	-1.99238500	-2.83043700	3.53324200	H	-0.43695400	4.80940600	-0.82892400
C	-1.70959000	-4.09474600	2.95391300	H	-0.90074600	3.12852200	-1.07925100
H	0.38640100	-2.97991100	0.47133100	H	-1.07068000	4.29708800	-2.40259900
H	-1.67933500	-0.72688900	3.48118900	C	2.11530800	2.58683700	-3.23348000
H	-2.65049100	-2.78521200	4.39870500	H	1.62835300	1.90917600	-2.52477700

H	1.41484800	3.40480500	-3.43493900	C	-2.24757700	-5.30567300	3.45766900
H	2.27790800	2.04214600	-4.17040700	H	-2.89989400	-5.26730300	4.32743500
C	4.12565600	4.03241000	-3.71253200	C	-1.95447300	-6.50982900	2.85917100
H	3.48025300	4.86071000	-4.02422100	H	-2.37302900	-7.43186100	3.25378200
H	5.05338300	4.46448800	-3.32390500				
H	4.36976200	3.45823800	-4.61277200				
C	4.97379400	3.45137000	2.94514600	Int-4_1a2c			
H	5.15639600	2.97882800	3.91682600	Mg	2.60241500	0.52031800	-0.06027800
H	5.73871000	3.09144200	2.25304200	Mg	-2.58622300	-0.50939200	-0.05581000
H	5.10649400	4.53252700	3.06693200	N	4.45061700	-0.37788100	0.37086100
C	2.53578800	3.47097400	3.54737900	N	3.42774600	2.03484900	-1.19815300
H	2.64908100	4.50248200	3.89935500	N	-3.38815300	-2.03003000	-1.20330800
H	1.50522500	3.34430400	3.20416600	N	-4.44135300	0.37034300	0.37056000
H	2.68862300	2.81986500	4.41433000	C	6.91604400	-0.57704600	0.12742800
C	3.05863200	-2.96215700	3.51295800	C	5.60113300	0.16195900	-0.02936100
H	2.01661200	-2.93179900	3.18340700	C	5.72101500	1.40836800	-0.67900800
H	3.27363000	-3.97850900	3.86119500	C	4.74958800	2.23132500	-1.27284000
H	3.16517900	-2.30124000	4.37998700	C	5.28913900	3.37327200	-2.10724700
C	5.47425000	-2.67916500	2.87666500	C	4.45060800	-1.69400800	0.94208200
H	5.72459400	-3.73689300	3.01773500	C	4.64652700	-1.88214500	2.33401400
H	6.18611400	-2.25543700	2.16400500	C	4.58661200	-3.18273000	2.84744200
H	5.61977800	-2.16913800	3.83561800	C	4.33419300	-4.27879800	2.03214700
C	2.36135000	-2.29626800	-3.28881400	C	4.14589500	-4.08349400	0.67041300
H	1.81759900	-3.23146000	-3.46219200	C	4.20413900	-2.80715100	0.10284000
H	1.76227800	-1.69405700	-2.59901700	C	2.58075600	2.83889000	-2.03149700
H	2.42575500	-1.76169400	-4.24359200	C	1.97771200	4.01245100	-1.52430000
C	4.60726900	-3.35274200	-3.74121200	C	1.12957300	4.74603800	-2.36099200
H	5.60058200	-3.59072100	-3.34776500	C	0.86688300	4.34234400	-3.66365100
H	4.13074800	-4.29709400	-4.02566500	C	1.46127900	3.18467000	-4.15164300
H	4.73623400	-2.76639100	-4.65750200	C	2.32463200	2.42215800	-3.36042200
C	0.86045800	0.23416600	2.58273900	C	-5.24934300	-3.36037600	-2.14840100
H	0.21268000	0.53378800	3.41628700	C	-4.70737400	-2.23176700	-1.29310100
H	1.63350300	-0.42655100	2.99872100	C	-5.68931700	-1.41875700	-0.70023900
H	1.33731700	1.15199900	2.21966700	C	-5.58438900	-0.17440800	-0.04584800
C	-0.56781500	-5.39226300	1.21836200	C	-6.90457500	0.55832400	0.09625500
H	0.08953500	-5.42114800	0.35325300	C	-2.52903100	-2.81068300	-2.04194300
C	-1.10658900	-6.55184200	1.72806700	C	-2.38539900	-2.46691800	-3.40751800
H	-0.88033700	-7.50756800	1.26228700	C	-1.53016400	-3.23148400	-4.20644000
				C	-0.83289900	-4.31339400	-3.68507800

C	-0.96658300	-4.63050700	-2.33813600	C	-5.01568500	0.69898000	3.28228100
C	-1.79754300	-3.88997500	-1.49129700	H	-4.82034000	-0.23357800	2.74061300
C	-4.45398800	1.68015600	0.95510000	C	-3.99251600	2.68019200	-1.37150300
C	-4.18878200	2.80195200	0.13315600	H	-4.01839300	1.61472800	-1.62585800
C	-4.14225200	4.07209600	0.71524300	C	-1.91721200	-4.26257100	-0.01941600
C	-4.35929800	4.25317400	2.07460400	H	-2.08729600	-3.33495100	0.54144800
C	-4.62906800	3.14879000	2.87298900	C	-3.09725900	-1.26642300	-4.01716400
C	-4.67878700	1.85371700	2.34490300	H	-3.87521400	-0.94452400	-3.31818400
H	7.67871300	0.09026700	0.53923700	C	0.71499200	-0.31419700	0.39559500
H	7.27068000	-0.89476400	-0.85926700	C	-0.69861400	0.32509900	0.39693800
H	6.83542600	-1.46169000	0.75750800	H	-0.64821300	1.40483300	0.20811400
H	6.74501600	1.71592700	-0.86194300	C	0.00359500	-0.00891900	1.70305600
H	4.72551500	4.29353400	-1.94170600	H	0.66401400	-1.39018000	0.18600600
H	5.19835900	3.14035600	-3.17370700	C	0.47111600	1.13851000	2.56671900
H	6.34278200	3.55453000	-1.88841900	C	-0.46059500	2.02099500	3.13476900
H	4.74616600	-3.33775400	3.91110500	C	1.82330700	1.35585700	2.85430200
H	3.95821300	-4.94051000	0.02854100	C	-0.05707500	3.06516600	3.96219100
H	0.66800500	5.65359000	-1.98012700	C	2.23944800	2.40906200	3.67271300
H	1.25426600	2.86704200	-5.17047600	C	1.29749500	3.26611100	4.23570300
H	-4.57751700	-4.21944700	-2.17485400	H	-1.51487700	1.89238900	2.90532600
H	-5.37867500	-3.02048400	-3.18188200	H	2.56482800	0.65218600	2.47822000
H	-6.22787300	-3.67980300	-1.78290600	H	-0.80264000	3.73308800	4.38608200
H	-6.70942900	-1.73251300	-0.89641500	H	3.29762400	2.54658700	3.88095900
H	-7.66965200	-0.11250800	0.49773400	H	1.61333400	4.08268400	4.87950100
H	-7.24813600	0.87608000	-0.89434200	C	-0.48221100	-1.17576100	2.53004500
H	-6.83531300	1.44260100	0.72822900	C	0.42977700	-2.10956900	3.04411400
H	-1.40975500	-2.97422800	-5.25553200	C	-1.83618200	-1.35911700	2.83552800
H	-0.40844900	-5.46919200	-1.93448500	C	0.00584200	-3.17212500	3.83788200
H	-3.93984700	4.93550100	0.08656200	C	-2.27287900	-2.43032700	3.61917800
H	-4.81063000	3.29292200	3.93470000	C	-1.34981300	-3.34050500	4.12811500
C	4.96317700	-0.73742600	3.29011500	H	1.48370400	-2.00391600	2.80152300
H	4.77537900	0.20070000	2.75551600	H	-2.56039900	-0.61820900	2.49906600
C	4.03961700	-2.67012500	-1.40423700	H	0.73621900	-3.87965000	4.22224400
H	4.07661900	-1.60268900	-1.64826100	H	-3.33106500	-2.54188800	3.84170700
C	2.22445800	4.51089400	-0.10838200	H	-1.68098300	-4.17166400	4.74495600
H	2.87460700	3.78412500	0.39025200	H	0.20441100	4.92718900	-4.29610500
C	2.94461600	1.15977200	-3.94341900	H	4.29065900	-5.27872400	2.45518100
H	3.70450900	0.80598300	-3.23940300	H	-0.18068400	-4.90386200	-4.32300700

H	-4.32390700	5.24851300	2.50906000	H	-3.05890200	-1.81182300	-6.14054300
C	0.91896000	4.59715500	0.69163200	H	-4.45467600	-2.45009400	-5.26697800
H	0.40060300	3.63535200	0.72049400	H	-4.37597200	-0.73077100	-5.68933400
H	1.12174300	4.89335700	1.72492500	C	-3.12419200	-5.17489200	0.24994800
H	0.23404700	5.33529100	0.25933200	H	-3.16755900	-5.44029600	1.31191600
C	2.94508900	5.86796800	-0.09235900	H	-4.06900800	-4.69205900	-0.00993000
H	3.90419700	5.83318000	-0.61808000	H	-3.04504700	-6.10362800	-0.32711900
H	2.33634400	6.64635700	-0.56603800	C	-0.64810200	-4.90488000	0.54924100
H	3.14026800	6.18242500	0.93878300	H	-0.49066000	-5.91592900	0.15553000
C	3.64666000	1.41049400	-5.28541200	H	0.24257300	-4.30909700	0.33145900
H	2.93592200	1.69265400	-6.06976600	H	-0.73527100	-4.98749300	1.63567800
H	4.39088200	2.20983700	-5.21228600	C	-4.15991300	0.70390500	4.55816500
H	4.15862700	0.50222800	-5.62173800	H	-3.08968200	0.74308900	4.34307900
C	1.89264900	0.05120700	-4.08776300	H	-4.40397400	1.55760800	5.19970900
H	1.40975400	-0.17683900	-3.13223000	H	-4.35028600	-0.20170700	5.14381600
H	1.10573900	0.35184000	-4.78770700	C	-6.50199600	0.70398700	3.67935000
H	2.34632500	-0.86992800	-4.47001100	H	-6.75453100	1.62321500	4.22002200
C	6.44237100	-0.74274700	3.71264000	H	-7.16426900	0.63534900	2.81387800
H	6.68920600	-1.66833500	4.24502500	H	-6.72318500	-0.14188700	4.33988200
H	7.11898000	-0.65984200	2.85942400	C	-2.63842500	3.23859200	-1.82699300
H	6.64899400	0.09488300	4.38820200	H	-2.55949000	4.31247300	-1.62687000
C	4.08329700	-0.75949600	4.54910300	H	-1.80661800	2.74543300	-1.31706100
H	3.01795500	-0.80349800	4.31186800	H	-2.50588400	3.09565400	-2.90439600
H	4.32071300	-1.61744300	5.18750600	C	-5.14134400	3.35512900	-2.13711300
H	4.25575700	0.14209400	5.14624100	H	-6.11481800	2.95311300	-1.84073400
C	5.19829900	-3.34631300	-2.15368200	H	-5.15938100	4.43491200	-1.95151900
H	6.16876100	-2.95616600	-1.83276100	H	-5.02501400	3.20585700	-3.21635100
H	5.20361900	-4.42828000	-1.98055600				
H	5.10555900	-3.18360200	-3.23323000				
C	2.69117400	-3.21600000	-1.89010900				
H	2.59913700	-4.28936500	-1.69280800	Int-4_1b2b			
H	1.85254400	-2.71531400	-1.39862000	Mg	2.78953600	-0.96693600	-0.11108600
H	2.58268800	-3.07178200	-2.96994500	Mg	-2.14324200	-0.00477700	0.86780300
C	-2.12262300	-0.09216700	-4.18939400	N	4.67792500	-0.16912300	-0.26636100
H	-1.64895400	0.18358900	-3.24189300	N	3.49105000	-2.87278500	0.20794300
H	-1.32281700	-0.35306000	-4.89076700	N	-2.40876900	1.26034800	2.46806200
H	-2.64035700	0.79007200	-4.58262000	N	-4.04865400	-0.77542300	1.01392000
C	-3.78468200	-1.58861200	-5.35103500	C	7.12579600	-0.13395800	-0.03522600
			C	5.79098400	-0.84533100	0.01896700	
			C	5.82111700	-2.20749000	0.37779900	

C	4.77663200	-3.14910400	0.44350700	H	5.05711300	3.12348600	-3.44709100
C	5.17344200	-4.56259900	0.81363800	H	4.60514600	4.33432700	0.63690700
C	4.77621400	1.19920600	-0.66050400	H	1.17359000	-6.29456000	-1.80128100
C	4.91235900	1.52799300	-2.02344700	H	0.28385700	-5.41482800	2.29575100
C	4.95232500	2.87398700	-2.39261200	H	-2.52411700	1.88979400	5.14470200
C	4.85420000	3.90338400	-1.45376700	H	-4.29369400	1.73747000	5.21387700
C	4.69726000	3.55017000	-0.11261300	H	-3.52891100	3.05600600	4.30735800
C	4.64952800	2.21700100	0.30303400	H	-5.21314500	0.23313500	3.98384500
C	2.54402500	-3.94096400	0.23133100	H	-6.81170300	-1.09591500	1.42006900
C	2.30783400	-4.69605600	-0.93531200	H	-6.58807500	-1.22073200	3.17443200
C	1.35148300	-5.71227600	-0.89869400	H	-5.93453600	-2.46111400	2.08213000
C	0.61811500	-5.99956100	0.25513300	H	1.62840300	2.65385900	4.16065000
C	0.85231300	-5.21953200	1.38813900	H	-0.77867900	5.54072800	2.10477000
C	1.79729400	-4.18979700	1.39719000	H	-4.19902900	-4.70017600	-1.36747200
C	-3.45055400	1.99646000	4.57165200	H	-6.38853400	-1.35052600	-2.89613700
C	-3.42099700	1.13186400	3.32900000	C	4.99282800	0.44869600	-3.07012000
C	-4.49461700	0.23328100	3.17277300	H	5.12240200	0.88083500	-4.06588800
C	-4.81218500	-0.61655600	2.09571600	H	5.82282600	-0.24311800	-2.89034700
C	-6.11011900	-1.38789600	2.20788300	H	4.08029700	-0.15925800	-3.08740000
C	-1.42247300	2.26236300	2.71793800	C	4.44247700	1.87808900	1.75520200
C	-0.23820700	1.92371700	3.39772100	H	3.45697600	1.42373000	1.91823400
C	0.72120700	2.91566600	3.61869800	H	5.18714400	1.16566900	2.12491400
C	0.54777400	4.22551300	3.16976000	H	4.49369000	2.77692100	2.37540400
C	-0.62495300	4.52822000	2.47423800	C	4.93531600	5.34731400	-1.87522900
C	-1.61195400	3.57110400	2.23202300	H	4.43367100	6.00298500	-1.15728700
C	-4.52503800	-1.58048800	-0.06282800	H	5.97754700	5.68241000	-1.94969900
C	-4.10205900	-2.91768700	-0.18083200	H	4.47440700	5.50509400	-2.85527500
C	-4.52779900	-3.66592100	-1.28125800	C	3.06429100	-4.40917300	-2.20554600
C	-5.35447100	-3.12804300	-2.26892000	H	2.91367700	-3.37564900	-2.53774900
C	-5.75043300	-1.79551800	-2.13423600	H	4.14540300	-4.53853000	-2.08362200
C	-5.35068500	-1.00873600	-1.05152800	H	2.73557400	-5.07066200	-3.01141700
H	7.32523400	0.24253800	-1.04372800	C	2.00367400	-3.35374100	2.63186500
H	7.94182100	-0.79753000	0.25489600	H	1.41421400	-3.73987700	3.46790600
H	7.12990500	0.73887400	0.62541900	H	3.05408800	-3.32478400	2.94043900
H	6.80515800	-2.59876300	0.60721500	H	1.69310000	-2.31497800	2.46197700
H	4.61330700	-4.90541300	1.68956300	C	-0.37848100	-7.12902100	0.27581500
H	6.24039600	-4.63015000	1.03130000	H	-0.96615100	-7.16245800	-0.64739800
H	4.93917600	-5.26262700	0.00545000	H	0.12258800	-8.10014300	0.37384400

H	-1.07350300	-7.03475000	1.11517200	H	-2.39617500	0.39455000	-2.45949300
C	-5.78328400	0.43015900	-0.95392300	C	-0.44015000	3.73128900	-2.12942800
H	-4.92359700	1.10902200	-0.93710700	H	1.11671900	2.54539200	-1.26867500
H	-6.41173600	0.70618100	-1.80491900	C	-3.73595200	2.54245000	-3.43401300
H	-6.35230500	0.63158400	-0.03976800	C	-1.73405200	3.75871700	-2.70831900
C	-3.19960700	-3.53100000	0.85603400	H	0.11200200	4.66411800	-2.03659600
H	-3.06686100	-4.60027000	0.67176000	C	-4.29037600	3.71747200	-3.88554500
H	-2.20448500	-3.06992400	0.84231200	H	-4.27250900	1.60296600	-3.54190700
H	-3.59593800	-3.40586200	1.86943000	C	-2.33618600	4.95421300	-3.17880000
C	-5.82542900	-3.96450000	-3.42993500	C	-3.58563800	4.93722800	-3.75351500
H	-5.10569600	-4.75151800	-3.67459400	H	-5.27319800	3.71254900	-4.34945900
H	-6.78089000	-4.45554900	-3.20578900	H	-1.78747900	5.88847500	-3.08161900
H	-5.97698900	-3.35611700	-4.32688800	H	-4.03398200	5.85959200	-4.11285500
C	-2.84714700	3.93143700	1.45048800				
H	-2.86239700	4.99938600	1.21783200				
H	-2.88712200	3.38736300	0.49974700				
H	-3.76779000	3.68781200	1.99092100	Mg	2.62163800	0.40339800	0.42157100
C	-0.00310900	0.51301700	3.86717800	Mg	-2.50295800	-0.57247400	0.39710200
H	0.08903400	-0.16952200	3.01252700	N	3.28724800	1.88408300	1.68385500
H	0.91951000	0.44461400	4.45052800	N	4.47945000	-0.47056300	0.26080100
H	-0.82513600	0.13960100	4.48712300	N	-4.30083100	0.42538400	0.25747900
C	1.60364400	5.27549700	3.39802200	N	-3.30410300	-2.07906300	1.55913400
H	2.26895400	5.00225700	4.22249400	C	4.82540800	2.87766900	3.32637500
H	2.22613100	5.41336400	2.50518600	C	4.48156400	1.83844800	2.28010500
H	1.15869000	6.24785100	3.63316900	C	5.47393300	0.87445300	2.01537400
C	0.92428500	-0.01248400	-0.13008400	C	5.49456300	-0.17068900	1.07135700
C	-0.46822900	-0.71399800	-0.17514200	C	6.76317800	-0.99425200	1.00753200
H	-0.38919700	-1.80032100	-0.30712800	C	2.40176100	2.95673900	2.01009200
C	0.07310700	0.02434400	-1.38210200	C	2.48360100	4.17520600	1.30783900
H	0.88480900	0.93643500	0.41863600	C	1.58635900	5.19681800	1.62568300
C	0.52634000	-0.79467800	-2.58348300	C	0.60625900	5.04521600	2.60904600
H	-0.31202500	-1.06373900	-3.23913900	C	0.52998600	3.81886200	3.27084900
H	1.25973300	-0.25368400	-3.19820300	C	1.40710800	2.76847500	2.98751400
H	0.97869600	-1.73658600	-2.24468700	C	4.63498100	-1.51254900	-0.70136000
C	-0.57997800	1.31740800	-1.80020100	C	5.17986900	-1.22540700	-1.96830600
C	-1.84955300	1.33149300	-2.35418500	C	5.25633200	-2.24764900	-2.91791400
C	0.11941000	2.55101700	-1.69904500	C	4.80559900	-3.54164500	-2.65234800
C	-2.45086200	2.52602000	-2.82915700	C	4.26969600	-3.79950100	-1.38901900
				C	4.16964900	-2.80949100	-0.40937500

Int-4_1b2c

C	-6.57993600	1.02587800	0.95849200	H	-2.36118700	-6.48095400	0.63574000
C	-5.34031200	0.16159300	1.04772600	C	0.74330300	-0.43118900	-0.04347400
C	-5.37982500	-0.89257400	1.98369000	C	-0.59221300	0.29419400	0.14387300
C	-4.46549000	-1.93871100	2.20470700	C	0.63705900	1.30976100	-1.94210100
C	-4.85111100	-2.95083200	3.26359200	C	0.00851000	0.12147200	-1.26243200
C	-4.38301500	1.51722900	-0.65812600	H	2.33654000	0.19364700	-2.65443900
C	-3.95261800	2.79751800	-0.25960700	C	1.86246900	1.17376400	-2.61790500
C	-3.99810500	3.84305400	-1.18600200	C	2.44789900	2.25619200	-3.27658200
C	-4.44546200	3.65443500	-2.49489000	C	1.82046400	3.50283700	-3.26680200
C	-4.85487600	2.37236700	-2.86652900	C	0.60553300	3.65292500	-2.59976200
C	-4.82604000	1.29655200	-1.97641000	C	0.01919900	2.56687700	-1.94859400
C	-2.54841800	-3.27311500	1.74903700	H	-0.93410700	2.68693100	-1.44183600
C	-1.41106700	-3.25996400	2.57902700	H	0.10820800	4.61947700	-2.58753000
C	-0.64901400	-4.42495800	2.70197300	H	2.27436900	4.34795900	-3.77751600
C	-0.97330500	-5.59897300	2.02073000	H	3.38826200	2.12381700	-3.80550600
C	-2.09549400	-5.58169100	1.18933800	C	-1.19806100	-2.05854800	-1.72342800
C	-2.89041400	-4.44331600	1.03835900	C	-0.73070500	-0.80654300	-2.17818600
H	4.83256800	3.88308800	2.89364300	C	-1.03092100	-0.46298400	-3.50808100
H	5.80365400	2.68463600	3.76922000	C	-1.75949200	-1.31576200	-4.33514700
H	4.07446300	2.89073200	4.12274600	C	-2.21302900	-2.54842400	-3.86799000
H	6.37522100	0.97216400	2.60880800	C	-1.92089200	-2.91508400	-2.55512400
H	6.54335300	-2.05561300	1.16166000	H	-0.91531000	-2.41330000	-0.73241900
H	7.48356100	-0.67246900	1.76115700	H	-2.23084000	-3.88456000	-2.17546500
H	7.23399800	-0.91714600	0.02256400	H	-2.77105600	-3.21660300	-4.51781700
H	1.65512700	6.13846400	1.08350500	H	-1.97166800	-1.01086400	-5.35716100
H	-0.23317300	3.67088900	4.03301900	H	-0.68991300	0.49019800	-3.89901600
H	5.67911200	-2.02178600	-3.89548900	C	-3.44602100	3.03866500	1.13763200
H	3.91306400	-4.80148700	-1.15669900	H	-4.18115000	2.75588800	1.89909700
H	-6.33849200	2.08247000	1.10926000	H	-2.54182000	2.45247100	1.33906100
H	-7.32651900	0.72657800	1.69572100	H	-3.19665200	4.09296200	1.28358200
H	-7.02752900	0.95129300	-0.03824300	C	-5.24874900	-0.07638800	-2.42673500
H	-6.27599300	-0.93141200	2.59165800	H	-5.68768300	-0.03812100	-3.42744600
H	-5.00215700	-3.94560400	2.83397200	H	-4.39393200	-0.76202300	-2.46978900
H	-5.76788100	-2.65536500	3.77629800	H	-5.98217200	-0.52591900	-1.74953800
H	-4.05095900	-3.05233500	4.00404600	C	-4.45645100	4.78933700	-3.48549100
H	-3.67425000	4.83377800	-0.87126800	H	-5.30167100	4.71052400	-4.17655000
H	-5.20546800	2.19925800	-3.88261800	H	-4.52113900	5.75932000	-2.98328100
H	0.22483600	-4.41023100	3.35111000	H	-3.54229900	4.79567700	-4.09218300

C	-1.01694500	-2.00836400	3.31612800
H	-1.85216000	-1.59257600	3.88980900
H	-0.19397900	-2.20730000	4.00832500
H	-0.68586800	-1.122790600	2.61858900
C	-4.08548900	-4.46971200	0.12207400
H	-4.09431800	-3.60475400	-0.54808300
H	-4.08906900	-5.37931300	-0.48517000
H	-5.03237500	-4.44173600	0.67417200
C	-0.15457400	-6.85185400	2.19180800
H	0.86647700	-6.62281600	2.51102100
H	-0.59231900	-7.51330000	2.95007800
H	-0.09648000	-7.42333000	1.26003500
C	3.57410400	-3.12638800	0.93652500
H	3.34908500	-4.19297000	1.02006400
H	4.24596400	-2.85449800	1.75789900
H	2.63750000	-2.57877900	1.09700900
C	5.67582300	0.15748600	-2.29861100
H	6.55995200	0.43117700	-1.71087700
H	5.94674900	0.23080100	-3.35552900
H	4.91801900	0.91798000	-2.08395000
C	4.86357500	-4.61747900	-3.70497500
H	3.92438000	-4.66971700	-4.26959000
H	5.66629300	-4.43155500	-4.42492600
H	5.02970200	-5.60415700	-3.26136100
C	3.50422100	4.37019400	0.21855700
H	3.47312400	5.39461600	-0.16226600
H	4.52381900	4.16773100	0.56289200
H	3.31625900	3.69743600	-0.62596000
C	1.28172200	1.45295700	3.70789300
H	1.00249700	0.65017500	3.01428400
H	2.22143600	1.15187700	4.18348100
H	0.51104200	1.50433700	4.48186100
C	-0.32154800	6.17921000	2.95959200
H	-0.58403800	6.77071400	2.07671000
H	-1.24943600	5.81375800	3.40952500
H	0.14191000	6.86426600	3.68076500
H	-0.45661600	1.32221400	0.50388200
H	0.66983800	-1.52285800	0.02302400

Int-5_1a2c

Mg	-2.90177400	-1.42085300	0.90652100
N	-2.52007100	-1.84979500	2.89665700
N	-4.49721800	-2.77438200	0.82549700
N	-0.69717100	4.59491900	-0.32193300
Mg	-0.29173000	2.59942900	-0.81641100
N	1.55300400	3.04687100	-1.68648400
C	-3.22966500	-2.39929200	5.18992700
C	-3.44924100	-2.39185600	3.69344700
C	-4.63589700	-2.98785800	3.24151700
C	-5.06805200	-3.26261000	1.92730600
C	-6.22889600	-4.23169600	1.83370100
C	-1.27904700	-1.43436300	3.47600100
C	-0.22286500	-2.36443400	3.62947000
C	1.02015600	-1.89434000	4.06530100
C	1.22250400	-0.55260200	4.36835800
C	0.16118800	0.34015400	4.26823800
C	-1.10117200	-0.07953100	3.83759900
C	-5.00857900	-3.21274100	-0.43979600
C	-4.52027200	-4.40738100	-1.01893300
C	-5.04584000	-4.82067100	-2.24764000
C	-6.03534500	-4.08917100	-2.89250500
C	-6.48976000	-2.90388800	-2.32567800
C	-5.98367500	-2.43492600	-1.10970300
C	-0.56227800	7.01445100	-0.83742500
C	-0.09729800	5.58134200	-0.99863800
C	1.01782000	5.41765000	-1.83687900
C	1.85556900	4.30175200	-2.03277400
C	3.20905000	4.63074400	-2.63164100
C	-1.61756800	4.97125200	0.71046500
C	-3.01292800	4.89580900	0.49016200
C	-3.87873200	5.22802800	1.53812400
C	-3.39804600	5.62135900	2.78046800
C	-2.02581200	5.70625800	2.98344800
C	-1.11717300	5.40112700	1.96608200
C	2.56934100	2.05746900	-1.91459200
C	2.56577500	1.32279800	-3.12655900

C	3.60853800	0.42040800	-3.35411000	H	7.49310900	-0.27761700	4.51149000
C	4.61880700	0.22349900	-2.41822500	C	7.14591800	-3.48988700	-1.85607100
C	4.58380200	0.91546300	-1.21520400	C	7.69289400	-3.10940300	-0.62543900
C	3.56760500	1.83741300	-0.94032500	C	5.31755000	-2.50567300	0.26611400
H	-2.37057400	-3.02123000	5.45714200	C	9.06043800	-3.33145500	-0.41253700
H	-4.10700000	-2.77947100	5.71532000	C	9.85259600	-3.91360300	-1.39943700
H	-3.00891200	-1.39164300	5.55477400	C	9.29511500	-4.28147900	-2.62360200
H	-5.26870600	-3.39477700	4.02157800	C	7.93652700	-4.06617900	-2.84827100
H	-6.85493000	-4.16820600	2.72651300	H	6.08350300	-3.33973200	-2.03383600
H	-5.84393000	-5.25630200	1.77694300	H	7.48948700	-4.34689700	-3.79841100
H	-6.84483700	-4.07008200	0.94866700	H	9.91382900	-4.73243100	-3.39459100
H	1.84328500	-2.59614100	4.17610900	H	10.90986400	-4.08094400	-1.21052000
H	0.31177900	1.38162200	4.53958800	H	9.50638200	-3.04271500	0.53534700
H	-4.67790400	-5.73777100	-2.70074900	H	4.50897800	-1.99749800	-0.23886000
H	-7.24975200	-2.32521300	-2.84244400	H	5.58820500	-4.26118400	1.72280600
H	-0.03686300	7.49611100	-0.00597800	C	-3.60518000	4.51916800	-0.85969600
H	-1.62986600	7.07935900	-0.62374900	H	-2.78427500	4.16354600	-1.49148900
H	-0.34027500	7.58702900	-1.74077000	C	0.37416300	5.55223800	2.24787000
H	1.37918800	6.33609500	-2.28542500	H	0.91004400	5.44392800	1.30038700
H	3.93621200	4.77088300	-1.82394900	C	3.56318000	2.55120400	0.40386200
H	3.16246700	5.56326300	-3.19780900	H	2.78617300	3.32230900	0.36896100
H	3.59369000	3.83867500	-3.27444900	C	1.46213400	1.49603200	-4.16588000
H	-4.95186200	5.18244000	1.37174600	H	0.52837600	1.64173800	-3.60679100
H	-1.65017300	6.02559300	3.95228900	C	-0.40803100	-3.85542500	3.37445200
H	3.62991800	-0.14434500	-4.28030900	H	-1.46329200	-4.02128100	3.13574500
H	5.36561100	0.74753500	-0.47877900	C	-2.25605100	0.90898500	3.78240500
C	5.76105000	-3.41791000	1.07095000	H	-3.17506000	0.32749700	3.64979900
C	7.43027100	-1.42914900	1.30022700	C	-3.43470500	-5.24560400	-0.35830300
H	6.55777600	-2.11103900	3.14320100	H	-3.24865900	-4.82464600	0.63509700
C	7.17710000	-1.35006100	2.67404800	C	-6.50454800	-1.12422300	-0.53453800
C	6.82004600	-2.52702200	0.46108700	H	-5.76839100	-0.77861900	0.20058900
C	7.69784600	-0.31234300	3.44454500	C	-1.81244600	1.15912900	-1.18123600
C	8.48031800	0.67638500	2.85032500	C	-1.79563800	-0.19680600	-1.88853600
C	8.73776600	0.61379500	1.48091400	C	-0.60337500	-1.08261200	-1.68140500
C	8.22130800	-0.42973100	0.71534400	H	-0.71892100	-2.12012400	-3.56596900
H	8.43710000	-0.47536300	-0.34864700	C	-0.18081400	-2.02890100	-2.62812600
H	9.34536000	1.37938900	1.00538600	H	1.21100000	-3.58262800	-3.14360000
H	8.88680400	1.48746800	3.44820400	C	0.91642400	-2.85777100	-2.38848300

C	1.62984700	-2.76335800	-1.19645000	H	-3.49911500	6.53634000	-1.72048400
H	2.47877800	-3.41487400	-1.00840200	H	-4.63197100	5.45078300	-2.53753700
C	1.23010900	-1.82492800	-0.24357200	C	3.20244900	1.57425700	1.53322800
H	1.76953700	-1.73289700	0.69521800	H	2.23479900	1.09293600	1.35917500
C	0.12819300	-1.00583000	-0.48012500	H	3.95263200	0.78070500	1.61899100
H	-0.17135400	-0.27403200	0.26813800	H	3.15496000	2.09329300	2.49668200
H	-1.80660400	1.60921600	-3.94090700	C	4.89487500	3.25005300	0.71295300
C	-2.38322800	0.71984800	-4.17987200	H	4.81323900	3.82983500	1.63900700
C	-2.47717400	-0.30534400	-3.22919900	H	5.70832600	2.53024000	0.85107800
C	-3.23716200	-1.43573000	-3.56734800	H	5.19078400	3.93445500	-0.08818600
C	-3.86905000	-1.53804600	-4.80538300	C	1.27207500	0.26160600	-5.05367400
C	-3.76223200	-0.50715700	-5.73875700	H	1.21828900	-0.65607200	-4.46392800
C	-3.01821900	0.62632700	-5.41866000	H	0.33935900	0.35396900	-5.61807600
H	-2.93025000	1.44140400	-6.13301700	H	2.08486900	0.15998900	-5.78266700
H	-4.25909500	-0.58450100	-6.70234700	C	1.65539300	2.72774000	-5.06624700
H	-4.45612700	-2.42357900	-5.03227600	H	1.60084400	3.66710000	-4.51322500
H	-3.34414500	-2.24223600	-2.84689600	H	2.62353400	2.68513400	-5.57863800
C	-2.68826100	0.01615100	-0.64803100	H	0.87486600	2.75289200	-5.83497500
H	-2.46926500	1.82022600	-1.77062900	C	0.41612000	-4.35202300	2.18012300
H	-3.72151000	0.17677500	-0.98970600	H	0.24415200	-5.42170500	2.01491600
H	-4.08777300	5.87134400	3.58213200	H	0.16299500	-3.81902200	1.26075900
H	5.42628100	-0.47409800	-2.62457400	H	1.48923500	-4.21354100	2.35531600
H	2.19789400	-0.20800700	4.70072800	C	-0.07423300	-4.68927700	4.62181800
H	-6.44573000	-4.43626700	-3.83707100	H	0.99102000	-4.62862400	4.87058100
C	0.89305700	4.45709500	3.19027700	H	-0.63426500	-4.35900300	5.50217200
H	0.36477600	4.48020400	4.15021500	H	-0.31092800	-5.74478300	4.44834700
H	0.76312900	3.45961400	2.76076800	C	-2.40752500	1.70317900	5.08707600
H	1.96085300	4.59717000	3.39288800	H	-3.30778200	2.32520100	5.04611500
C	0.71950600	6.93628800	2.81903400	H	-2.48745100	1.04385800	5.95777300
H	0.32134500	7.74559100	2.19952600	H	-1.55886400	2.37450900	5.25592300
H	0.31745600	7.06966600	3.82922900	C	-2.13239700	1.85577100	2.58328400
H	1.80601200	7.06029600	2.88277800	H	-1.22763200	2.46482600	2.67138400
C	-4.63515400	3.38842100	-0.74782100	H	-2.09301200	1.31480300	1.62998200
H	-4.96871000	3.08074800	-1.74448300	H	-2.98051600	2.54641400	2.54085100
H	-4.21150800	2.51327200	-0.24935100	C	-7.83795000	-1.30802300	0.20728500
H	-5.52331000	3.70757700	-0.19063100	H	-7.74670100	-1.99210800	1.05472100
C	-4.22868500	5.73724400	-1.55991400	H	-8.19660800	-0.34675000	0.59215800
H	-5.05219300	6.15217400	-0.96772200	H	-8.60537600	-1.70629800	-0.46643000

C	-6.64634600	-0.02986300	-1.60043900	C	-2.07839500	-3.59066600	-2.16553800
H	-5.73652000	0.07207400	-2.19820500	C	-1.27543200	-3.09817800	-3.23696600
H	-7.47721500	-0.23427300	-2.28493100	C	-1.29778800	-1.80271900	-3.79228900
H	-6.85477800	0.93275300	-1.12221000	C	-0.57786300	-1.63326800	-5.11306800
C	-3.85686700	-6.70968400	-0.16867700	C	-3.51165000	-3.22341200	-0.29107200
H	-3.09122200	-7.25686600	0.39199500	C	-3.21908100	-3.81967700	0.95060800
H	-4.80181000	-6.79477900	0.37668800	C	-4.27700200	-4.14291500	1.80761500
H	-3.98437900	-7.22044700	-1.12939100	C	-5.60853300	-3.88403500	1.48216200
C	-2.12121600	-5.16744000	-1.15015100	C	-5.87018100	-3.28136100	0.24909100
H	-1.33225100	-5.73959200	-0.65007200	C	-4.85071600	-2.95194600	-0.64632500
H	-2.24482800	-5.58015600	-2.15777900	C	-2.36326800	0.37011600	-3.81159400
H	-1.76965100	-4.13723600	-1.26150800	C	-2.24572300	1.62534200	-3.16151800

Int-5_1b2c

Mg	2.88992300	1.19734600	0.28707200	C	-3.41686100	2.73741500	-4.99002000
Mg	-1.21518900	-1.13620100	-1.22506100	C	-3.61450100	1.48645000	-5.56724200
N	2.72078100	3.26024400	0.26617100	C	-3.12986000	0.30058900	-5.00249200
N	4.90983300	1.23321300	0.72427100	H	3.13395900	5.99830700	-0.19758700
N	-2.47685200	-2.80543900	-1.17648400	H	4.38779200	6.08067400	1.05392900
N	-1.84640600	-0.75217400	-3.15137800	H	2.69734100	5.74919900	1.48003900
C	3.48257100	5.55845600	0.74110900	H	5.73846400	4.44939500	1.11364000
C	3.73254000	4.06967100	0.60604600	H	7.22458400	1.71915800	2.21073800
C	5.04470400	3.64991800	0.88331100	H	7.50202700	3.27140800	1.39624300
C	5.59680600	2.35601300	0.93650900	H	7.62388500	1.74039500	0.50537100
C	7.06917200	2.27655800	1.28149000	H	-0.21593500	5.52267200	-2.45678800
C	1.46170200	3.88220300	0.00103700	H	-1.46289600	4.65893700	1.55124500
C	1.19308200	4.42410400	-1.27032400	H	7.33808200	-2.30567300	-0.91898600
C	-0.02005300	5.08793000	-1.47802200	H	6.32989300	-2.33561500	3.24410200
C	-0.98048000	5.20963100	-0.47145200	H	-1.84541700	-5.60463300	-2.90098200
C	-0.71547800	4.60775100	0.76206100	H	-3.51689600	-5.12438200	-2.59141600
C	0.48728300	3.94519500	1.01672100	H	-2.46686200	-5.50871300	-1.23140800
C	5.59860300	-0.00925400	0.87793100	H	-0.76231300	-3.84762200	-3.83078500
C	6.21236500	-0.61560300	-0.23338600	H	-0.93112800	-2.34431000	-5.86509800
C	6.86125600	-1.84024700	-0.05815500	H	0.48657700	-1.82991200	-4.94483900
C	6.91606400	-2.48086200	1.18067900	H	-0.67767400	-0.61954300	-5.50173900
C	6.29792600	-1.85744300	2.26639800	H	-4.04400000	-4.60668600	2.76454400
C	5.63082100	-0.63672400	2.13797800	H	-6.89967300	-3.06182800	-0.02898300
C	-2.48856000	-5.04329000	-2.22012500	H	-2.62959300	3.72398400	-3.24500300

C	-2.16488300	0.14574900	2.18732700	H	-7.09396400	-5.27806900	2.20162800
C	-3.32858100	-0.42479400	2.23979600	C	-3.53276500	-0.99843300	-5.65448500
C	-2.87932500	0.27156400	4.68962600	H	-3.51237500	-1.83372000	-4.95039300
C	-3.10418200	0.67652400	3.25151100	H	-4.55061600	-0.91495700	-6.04814100
H	-0.94696100	-0.59984200	4.32602100	H	-2.88548600	-1.26581000	-6.49818600
C	-1.71141500	-0.39683300	5.07243000	C	-1.62890300	1.71558900	-1.79590200
C	-1.51853900	-0.81237500	6.38852600	H	-0.61033800	1.31403100	-1.76076300
C	-2.49842700	-0.57096100	7.34981600	H	-1.56801600	2.74756700	-1.44581200
C	-3.67003200	0.09001800	6.98157500	H	-2.23746500	1.18179000	-1.04564400
C	-3.85673000	0.50865800	5.66629400	C	-3.91778000	3.99677200	-5.64524800
H	-4.77093600	1.02743500	5.39039700	H	-3.11495600	4.51251400	-6.18755600
H	-4.44370600	0.27969000	7.72125300	H	-4.71214600	3.78387700	-6.36694700
H	-2.35148100	-0.89546700	8.37640500	H	-4.31356000	4.70381300	-4.90855500
H	-0.60004500	-1.32505500	6.66239900	C	2.19816300	4.31042800	-2.38602700
C	-4.66366700	2.22083700	1.99035200	H	3.09335400	4.91638000	-2.20259500
C	-3.74728700	2.02487700	3.02944300	H	2.54788700	3.27987100	-2.50654200
C	-3.41536600	3.12561300	3.83282000	H	1.76448400	4.63900800	-3.33443600
C	-3.97874000	4.37882800	3.60015800	C	0.74693400	3.32990300	2.36617400
C	-4.89279900	4.55783400	2.56126500	H	0.91858500	2.24888600	2.28755400
C	-5.23393400	3.47094600	1.75718000	H	1.63541400	3.75633900	2.84531100
H	-4.93315600	1.37961200	1.35599900	H	-0.10628500	3.48007100	3.03211300
H	-5.95139400	3.59345900	0.94983400	C	-2.25814300	5.97643300	-0.69448200
H	-5.33959800	5.53263700	2.38548600	H	-2.48810900	6.07589100	-1.75958400
H	-3.70692600	5.21714100	4.23665100	H	-3.10670800	5.48979000	-0.20416800
H	-2.71638900	2.99310900	4.65418300	H	-2.18517400	6.99082500	-0.28260900
H	-4.02358500	-1.17913900	1.89966200	C	6.17920000	0.04654100	-1.58436800
H	-1.17704700	0.22865100	1.75186100	H	6.58490200	1.06371500	-1.55343400
C	-1.80572000	-4.08431500	1.39253100	H	6.75930700	-0.52713100	-2.31181300
H	-1.13550500	-4.30847900	0.56045000	H	5.15617500	0.12363400	-1.96909200
H	-1.38945100	-3.20965700	1.90643400	C	4.95540600	-0.00842400	3.32872600
H	-1.76841500	-4.91949400	2.09778400	H	3.87419300	0.08614000	3.16976700
C	-5.18407000	-2.31549500	-1.96920900	H	5.10729400	-0.61356800	4.22663000
H	-4.53035400	-1.46598400	-2.18700400	H	5.32873300	1.00066900	3.53449600
H	-5.05655500	-3.02238300	-2.79865800	C	7.58595800	-3.82090300	1.33319400
H	-6.22314800	-1.97556900	-1.98709900	H	8.40049700	-3.94718600	0.61341700
C	-6.72780100	-4.26597300	2.41506000	H	7.99962900	-3.95166900	2.33801500
H	-6.40167900	-4.25197600	3.45928200	H	6.87160800	-4.63614500	1.16469200
H	-7.58003400	-3.58638100	2.31806100	C	0.42579000	-1.16537600	0.10074700

C	1.81482600	-1.69710700	-0.32531800	C	-7.41633500	-0.81017000	0.40265700
C	2.31279300	-1.34750400	-1.69485000	C	-3.32232000	3.35227200	-0.45826600
H	3.49879900	-3.11857200	-2.00481600	C	-2.64627600	4.25345600	0.39837900
C	3.18123500	-2.17196100	-2.42901000	C	-2.01506700	5.36771800	-0.16263300
H	4.32057800	-2.46302500	-4.22496900	C	-2.03483800	5.59974800	-1.53128600
C	3.64923300	-1.79688200	-3.68836600	C	-2.68793500	4.70333500	-2.36562000
C	3.27556300	-0.57976400	-4.25791600	C	-3.34313500	3.57941900	-1.85514600
H	3.64323600	-0.29055400	-5.23839900	C	-5.01730800	-2.12760400	0.08321500
C	2.42013000	0.26011500	-3.54537900	C	-4.97928200	-3.04031600	1.16861400
H	2.10201500	1.20712700	-3.97396800	C	-5.12647000	-4.40353000	0.89160400
C	1.95147300	-0.11863300	-2.28643200	C	-5.27314600	-4.87499100	-0.40852800
H	1.24837800	0.52329800	-1.75830700	C	-5.26399000	-3.97566300	-1.46436500
H	0.98577400	-4.05745700	-1.34796400	C	-5.14669000	-2.59873000	-1.24423000
C	1.62926800	-4.20417600	-0.48286700	C	4.20718800	-4.38927400	-1.04822400
C	2.16214300	-3.07587100	0.16508700	C	3.86467000	-3.08313100	-0.35673200
C	2.99451000	-3.29158500	1.26801300	C	4.19706500	-3.06932900	1.01518500
C	3.26878400	-4.58214500	1.72428600	C	4.35607600	-2.00122300	1.91770900
C	2.72771500	-5.68921500	1.07563300	C	5.20212500	-2.34766900	3.13019300
C	1.90816200	-5.49361200	-0.03766100	C	3.27626400	-2.16104900	-2.46858100
H	1.48051000	-6.34885700	-0.55566000	C	2.27072900	-2.87945600	-3.15900300
H	2.94194000	-6.69423500	1.42973500	C	2.31870300	-2.93656500	-4.55720500
H	3.91564300	-4.71909800	2.58744000	C	3.32493000	-2.31615800	-5.27957800
H	3.44360800	-2.43909200	1.76690200	C	4.30843100	-1.61268100	-4.59722300
C	1.69359900	-0.51559100	0.65415400	C	4.30653900	-1.51833000	-3.20313900
H	0.04712900	-1.86962500	0.85770600	C	4.38581800	0.27671700	2.57331500
H	1.86814400	-0.86756200	1.68075800	C	3.61034000	0.78832300	3.64397900
				C	4.13753600	1.82095900	4.42620100
				C	5.39485900	2.35727400	4.17819200
				C	6.14445900	1.85845400	3.12477900
Mg	-3.11476600	0.33322300	0.28269900	C	5.66747400	0.82427100	2.31100000
Mg	2.47501900	-0.52846200	0.16116300	H	-5.30273100	4.54958800	0.36677000
N	-4.01656300	2.21103400	0.07427300	H	-6.86214900	3.79817100	0.78336000
N	-4.93502000	-0.71569200	0.33083700	H	-6.31469700	3.86062400	-0.89190000
N	3.30413300	-2.07272700	-1.02903100	H	-7.25006500	1.66297600	0.75243900
N	3.86620200	-0.77029500	1.74127500	H	-7.76518600	-0.83888600	-0.63558700
C	-5.98018600	3.72642900	0.14288400	H	-8.17637800	-0.28515900	0.98575700
C	-5.32805800	2.36603700	0.29594200	H	-7.34665900	-1.84012500	0.75068700
C	-6.23180100	1.32968500	0.58599800	H	-1.49430400	6.06736900	0.48476400

TS-4_1a2c

Mg	-3.11476600	0.33322300	0.28269900				
Mg	2.47501900	-0.52846200	0.16116300				
N	-4.01656300	2.21103400	0.07427300				
N	-4.93502000	-0.71569200	0.33083700				
N	3.30413300	-2.07272700	-1.02903100				
N	3.86620200	-0.77029500	1.74127500				
C	-5.98018600	3.72642900	0.14288400				
C	-5.32805800	2.36603700	0.29594200				
C	-6.23180100	1.32968500	0.58599800				
C	-6.09500200	-0.06607300	0.46484500				

H	-2.69736000	4.88134000	-3.43790500	H	1.19690700	4.50321400	-2.68057300
H	-5.11305700	-5.11632100	1.70896900	H	3.66367800	1.97946800	0.66959900
H	-5.36307600	-4.34389800	-2.48239600	H	0.70850900	1.83222400	1.02232500
H	5.08920800	-4.84721000	-0.59576600	C	1.13238800	-3.61865300	-2.47314000
H	4.38096300	-4.26410000	-2.11689000	H	1.24865100	-3.51116100	-1.38980000
H	3.37189900	-5.08703100	-0.92366300	C	5.44903000	-0.78629200	-2.51424800
H	4.59230800	-4.01203300	1.37951000	H	5.06215400	-0.39166500	-1.56743000
H	6.25098400	-2.45659300	2.83734500	C	6.56646700	0.35286300	1.17653000
H	4.88456600	-3.31382500	3.53401900	H	6.05959300	-0.46309300	0.65297600
H	5.14611700	-1.59753900	3.91826400	C	2.24545000	0.21426800	3.99074000
H	1.54850200	-3.49233500	-5.08577200	H	1.75492100	-0.07701000	3.05258500
H	5.09930900	-1.12839000	-5.16073000	C	-2.62067300	4.08072300	1.91068000
H	3.55285000	2.21338100	5.25115700	H	-3.02626800	3.08662700	2.12856200
H	7.12745300	2.27693900	2.92419000	C	-4.05226400	2.64487100	-2.82534700
C	1.45586200	1.68497000	0.26057800	H	-4.62573800	1.92190200	-2.23644600
C	2.79847700	1.74032700	0.05907100	C	-4.77216200	-2.57965400	2.60918400
C	1.78820800	2.03303100	-2.33495700	H	-4.06207800	-1.74299300	2.57982200
C	1.93494000	2.50659100	-0.91536700	C	-5.16507000	-1.66958600	-2.45016800
H	0.02783700	0.86523000	-1.96615600	H	-5.12850500	-0.63950300	-2.08049000
C	0.74079000	1.19202800	-2.71902800	C	0.22679200	-0.67253000	0.14106000
C	0.61839100	0.77217900	-4.04556200	C	-0.66676600	-1.48037600	1.10969200
C	1.52916300	1.20013300	-5.00698000	C	-1.07965100	-0.94559300	2.45324000
C	2.57493500	2.04561300	-4.63433800	H	-0.90883000	-2.81657100	3.50530000
C	2.70560400	2.45247100	-3.30975900	C	-1.21801800	-1.77967800	3.57502200
H	3.52049500	3.11295800	-3.02369600	H	-1.87127000	-2.00639900	5.60709300
H	3.29305200	2.38445400	-5.37673900	C	-1.77914500	-1.32160800	4.76774400
H	1.43061400	0.87396000	-6.03842100	C	-2.24012400	-0.01246000	4.88244500
H	-0.19655100	0.11157200	-4.32710700	H	-2.69772800	0.33846200	5.80273100
C	2.24868800	4.55188900	0.54163100	C	-2.07039300	0.84966200	3.80035000
C	1.88176300	4.00418300	-0.69944900	H	-2.37467300	1.88818400	3.88423800
C	1.50132400	4.89330100	-1.71565200	C	-1.48264200	0.39809300	2.61746200
C	1.52035700	6.27089200	-1.51051000	H	-1.28153100	1.11068500	1.81961400
C	1.89838900	6.79903500	-0.27733800	H	1.44785500	-2.93590100	2.01327900
C	2.25478000	5.92893000	0.75129900	C	0.67224000	-3.56707600	1.58586000
H	2.54625000	3.89535300	1.35342000	C	-0.48937000	-2.97643500	1.06422700
H	2.55219700	6.32101900	1.72049000	C	-1.46810000	-3.82008800	0.52581700
H	1.91822400	7.87426100	-0.12109800	C	-1.29248900	-5.20518900	0.50544300
H	1.23927100	6.93522100	-2.32384000	C	-0.13294600	-5.77604900	1.02717500

C	0.85215200	-4.94863800	1.56786500	H	0.33047800	0.80696500	4.79086900
H	1.76540400	-5.37564400	1.97385200	H	1.68655600	1.44802200	5.70862600
H	0.00288800	-6.85428600	1.01337400	C	2.36064900	-1.05155000	4.85522200
H	-2.07291200	-5.83448300	0.08614100	H	2.88815600	-1.85535400	4.33817300
H	-2.38143900	-3.39075200	0.12570700	H	2.89896000	-0.83528600	5.78546300
C	-1.27728500	-0.72769000	-0.08871300	H	1.36324500	-1.41952200	5.11557400
H	0.63881700	-1.41043500	-0.58331000	C	-1.19611600	4.16142100	2.47497200
H	-1.49879500	-1.43306600	-0.90000900	H	-1.19055400	3.93690700	3.54699700
H	3.34634300	-2.38057800	-6.36428800	H	-0.52050800	3.46309400	1.97505600
H	5.78321100	3.15819200	4.80157000	H	-0.77015200	5.16190000	2.35085000
H	-1.53603900	6.47143100	-1.94321900	C	-3.51183000	5.10927000	2.62649600
H	-5.38540400	-5.93988700	-0.59421100	H	-3.17725800	6.13054000	2.41280500
C	5.98465200	0.39569900	-3.33030200	H	-4.55911100	5.03030000	2.32427300
H	6.53992500	0.06374200	-4.21479300	H	-3.46764500	4.96501300	3.71205700
H	5.17465200	1.05049800	-3.66132800	C	-5.04456700	3.38350100	-3.73527500
H	6.67813900	0.98729100	-2.72630000	H	-5.60737400	2.66744500	-4.34405200
C	6.59704000	-1.75322200	-2.18082900	H	-5.76260800	3.97531900	-3.15931400
H	6.27838200	-2.54704900	-1.50058900	H	-4.53334600	4.06484400	-4.42385100
H	6.97932500	-2.22347300	-3.09422800	C	-3.03635000	1.86159000	-3.66762900
H	7.42810100	-1.21912500	-1.70623300	H	-2.40062700	2.53696900	-4.24974500
C	-0.22157700	-3.01327700	-2.86662500	H	-2.37572100	1.25864200	-3.03783800
H	-1.03220100	-3.50418000	-2.31997200	H	-3.54659000	1.19267100	-4.36923200
H	-0.25532600	-1.94258700	-2.64875600	C	-6.44943900	-1.81775300	-3.27973600
H	-0.41250200	-3.14099100	-3.93831900	H	-7.34759900	-1.67794200	-2.67123000
C	1.12853500	-5.12068700	-2.80218200	H	-6.46943900	-1.07824800	-4.08768500
H	0.89450800	-5.29472500	-3.85857100	H	-6.51631500	-2.80904300	-3.74121900
H	2.09382500	-5.59227700	-2.60058200	C	-3.93355600	-1.89596400	-3.33829800
H	0.36795700	-5.63229300	-2.20399500	H	-3.00465400	-1.72640700	-2.78678900
C	6.81453900	1.48103200	0.16462800	H	-3.90661800	-2.92151400	-3.72230500
H	5.88498000	1.81753800	-0.30296300	H	-3.94631400	-1.21995900	-4.19965100
H	7.28170400	2.34855400	0.64313300	C	-6.05554400	-2.06174500	3.27946400
H	7.48968100	1.14192400	-0.62786000	H	-5.85492000	-1.82537000	4.33017900
C	7.91201100	-0.18054200	1.69442800	H	-6.43564300	-1.15393500	2.80852500
H	8.49490400	-0.60993300	0.87230100	H	-6.84501400	-2.82189100	3.25307300
H	8.51327700	0.62004900	2.13946500	C	-4.15912900	-3.67008200	3.49521300
H	7.78170400	-0.95300900	2.45705200	H	-3.87077100	-3.23868500	4.45738100
C	1.33448100	1.22231700	4.69543000	H	-4.87608800	-4.47236900	3.70533400
H	1.26394900	2.16568400	4.14446400	H	-3.26896200	-4.11378500	3.04066800

TS-4_1b2c

Mg	3.03232600	-0.01086600	0.32023600	C	-1.78194700	4.17686500	-3.40161600
Mg	-2.32095000	-0.06938100	-0.67885500	C	-2.60031600	5.10935500	-2.75928500
N	4.09567300	1.65992000	0.92608500	C	-3.67214200	4.62502900	-2.01072300
N	4.64694300	-1.27971300	0.62585000	C	-3.92505000	3.25618300	-1.87173100
N	-3.73697100	-1.60817300	-0.69371600	H	6.10505800	3.58276000	1.40087000
N	-3.22816900	0.92984000	-2.28309400	H	6.80033400	2.59561500	2.69837200
C	5.88007300	2.82852800	2.16065000	H	5.17544500	3.29396900	2.85708400
C	5.27808000	1.58079300	1.54712100	H	6.97610500	0.52778100	2.20887700
C	6.03264100	0.40446700	1.69097100	H	6.51870300	-2.76284700	2.05719400
C	5.77296600	-0.90111000	1.23398000	H	7.72360100	-1.46084400	1.98178500
C	6.87524900	-1.91357500	1.46651600	H	7.22613800	-2.32662900	0.51519700
C	3.52332900	2.95845200	0.76497200	H	3.64282700	5.66819400	-1.28073700
C	3.92484800	3.77792100	-0.30844600	H	1.21579200	5.00217200	2.18959900
C	3.32602200	5.03225600	-0.45545300	H	5.13261200	-4.71876200	-2.38431600
C	2.34381600	5.49397800	0.42337300	H	3.54180900	-5.65804500	1.48069300
C	1.96968600	4.66403300	1.48216400	H	-5.51996400	-3.33514200	-2.96971200
C	2.54259900	3.40355000	1.67062400	H	-6.04110500	-3.13455100	-1.28726700
C	4.53777100	-2.65236500	0.24545500	H	-4.58588000	-4.04934400	-1.63675500
C	4.92559900	-3.05821400	-1.04630000	H	-4.89511500	-1.51281200	-3.84040000
C	4.82506800	-4.40829000	-1.38732600	H	-5.45848000	1.53600900	-4.04289900
C	4.34497600	-5.36690500	-0.49165900	H	-4.90256800	0.23755100	-5.10266500
C	3.93512900	-4.93313900	0.77006000	H	-3.88292200	1.66502900	-4.80812100
C	4.01852300	-3.59166500	1.15641700	H	-3.46172200	-5.22961900	2.17040000
C	-5.16931600	-3.17848100	-1.94835900	H	-6.62950200	-2.41283500	2.76860200
C	-4.35124600	-1.90651100	-1.84471100	H	-0.95839100	4.52777500	-4.02114200
C	-4.35815900	-1.09546600	-2.99673400	H	-4.34627800	5.33080300	-1.52741000
C	-3.98589700	0.25436900	-3.14719700	C	-1.16487500	1.40246400	0.90864500
C	-4.57837800	0.95924200	-4.35049300	C	-2.50136800	1.57292400	1.01001300
C	-4.14027400	-2.38517800	0.44496900	C	-1.87495100	-0.06646600	2.98815800
C	-3.47189500	-3.56297900	0.82486100	C	-1.76564500	1.26065300	2.28879900
C	-3.97429900	-4.30820500	1.89799400	H	0.10370400	-0.70726300	2.46121300
C	-5.10735900	-3.92493400	2.61066100	C	-0.78973000	-0.94682300	3.03040100
C	-5.74121200	-2.74007100	2.23030900	C	-0.85768000	-2.12220600	3.77895500
C	-5.27733500	-1.96347700	1.16896000	C	-2.00892900	-2.42539200	4.50256300
C	-3.05451000	2.33409500	-2.48581700	C	-3.09847300	-1.55527800	4.46219100
C	-1.99041300	2.80130300	-3.28663000	C	-3.03145700	-0.38657200	3.70886400
				H	-3.87763900	0.29543500	3.68575300
				H	-4.00354400	-1.78894600	5.01543100

H	-2.06059400	-3.33759400	5.09082000	H	-1.59445000	6.91407100	-2.12127800
H	-0.00713100	-2.79869000	3.79971600	C	4.98456300	3.32331500	-1.27676300
C	-1.60617200	3.75138100	2.73409100	H	5.95154200	3.16061600	-0.78791100
C	-1.51468700	2.43466200	3.21326100	H	4.71020600	2.37630000	-1.75228000
C	-1.19692500	2.25319800	4.56837900	H	5.13250100	4.06649800	-2.06524700
C	-0.98430000	3.34295200	5.40994800	C	2.14476700	2.54983400	2.84471200
C	-1.08581000	4.64459500	4.92091100	H	1.65470900	1.62117500	2.52590300
C	-1.39955000	4.84175400	3.57701200	H	3.01402600	2.25418900	3.44254800
H	-1.84662800	3.92772800	1.68999900	H	1.44356200	3.07697100	3.49450300
H	-1.48934700	5.84986200	3.18012700	C	1.69338000	6.83806700	0.22491900
H	-0.92692800	5.49413600	5.57942300	H	2.34657900	7.52299600	-0.32414100
H	-0.74160100	3.17137000	6.45546300	H	0.76145000	6.74715500	-0.34697300
H	-1.12018200	1.24767100	4.96811100	H	1.44113900	7.30605300	1.18155800
H	-3.24149100	2.29437400	0.68576900	C	5.44161200	-2.05637700	-2.04459000
H	-0.26375200	1.85221300	0.51968800	H	6.26174500	-1.45519400	-1.63855300
C	-2.24901200	-4.06350900	0.10591900	H	5.80160400	-2.55794900	-2.94696800
H	-2.16729800	-3.67347000	-0.90973500	H	4.65577000	-1.35517000	-2.35052900
H	-1.33687000	-3.76976900	0.63843700	C	3.56792100	-3.16532400	2.52842600
H	-2.24753600	-5.15670900	0.05389500	H	2.78675700	-2.39856200	2.47124600
C	-5.99703100	-0.69530300	0.79750900	H	3.16640400	-4.01493600	3.08739800
H	-5.34075000	0.17346200	0.92346600	H	4.38510400	-2.73274200	3.11660800
H	-6.32471500	-0.69353000	-0.24764600	C	4.29241400	-6.82342700	-0.87328900
H	-6.87714900	-0.54746700	1.42978100	H	5.28665500	-7.28409600	-0.81942500
C	-5.61662600	-4.74402000	3.76747200	H	3.63485600	-7.38913100	-0.20671300
H	-5.37823800	-5.80491600	3.64326100	H	3.93131000	-6.95677000	-1.89818100
H	-5.16637500	-4.42012900	4.71451500	C	-0.26299200	-0.73112100	-0.32121900
H	-6.70181700	-4.65285700	3.87763100	C	0.73531600	-1.21241400	-1.40353100
C	-5.15889000	2.80339600	-1.13485000	C	1.36113500	-0.22779200	-2.34358400
H	-5.04429100	1.79870200	-0.72393500	H	1.89046300	-1.66242600	-3.86215200
H	-5.41469600	3.49235800	-0.32354300	C	1.95090300	-0.62300500	-3.55647300
H	-6.02441000	2.77135100	-1.80929700	H	3.05587100	-0.04820800	-5.30582400
C	-1.13962200	1.83859500	-4.06682200	C	2.61215600	0.29370400	-4.37393800
H	-1.69626000	1.41102100	-4.91016700	C	2.70944400	1.63478000	-4.00569300
H	-0.25374900	2.33165000	-4.47151100	H	3.22226700	2.34745800	-4.64565300
H	-0.80435400	0.99965300	-3.45385800	C	2.13096200	2.04863500	-2.80585200
C	-2.32865000	6.58694900	-2.86830800	H	2.17822600	3.09016800	-2.50182300
H	-1.92571800	6.84899100	-3.85171800	C	1.47436400	1.13066300	-1.98676100
H	-3.23762400	7.17477200	-2.70862200	H	0.97839800	1.47417200	-1.08361300

H	-0.95398100	-1.79747200	-3.42757400	C	5.16031000	-3.31062800	0.56517000
C	-0.46773500	-2.69034400	-3.04080100	C	-5.61603500	-3.94410700	0.60625300
C	0.45441400	-2.56871900	-1.98589600	C	-5.11602400	-2.63288300	0.03693100
C	1.06792400	-3.73447900	-1.51489700	C	-5.46987200	-2.39009300	-1.30295300
C	0.75917600	-4.97990500	-2.06493700	C	-5.44251000	-1.19713100	-2.05987200
C	-0.15857900	-5.08536400	-3.10720800	C	-6.29715700	-1.22201300	-3.31054200
C	-0.77054300	-3.92999800	-3.59695300	C	-4.37049000	-2.10105100	2.22260500
H	-1.49065900	-3.99466000	-4.40875600	C	-3.38526600	-2.95655700	2.76865700
H	-0.39552300	-6.05558400	-3.53594200	C	-3.43632500	-3.25684700	4.13397300
H	1.24848300	-5.86952300	-1.67738400	C	-4.42593800	-2.73910800	4.95790000
H	1.80077800	-3.66996000	-0.71655000	C	-5.37015500	-1.87298700	4.42081600
C	1.16750400	-1.02339900	0.06471100	C	-5.35522800	-1.52770600	3.06549300
H	-0.84647700	-1.61825600	-0.00120100	C	-5.01224400	1.10787600	-2.44776200
H	1.23621000	-1.98781500	0.58632000	C	-4.07047900	1.53895600	-3.41336500
				C	-4.33664700	2.70948500	-4.13077500
				C	-5.48218200	3.46123900	-3.90079700
				C	-6.37825400	3.05158800	-2.92417200

Int-6_1a2c

Mg	3.70125700	0.16705700	-0.15887600	C	-6.16688200	1.88282700	-2.18576500
Mg	-3.44834000	-0.21030600	-0.10979200	N	6.42037200	3.92285400	0.74626400
N	4.85454000	1.81186100	0.36689200	H	7.84833200	3.15700000	0.00701600
N	5.33638600	-1.08152900	-0.47218600	H	7.42334200	2.81500300	1.68123800
N	-4.40462900	-1.80109700	0.81525000	H	8.01451100	0.91902100	-0.27168900
N	-4.77922600	-0.09797200	-1.70632200	H	8.03019700	-1.94437600	0.44336100
C	7.00539600	3.00554100	0.68645900	H	8.64152200	-1.05150700	-0.94893100
C	6.18428600	1.81152700	0.24138200	H	7.55049100	-2.43761700	-1.17604300
C	6.94881000	0.72414800	-0.21944200	H	2.45480100	5.75307400	0.49922700
C	6.59076700	-0.61893900	-0.43621300	H	3.48902800	3.93254600	4.21973700
C	7.76619900	-1.57029600	-0.55203600	H	4.72671700	-4.92951000	-2.93766800
C	4.23406200	2.90525500	1.05903000	H	5.01101500	-5.32434400	1.30546700
C	3.61428200	3.94867700	0.33052100	H	-6.23579900	-4.47654400	-0.11636200
C	2.95245500	4.95513400	1.04035700	H	-6.19844500	-3.78376300	1.51734700
C	2.89770400	4.94806200	2.42838900	H	-4.77661700	-4.58626200	0.88574300
C	3.52740200	3.93161900	3.13336600	H	-6.00475400	-3.20366300	-1.77935700
C	4.20899400	2.90429800	2.47420100	H	-7.33293300	-0.96972700	-3.05857300
C	5.16243700	-2.49991100	-0.59402500	H	-6.30479000	-2.22535900	-3.74363600
C	4.97817400	-3.07731000	-1.87626600	H	-5.95908100	-0.50703700	-4.06132300
C	4.85632700	-4.46778700	-1.96464800	H	-2.68228200	-3.91633400	4.55558000
C	4.88063900	-5.27649000	-0.83314800	H	-6.13949300	-1.45700600	5.06611100
C	5.01318300	-4.69448500	0.41939800				

H	-3.62768900	3.04280200	-4.88179400	H	3.88127700	3.01181500	-1.55926000
H	-7.26284800	3.65122400	-2.72525300	C	4.90056600	1.82947700	3.30352300
C	-0.38952200	1.14554300	-0.22281800	H	5.50114100	1.21344700	2.62708600
C	-1.90415800	1.23746200	-0.17026800	C	4.89801100	-2.22472500	-3.13940800
C	-1.07132300	1.19665400	2.30339900	H	4.36290100	-1.30418900	-2.87143300
C	-1.06597100	1.85641000	0.95044000	C	5.29842900	-2.73661800	1.96877500
H	1.06537900	1.13903400	2.48155800	H	5.47755500	-1.66036500	1.87374500
C	0.12497500	0.91888000	2.97723500	C	0.26527100	-0.19767800	-0.06091300
C	0.11396700	0.37238400	4.25987500	C	0.90605300	-1.01219200	-1.19211000
C	-1.09512000	0.10075200	4.89909000	C	1.29094600	-0.38554800	-2.50470000
C	-2.29418000	0.37962700	4.24620800	H	0.57799400	-2.01424800	-3.72339400
C	-2.27454300	0.92215900	2.96228800	C	1.07206100	-1.04912500	-3.72509000
H	-3.21221000	1.16395600	2.46421900	H	1.30375300	-1.06368300	-5.85810700
H	-3.24248600	0.16280000	4.72844200	C	1.49106800	-0.51064200	-4.94108900
H	-1.10377100	-0.33003700	5.89668100	C	2.15162800	0.71455400	-4.98721300
H	1.05304800	0.15390200	4.76096500	H	2.48321600	1.13269900	-5.93327000
C	-1.01792000	4.14522500	-0.16189800	C	2.36850300	1.39934500	-3.79366700
C	-0.99089700	3.36394500	1.00710600	H	2.86641300	2.36434500	-3.80318000
C	-0.94703700	4.05276900	2.22965400	C	1.94121800	0.86225400	-2.57955300
C	-0.93834800	5.44634900	2.28213200	H	2.07401500	1.45303900	-1.67615700
C	-0.96577100	6.20106000	1.11268700	H	-1.56793900	-1.86674400	-1.91402500
C	-1.00244700	5.53610100	-0.11279300	C	-0.90403200	-2.70240500	-1.70123500
H	-1.06822100	3.66181900	-1.13348900	C	0.41666500	-2.43383300	-1.31110900
H	-1.03096100	6.10229000	-1.04060800	C	1.26470900	-3.52133500	-1.07466300
H	-0.96706700	7.28706000	1.15288300	C	0.80845900	-4.83242300	-1.22035900
H	-0.91600100	5.94117000	3.25027900	C	-0.50646500	-5.08197000	-1.61016000
H	-0.92610600	3.49168700	3.15759800	C	-1.36558400	-4.00879300	-1.85149400
H	-2.28073600	2.02108800	-0.83690800	H	-2.39447700	-4.18543800	-2.15394500
H	0.11482400	1.82854400	-0.90431000	H	-0.86006200	-6.10297900	-1.72686600
C	-2.25168600	-3.54376700	1.94353200	H	1.48961800	-5.65781100	-1.03172500
H	-2.40735300	-3.25451700	0.89919900	H	2.29296700	-3.34112700	-0.77492900
C	-6.41281000	-0.56195700	2.54780000	C	1.72324700	-0.59293300	0.05138700
H	-6.11785800	-0.26241300	1.53603600	H	-0.38734400	-0.83906500	0.53315700
C	-7.16807200	1.52506000	-1.09720200	H	1.78368800	-1.44553200	0.73978200
H	-6.90436700	0.53840300	-0.70373400	H	-4.45648900	-2.99991200	6.01246900
C	-2.79441000	0.76010300	-3.69697200	H	-5.66649400	4.36773500	-4.47095000
H	-2.50594300	0.26127800	-2.76352500	H	2.35971600	5.73055900	2.95460700
C	3.69720400	4.02797500	-1.18883600	H	4.78548400	-6.35469200	-0.93055900

C	-6.50182800	0.70699800	3.40740900	H	5.84183800	4.48988100	-1.31155500
H	-6.85682300	0.48862100	4.42010700	H	4.91272000	4.95591200	-2.74009600
H	-5.53122200	1.20444600	3.49755600	C	5.85552000	2.42884200	4.34667100
H	-7.20556300	1.41930800	2.96601300	H	6.42104300	1.63471400	4.84652100
C	-7.79182400	-1.23087300	2.44174300	H	6.57019000	3.12104000	3.89126700
H	-7.77504700	-2.08667000	1.76100400	H	5.31290700	2.97990500	5.12224100
H	-8.13050300	-1.58768700	3.42106400	C	3.88452600	0.90352100	3.98526900
H	-8.53849000	-0.52113900	2.06816300	H	3.22788600	1.46890600	4.65526600
C	-0.90141000	-2.96860700	2.39663300	H	3.24998100	0.39376100	3.25344600
H	-0.10235900	-3.30360900	1.72747100	H	4.39540100	0.13892400	4.58133700
H	-0.90982800	-1.87570400	2.41115500	C	6.48794000	-3.33743800	2.73253200
H	-0.65521500	-3.30275000	3.41097300	H	7.42556300	-3.23088500	2.17909100
C	-2.20027800	-5.07800600	2.00039700	H	6.60866500	-2.84164200	3.70188600
H	-1.96581600	-5.43215900	3.01052400	H	6.34119100	-4.40539200	2.92745100
H	-3.14649500	-5.54144000	1.70415500	C	4.00371000	-2.92879300	2.77275400
H	-1.41966000	-5.44861400	1.32881400	H	3.14725600	-2.46538800	2.27466000
C	-7.07734800	2.53068600	0.06047400	H	3.77351300	-3.99207200	2.90158500
H	-6.07289900	2.55502400	0.49492600	H	4.09707100	-2.48570400	3.77006800
H	-7.31000300	3.54511900	-0.28113100	C	6.27557100	-1.80750800	-3.68021700
H	-7.78839900	2.27557600	0.85357800	H	6.15594100	-1.26193200	-4.62273300
C	-8.60993500	1.44609200	-1.61947200	H	6.81425200	-1.15509500	-2.99093200
H	-9.28287700	1.09379800	-0.83013100	H	6.89806700	-2.68731800	-3.88055600
H	-8.97562900	2.42561000	-1.94615900	C	4.10644100	-2.90131000	-4.26401400
H	-8.69887100	0.76300000	-2.46952500	H	3.91788500	-2.17982600	-5.06347700
C	-1.62427900	1.66284100	-4.10035700	H	4.66256200	-3.73710100	-4.70469900
H	-1.50436600	2.49863800	-3.40495100	H	3.14040600	-3.27531900	-3.91445400
H	-0.69500100	1.08940800	-4.10689500				
H	-1.75545200	2.07637500	-5.10690800				
C	-3.00424600	-0.32990900	-4.75916600				
H	-3.74326600	-1.07171200	-4.44582400				
H	-3.34592800	0.11044200	-5.70308900				
H	-2.06302300	-0.85515200	-4.95333400				
C	2.40834100	4.54932200	-1.83385800				
H	2.46544800	4.46056100	-2.92369900				
H	1.52618300	4.00601100	-1.48676300				
H	2.24735300	5.60962900	-1.61289400				
C	4.88364300	4.89328400	-1.64628400				
H	4.79040500	5.91232400	-1.25404500				

Int-6_1b2c

Mg	3.62499500	0.09949300	-0.01109400
Mg	-3.33622200	-0.31988600	-0.08351600
N	4.71295300	1.83519000	0.00464000
N	5.29314900	-1.10694300	-0.09056900
N	-4.34658900	-1.37855700	1.36918700
N	-4.47778600	-1.07214500	-1.62388300
C	6.71943600	3.21396100	-0.34307700
C	6.02060200	1.87396700	-0.26606000
C	6.82794700	0.73839200	-0.46267700
C	6.52090700	-0.62711300	-0.30182300

C	7.69827600	-1.57880900	-0.33031700	H	3.43716000	4.82003300	3.23927500
C	4.06578000	3.04740400	0.40403800	H	4.67679600	-5.42458900	-1.54944900
C	3.39101800	3.85968500	-0.52138900	H	4.91988200	-4.75584600	2.67479400
C	2.73884900	5.01108500	-0.06193900	H	-6.02121800	-4.27535900	1.72824900
C	2.74727700	5.38223800	1.27933200	H	-6.41751100	-2.81644100	2.65149000
C	3.42231300	4.55472800	2.18334100	H	-4.86513800	-3.59375400	2.89501000
C	4.07031500	3.39144400	1.77538800	H	-5.78979200	-3.87083800	-0.35394000
C	5.14079700	-2.51035900	0.13240800	H	-6.62504700	-2.26200400	-3.04813800
C	4.97408600	-3.38840300	-0.95809500	H	-6.12392300	-3.86899900	-2.49547900
C	4.80142400	-4.74973700	-0.70440100	H	-5.07302300	-2.90047600	-3.55597600
C	4.78108800	-5.26918100	0.59274000	H	-2.67039500	-1.28462500	5.66040700
C	4.93337500	-4.37718600	1.65418700	H	-6.30246100	0.84616000	4.87720900
C	5.10759100	-3.00419100	1.44952400	H	-2.84743800	0.16371500	-5.74566600
C	-5.61209200	-3.34911600	2.13466000	H	-6.53378700	1.91215700	-4.44196600
C	-5.02261600	-2.48688700	1.03766100	C	-0.35927400	0.94119300	-0.63084000
C	-5.27422300	-2.92061600	-0.27877700	C	-1.87045300	1.06770800	-0.69801000
C	-5.12160700	-2.23084000	-1.50023700	C	-1.08363700	2.17877300	1.54673400
C	-5.77037800	-2.85997900	-2.71410700	C	-1.04579000	2.12256000	0.04368900
C	-4.38138100	-0.97739400	2.74412700	H	1.05226700	2.29298500	1.75258600
C	-3.36838600	-1.37295400	3.63799900	C	0.10407700	2.29314800	2.28172000
C	-3.45365600	-0.97053800	4.97301800	C	0.07659000	2.41010800	3.66997400
C	-4.50321200	-0.18312800	5.44891800	C	-1.14100900	2.42351500	4.35064400
C	-5.47898500	0.22087100	4.53608800	C	-2.33086500	2.32088500	3.63228200
C	-5.43686500	-0.15879000	3.19187500	C	-2.29581600	2.19983700	2.24351800
C	-4.56126200	-0.36093700	-2.86097700	H	-3.22648800	2.14208100	1.68218000
C	-3.54145300	-0.47912000	-3.82323200	H	-3.28571400	2.32403300	4.14929300
C	-3.63567200	0.26605800	-5.00183100	H	-1.16253800	2.51326100	5.43367500
C	-4.70036700	1.13279300	-5.25032700	H	1.00989100	2.49403300	4.22115300
C	-5.69362900	1.24016800	-4.27497900	C	-0.74865900	3.59365000	-2.01434700
C	-5.64310800	0.51445800	-3.08321300	C	-0.93455300	3.47216200	-0.62459900
H	6.23315700	3.86247200	-1.07831900	C	-1.07884600	4.66301400	0.10368200
H	7.76941100	3.09799900	-0.61608300	C	-1.04340800	5.90963300	-0.52125200
H	6.66457300	3.73865000	0.61627000	C	-0.84808900	6.00920900	-1.89611600
H	7.86792300	0.94983200	-0.68105600	C	-0.69904400	4.83704400	-2.63821600
H	7.82854500	-2.04769100	0.65125900	H	-0.65997600	2.70264700	-2.62970100
H	8.62143300	-1.05679700	-0.58633600	H	-0.55627200	4.88791500	-3.71506400
H	7.54394300	-2.39363200	-1.04272900	H	-0.82302200	6.97971300	-2.38441500
H	2.19946900	5.62482900	-0.78007900	H	-1.17394600	6.80800900	0.07724800

H	-1.22960300	4.61424000	1.17688600	H	2.69876800	7.25300400	2.36099700
H	-2.20156800	1.46410600	-1.66429900	C	4.98227800	-2.87286800	-2.37136300
H	0.19222400	1.21748100	-1.52489400	H	5.92372200	-2.37183000	-2.62296300
C	-2.21098800	-2.21452200	3.17757600	H	4.83673500	-3.68995000	-3.08225400
H	-2.53073800	-3.11551300	2.64611400	H	4.18398400	-2.14259800	-2.53649800
H	-1.56546700	-1.66366500	2.48469800	C	5.25555300	-2.07531500	2.62582100
H	-1.59150300	-2.52062100	4.02445600	H	4.39915300	-1.39395800	2.70965600
C	-6.51149500	0.30334100	2.24366700	H	5.31616800	-2.63805400	3.56128200
H	-6.09807200	0.91935000	1.43613600	H	6.14896200	-1.44757900	2.54666600
H	-7.02505900	-0.53387300	1.75898700	C	4.58631300	-6.74425200	0.82837200
H	-7.26082800	0.90318300	2.76710200	H	5.30367400	-7.33977300	0.25287100
C	-4.59061700	0.19778100	6.90382700	H	4.71069300	-7.00084500	1.88429300
H	-3.59858300	0.36499500	7.33475100	H	3.58374200	-7.06601400	0.52296500
H	-5.17855100	1.10954300	7.04568400	C	0.23394000	-0.19566100	0.15217900
H	-5.07006400	-0.59366600	7.49355500	C	0.89630800	-1.42271000	-0.49184300
C	-6.72493000	0.68360500	-2.04975300	C	1.33360500	-1.38817600	-1.93178800
H	-6.31908600	1.06847800	-1.10702300	H	0.70838000	-3.39993400	-2.38283000
H	-7.48678600	1.38697400	-2.39624800	C	1.17127000	-2.50123500	-2.77536000
H	-7.22283900	-0.26141600	-1.80706200	H	1.45839800	-3.37329700	-4.71404700
C	-2.35860500	-1.37674700	-3.58870700	C	1.60080500	-2.48648500	-4.10132300
H	-2.65768600	-2.39052100	-3.30231400	C	2.21264600	-1.35714300	-4.64191400
H	-1.73488600	-1.44847300	-4.48308000	H	2.54560300	-1.34688400	-5.67580600
H	-1.72486900	-0.98689900	-2.78334300	C	2.38998300	-0.24094900	-3.82790700
C	-4.76045000	1.95164000	-6.51314700	H	2.85607300	0.65766500	-4.22402000
H	-4.21852400	1.46717800	-7.33096600	C	1.96268100	-0.26059700	-2.50015600
H	-5.79289500	2.11089700	-6.83976000	H	2.07223200	0.64981300	-1.91525000
H	-4.31088700	2.94147800	-6.36537300	H	-1.55307700	-2.53630700	-0.92817400
C	3.36688400	3.54295300	-1.99431200	C	-0.91930100	-3.17950100	-0.32116500
H	3.96330900	4.26700500	-2.56333500	C	0.38382200	-2.75882500	-0.01606200
H	3.77667400	2.55192200	-2.20263200	C	1.19256200	-3.62236100	0.73084800
H	2.34486400	3.59413000	-2.38323900	C	0.71123000	-4.85544400	1.17148500
C	4.76286100	2.51533600	2.78623300	C	-0.58802700	-5.25598700	0.86441400
H	4.30709400	1.51864600	2.83434400	C	-1.40445700	-4.41311300	0.10961000
H	5.82072600	2.35983900	2.54841100	H	-2.42109400	-4.70665000	-0.13833900
H	4.70233200	2.95489900	3.78557400	H	-0.96223900	-6.21651800	1.20893400
C	2.03726200	6.62054400	1.75815700	H	1.35777700	-5.50389000	1.75700000
H	1.66859400	7.21708000	0.92002100	H	2.21016000	-3.32588500	0.96894600
H	1.17575500	6.36225800	2.38462800	C	1.66958000	-0.51999100	0.49496800

H -0.46586900 -0.49977000 0.93417900

H 1.68611700 -0.99376100 1.48422500

