Mono-BHT heteroleptic magnesium complexes: synthesis, molecular structure and catalytic behavior in the ring-opening polymerization of cyclic esters

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Supplementary Information

S1. Synthesis of BHT-Mg complexes

S1.1. General remarks

All synthetic manipulations were carried out in an argon box (6-9 ppm O_2, 0 ppm H_2O) in 20 or 40 mL vials. Tetrahydrofuran (THF) and 1,2-dimethoxyethane (DME) were predried over NaOH and distilled from sobium/benzophenone. Hexane was distilled from Na/K alloy. Toluene was distilled from sodium/benzophenone ketyl in the presence of dibenzo-18-crown-6. DMSO was distilled over CaH_2 under reduced pressure. Benzyl alcohol was distilled over CaH_2 under reduced pressure and stored under argon. 2,6-di-*tert*-butyl-4-methylphenol (BHT-H), di-n-butylmagnesium (1M in heptane), ethyl glycolate and γ-hydroxybutyroyl N,N-dimethylamide (Sigma-Aldrich) were used as purchased.

$(BHT)_2Mg(THF)_2$ (**1**) was prepared using modified method of Ittel.[1] [(BHT)Mg(n-Bu)$(THF)_2$] (**2**) and $[(BHT)Mg(n\text{-}Bu)]_2$ were synthesized according to the literature procedure.[2]

$CDCl_3$ (Cambridge Isotope Laboratories, Inc., D 99.8 %) was washed by solution of K_2CO_3 in D_2O, distilled over P_2O_5, CaH_2 and stored over 4Å molecular sieves. CD_2Cl_2 was distilled over P_2O_5 and then over CaH_2. DMSO-d_6 (Aldrich, ≥99.5 atom % ^2H) was distilled over CaH_2 and stored over 4Å molecular sieves. THF-d_8 was stored over Na/benzophenone and condensed into NMR vials using Schlenck technique. The ^1H and ^{13}C NMR spectra were recorded on a Bruker AVANCE 400 spectrometer (400 MHz) or on Bruker Avance III (600 MHz) at 20 °C. The chemical shifts are reported in ppm relative to the solvent residual peaks. Synthesized complexes slowly decompose in THF (**2**) and chloroform (all obtained complexes). Therefore, their NMR spectra were recoded right after sample preparation.

Elemental analysis (C, H) was performed on a Perkin Elmer Series II CHNS/O Analyzer 2400.

S1.2. Synthesis of $[(BHT)_2Mg(THF)_2]$ (1)

A solution of BHT-H (3.085 g, 14 mmol) in THF (10 mL) was added dropwise to a stirred solution of Bu_2Mg in heptane (1M, 7 mL, 7 mmol). The reaction mixture was stirred for 1 hour, then all solvent was evaporated under reduced pressure. The residue was washed with hexane (2×10 mL), recrystallized from THF/toluene/hexane mixture (1:10:50). The precipitated crystals were dried under vacuum. The yield was 3.855 g (6.35 mmol, 90.7%). ^{1}H NMR ($CDCl_3$, 400MHz, 20°C): δ 6.94 (s, 4H), 4.17 (m, 8H), 2.23 (s, 6H), 1.98 (m, 8H), 1.42 (s, 36H). ^{1}H NMR (400 MHz, C_6D_6, 20°C): δ 7.28 (s, 4H), 3.58-3.63 (m, 8H), 2.43 (s, 6H), 1.62 (s, 36H), 1.13-1.18 (m, 8H).

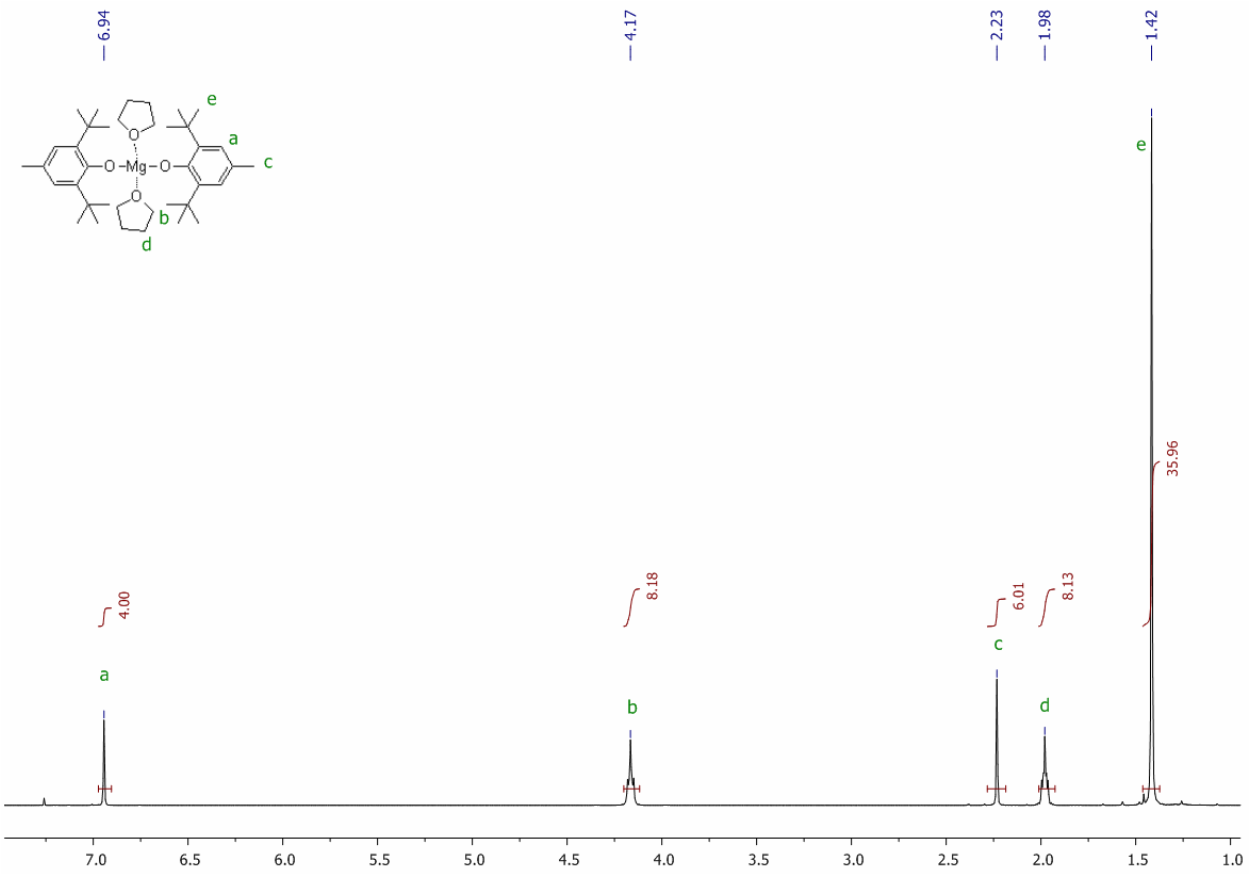

Fig. S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of $(BHT)_2Mg(THF)_2$ (**1**).

S1.3. Synthesis of [(BHT)Mg(μ-OBn)(THF)]$_2$ (3)

Method I. From BHT$_2$Mg. A solution of BnOH (325 mg, 3.0 mmol) in THF (2 mL) was added dropwise to a stirred solution (BHT)$_2$Mg(THF)$_2$ (1.822 g, 3.0 mmol) in THF (4 mL). The reaction mixture was stirred for 30 min. All solvent was evaporated under reduced pressure to provide precipitate and viscous oil. The residue was washed with toluene (1 mL), with hexane (2×7 mL), centrifuged, dried under dynamic vacuum. The yield of microcrystalline powder was 1.043 g (1.23 mmol, 82.2%).

Method II. From BHT-Mg-Bu. A solution Bu$_2$Mg in heptane (20.2 mL, 1 M, 20.2 mmol) was added dropwise to a stirred solution of BHT-H (4.410 g, 20 mmol) in a toluene/THF mixture (8 mL and 4.5 mL, correspondingly). After 40 min, a solution of BnOH (2.168 g, 20 mmol) in THF (1 mL) was added dropwise to the stirred reaction mixture. The formed solution was then stirred for 3 min. After 5 min, crystals of **3** started to form. Two hours later, the mother liquor was decanted. Some of formed crystals were taken for the X-ray diffraction studies. The remaining crystals were washed with toluene (2×5 mL) and hexane (2×5 mL), dried under dynamic vacuum till the constant weight. The yield was 6.785 g (8.02 mmol, 80%). The mother liquor was concentrated under reduced pressure to 5 mL of residual volume, hexane (10 mL) was added. Crystallization at -20 °C gave additional 0.69 g of the product. The total yield 88%.

Complex **3** with the same yield (~90%) was obtained by the reaction of **2** or [(BHT)Mg(n-Bu)]$_2$ (for NMR, see fig. S2) in the presence of THF with BnOH in hexane with subsequent low temperature crystallization.

Anal. found (calcd for $C_{26}H_{38}MgO_3$): C, 73.28 (73.85%); H, 9.15 (9.06%). ^{1}H NMR (400 MHz, THF-d$_8$, 20 °C): δ 7.36 (d, ^3J = 7.3 Hz, 2H, o-H$_{Ph}$); 7.18 (t, ^3J = 7.3 Hz, 2H, m-H$_{Ph}$); 7.13 (t, ^3J = 7.3 Hz, 1H, p-H$_{Ph}$); 6.78 (s, 2H, m-H$_{BHT}$); 5.02 (s, 1H, O-CH$_2$-Ph); 3.62 (m, 4H, CH$_2$CH$_2$O$_{THF}$); 2.13 (s, 3H, -CH$_3$ $_{BHT}$); 1.78 (m, 4H, CH$_2$CH$_2$O$_{THF}$); 1.38 (s, 18H, 2,6-^{t}Bu$_{2\ BHT}$). ^{1}H NMR (400 MHz, C$_6$D$_6$, 20 °C): δ 7.45 (d, ^3J = 7.5 Hz, 2H, o-H$_{Ph}$); 7.29 (s, 2H, m-H$_{BHT}$); 7.10 (t, ^3J = 7.5 Hz, 2H, m-H$_{Ph}$); 7.02 (t, ^3J = 7.5 Hz, 1H, p-H$_{Ph}$); 5.09 (s, 1H, O-CH$_2$-Ph); 3.46 (br.s, 4H, CH$_2$CH$_2$O$_{THF}$); 2.45 (s, 3H, -CH$_3$ $_{BHT}$); 1.61 (s, 18H, 2,6-^{t}Bu$_{2\ BHT}$); 1.11 (br.s, 4H, CH$_2$CH$_2$O$_{THF}$). ^{13}C{^{1}H} NMR (101 MHz, THF-d$_8$, 20 °C): δ 161.4 (ipso-C-O$_{BHT}$); 145.8; 137.7; 129.1; 128.1; 127.6; 125.7; 121.0; 68.4 (CH$_2$CH$_2$O$_{THF}$); 66.6 (Ph-CH$_2$-O); 35.7 (-CMe$_{3\ BHT}$); 31.4 (-C(CH$_3$)$_{3\ BHT}$); 26.5 (CH$_2$CH$_2$O$_{THF}$); 21.6 (p-CH$_{3\ BHT}$). ^{13}C{^{1}H} NMR (101 MHz, C$_6$D$_6$, 20 °C): δ 161.3 (ipso-C-O$_{BHT}$); 145.3; 137.7; 128.8; 127.7; 127.4; 126.1; 121.8; 70.2 (CH$_2$CH$_2$O$_{THF}$); 66.2 (Ph-CH$_2$-O); 35.7 (-CMe$_{3\ BHT}$); 31.5 (-C(CH$_3$)$_{3\ BHT}$); 25.3 (CH$_2$CH$_2$O$_{THF}$); 22.1 (p-CH$_{3\ BHT}$).

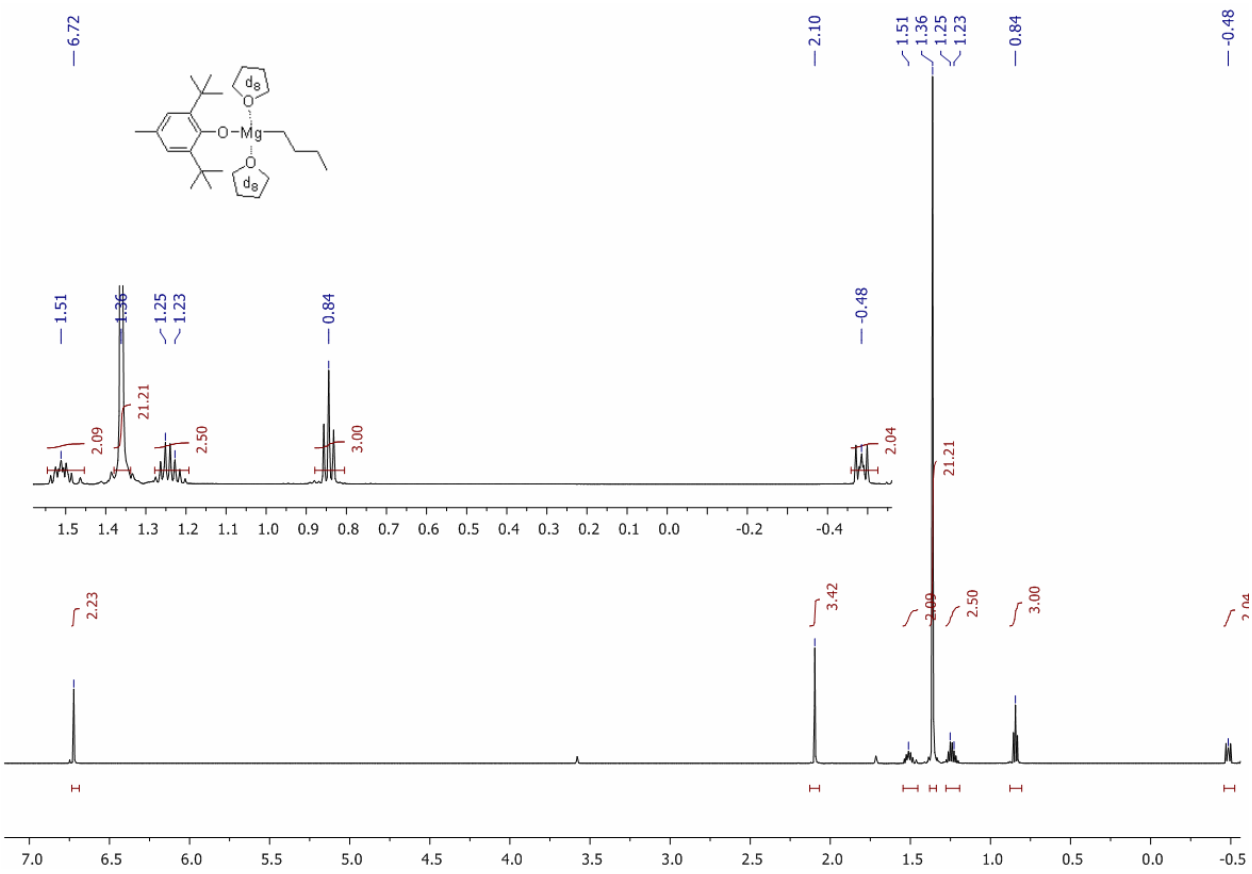

Fig. S2. ^{1}H NMR spectrum (600 MHz, THF-d_8, 20 °C) of $[(BHT)Mg(n\text{-}Bu)]_2$.

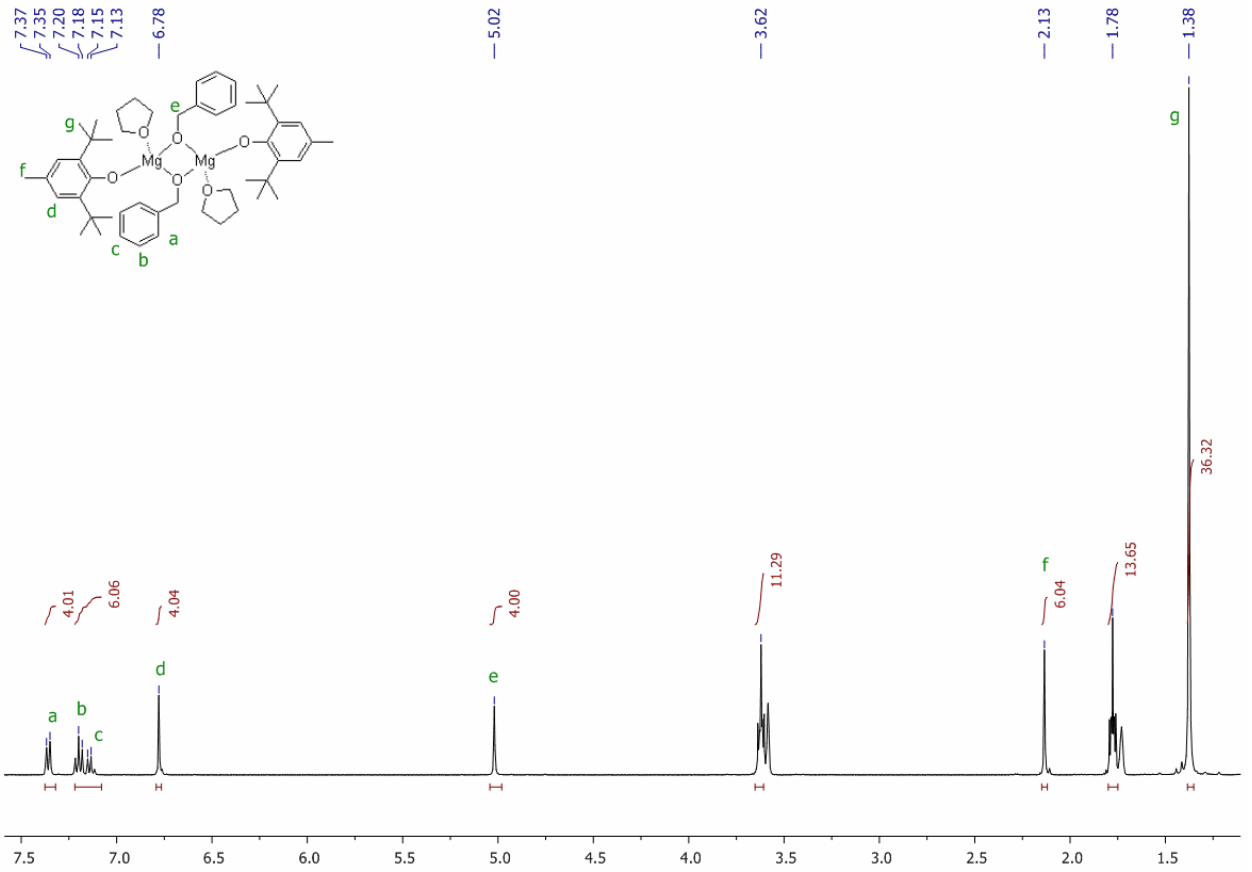

Fig. S3. ^{1}H NMR spectrum (400 MHz, THF-d_8, 20 °C) of $[(BHT)Mg(\mu\text{-}OBn)(THF)]_2$ (**3**).

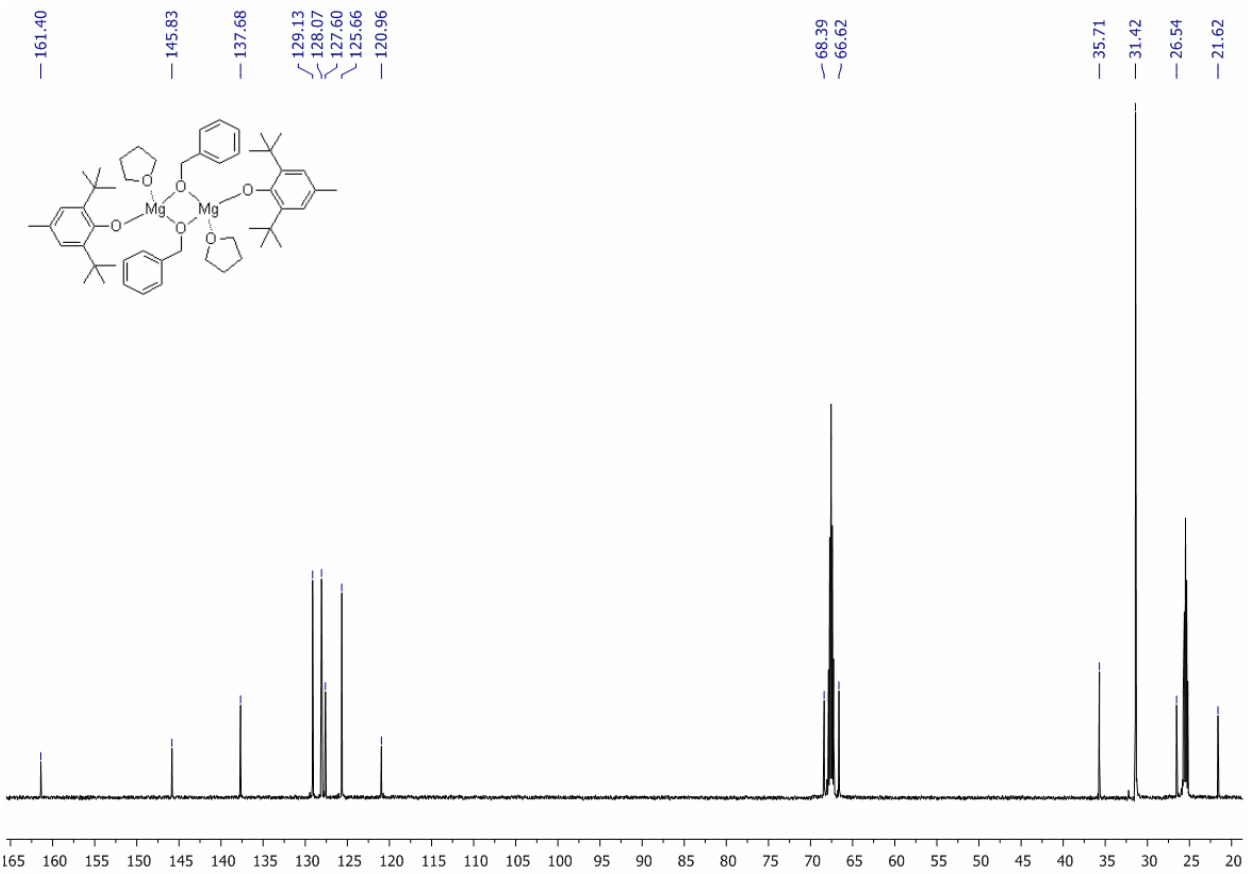

Fig. S4. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, THF-d_8, 20 °C) of $[(BHT)Mg(\mu\text{-}OBn)(THF)]_2$ (**3**).

S1.4. Synthesis of $[(BHT)Mg(\mu\text{-}OC_6H_4\text{-}4\text{-}^{t}Bu)(THF)]_2$ (4)

A solution Bu_2Mg in heptane (5.0 mL, 1 M, 5 mmol) was added dropwise to a stirred solution of BHT-H (1.102 g, 5 mmol) in a hexane (3.5 mL) /THF (1.5 mL) mixture. In 20 min, 4-*tert*-butylphenol (0.751 g, 5 mmol) in a hexane (3.5 mL) /THF (1.5 mL) mixture was added dropwise. After the beginning of the product precipitation, the stirring was stopped. Next day, the mother liquor was decanted. Some of crystals were taken for the X-ray diffraction studies. The remaining crystals were washed with toluene (2×5 mL) and hexane (2×10 mL), dried under dynamic vacuum till the constant weight. The yield was 2.132 g (2.29 mmol, 91.7%).

Anal. found (calcd for $C_{29}H_{44}MgO_3$): C, 75.06 (74.91%); H, 9.66 (9.54%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.16 (d, ^{3}J = 8.4 Hz, 4H); 6.87 (s, 4H, *m*-$\underline{H}_{(BHT)}$); 6.56 (d, ^{3}J = 8.4 Hz, 4H); 4.23 (bs, 8H); 2.19 (s, 6H, $C\underline{H}_{3(BHT)}$); 2.06 (bs, 8H); 1.31 (s, 18H, $^{t}\underline{Bu}_{(C6H4\text{-}tBu)}$); 1.09 (s, 36H, $^{t}\underline{Bu}_{(BHT)}$). ^{1}H NMR (600 MHz, C_6D_6): δ 7.33 (d, 4H); 7.24 (s, 4H); 6.82 (d, 4H); 3.72 (br. s, 8H); 2.40 (s, 6H, $C\underline{H}_{3(BHT)}$); 1.44 (s, 18H, $^{t}\underline{Bu}_{(C6H4\text{-}tBu)}$); 1.32 (s, 36H, $^{t}\underline{Bu}_{(BHT)}$); 1.29 (bs, 8H). $^{13}C\{^{1}H\}$ NMR (150 MHz, C_6D_6, 20 °C): δ 160.3; 157.2; 142.8; 137.6; 126.3; 125.6; 121.9; 120.5; 69.7 ($CH_2\underline{C}H_2O_{(THF)}$); 35.1; 34.2; 31.9 ($-C(\underline{C}H_3)_{3(C6H4\text{-}tBu)}$); 30.9 ($-C(\underline{C}H_3)_{3\,(BHT)}$); 25.2 ($\underline{C}H_2CH_2O_{(THF)}$); 21.6 (p-C-$\underline{C}H_{3\,(BHT)}$).

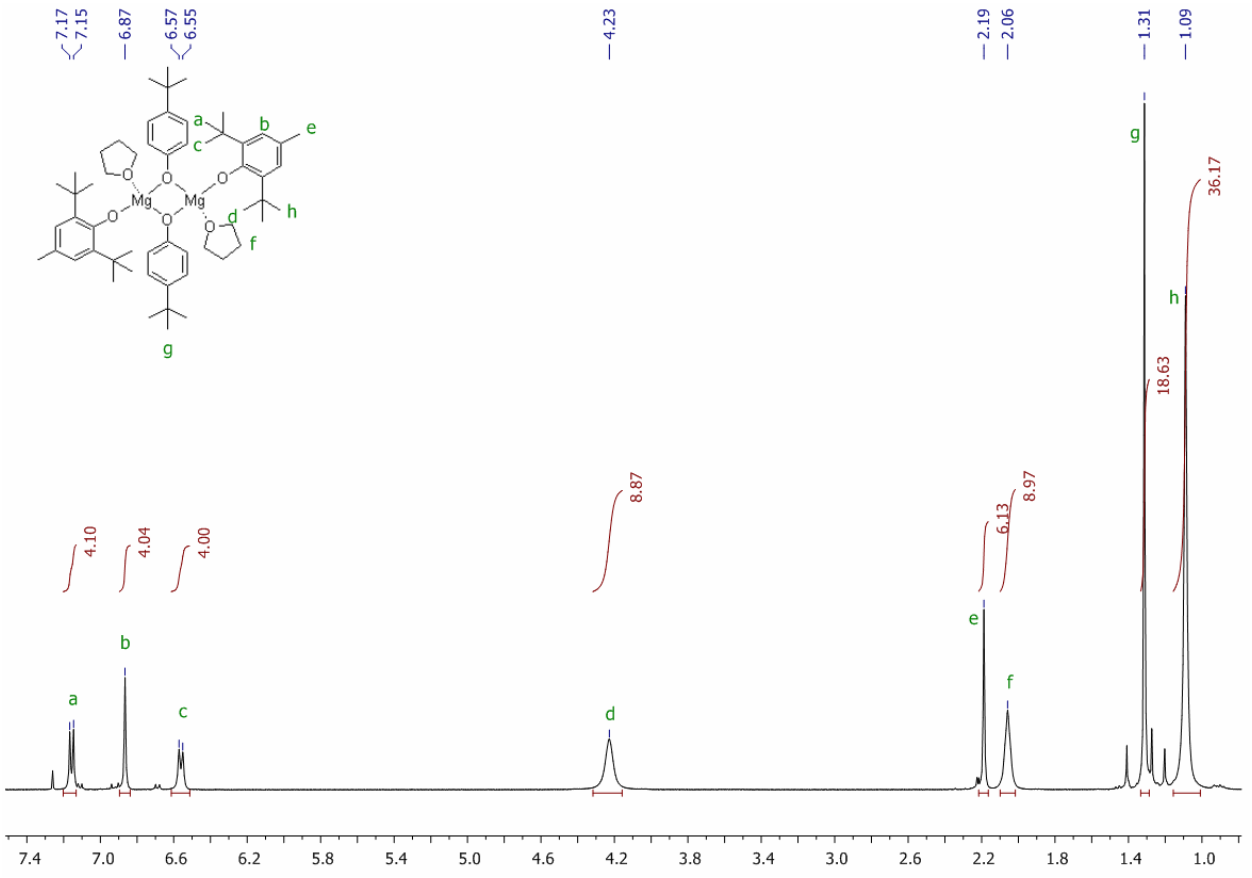

Fig. S5. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**)

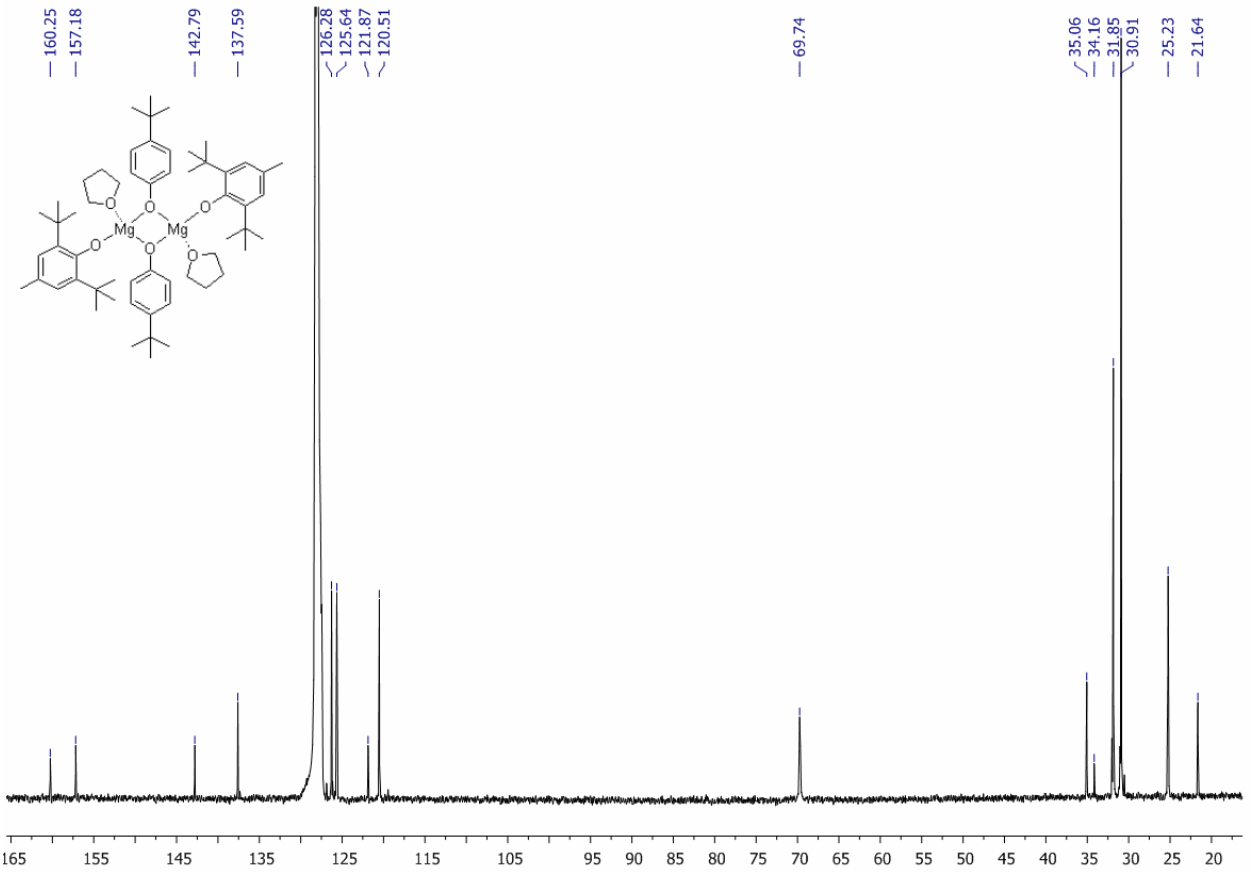

Fig. S6. ^{13}C{^{1}H} NMR spectrum (151 MHz, C_6D_6, 20 °C) of [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**)

S1.5. Synthesis of [(BHT)Mg(μ-OCH_2COOEt)(THF)]$_2$ (5)

A solution of BHT-H (220 mg, 1 mmol) in THF (1 mL) was added dropwise to a stirred solution of Bu_2Mg in heptane (1.0 mL, 1.0M, 1 mmol). After 30 min, a solution of $HOCH_2COOEt$ (104 mg, 1 mmol) in THF (1 mL) was added dropwise to the stirred reaction mixture. The stirring was stopped after 30 min. Hexane (8 mL) was slowly layered on a top of the formed solution. After 14 days, some (55 mg) of formed crystals were taken out for X-ray diffraction analysis. The mother liquor was decanted. The remaining crystals were washed with toluene (2×1 mL), hexane (2×5 mL), dried under vacuum. Total product yield was 305 mg (61%, 0.31 mmol). Anal. found (calcd for $C_{56}H_{98}Mg_2O_{11}$): C, 67.47 (67.53); H, 10.01 (9.92). After prolonged drying *in vacuo* (removing of hexane) ^{1}H NMR (400 MHz, $CDCl_3$, 20 °C): δ 6.93 (s, 4H, m-H_{BHT}); 4.40 (br. s, 4H, OCH_2COO); 4.27 (q, 4H, ^3J = 7.15 Hz, CH_3CH_2O-); 3.90 (m, 12H, $OCH_{2\ THF}$); 2.24 (s, 6H, $CH_{3\ BHT}$); 1.89 (m, 12H, $CH_{2\ THF}$); 1.38 (s, 36H, $(CH_3)_3C_{\ BHT}$); 1.29 (t, ^3J = 7.15 Hz, 6H, CH_3CH_2O-). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$, 20 °C): δ 187.0 (C=O); 161.6 (ipso-C-O_{BHT}); 136.9; 125.4; 118.6; 69.0 (THF); 63.1; 62.6; 34.8 ($(CH_3)_3C_{BHT}$); 30.1 ($(CH_3)_3C_{BHT}$); 25.5 (THF); 21.3 (CH_3-$_{BHT}$) ; 14.2 (CH_3CH_2O-).

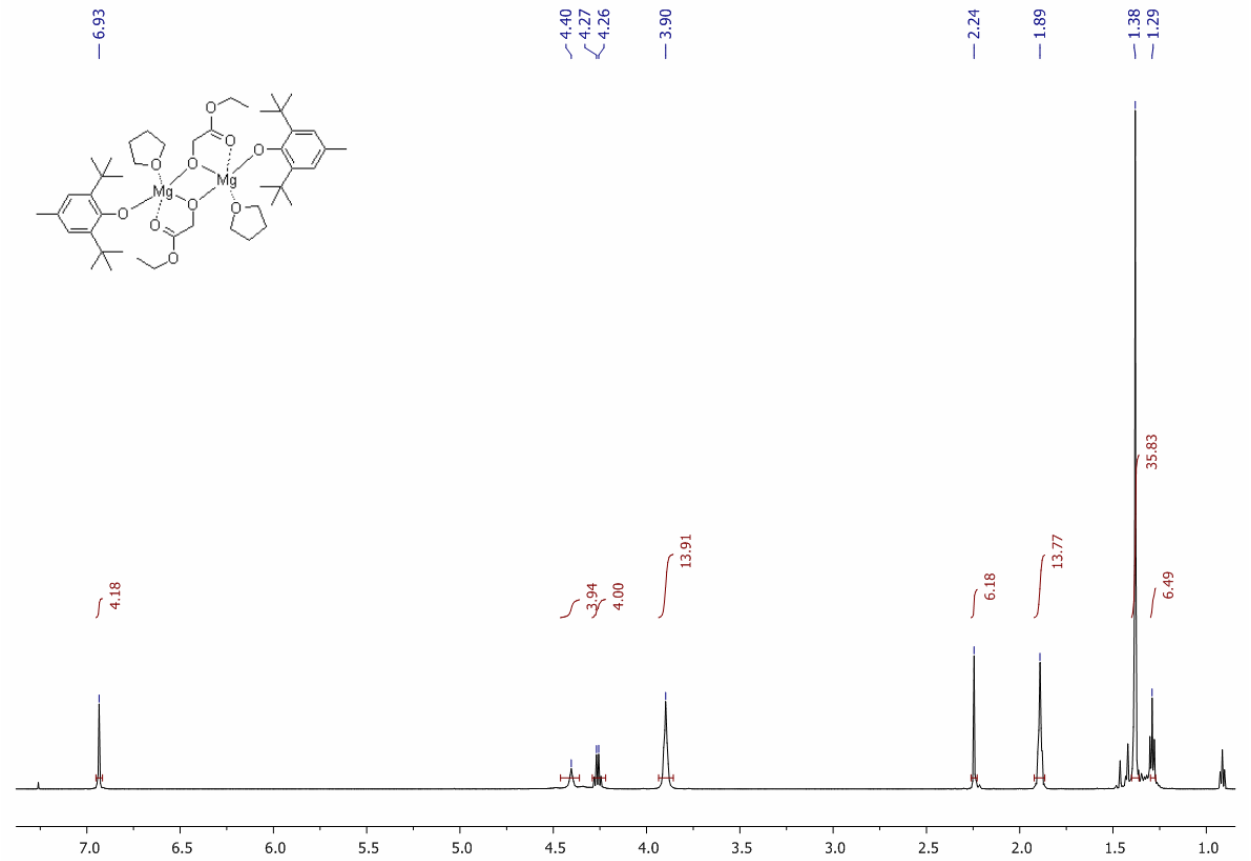

Fig. S7. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 20 °C) of [(BHT)Mg(μ-OCH_2COOEt)(THF)]$_2$ (**5**).

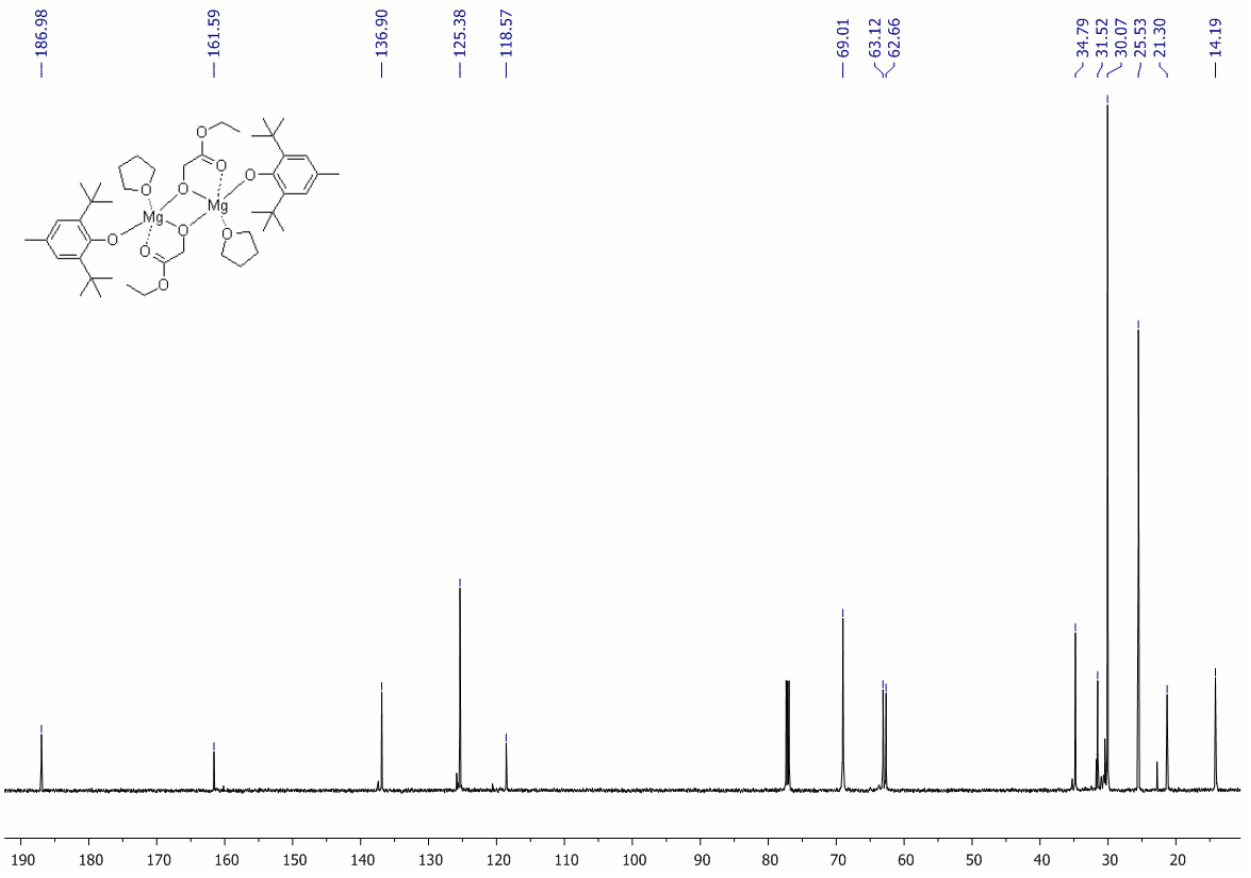

Fig.S8. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 20 °C) of $[(BHT)Mg(\mu\text{-}OCH_2COOEt)(THF)]_2$ (**5**)

S1.6. Synthesis of $[(BHT)Mg(THF)(\mu\text{-}OCH(CH_3)COOCH_2COO^tBu)]_2$ (6)

A solution of BHT-H (220 mg, 1.0 mmol) in THF (1 mL) was added dropwise to a stirred Bu_2Mg solution in heptane (1.0 M, 1.0 mL, 1.0 mmol). After 40 min, a solution of $HOCH(CH_3)COOCH_2COO^tBu$ (204 mg, 1.0 mmol) in THF (1 mL) was added dropwise to the formed reaction mixture. The stirring was stopped 5 min later. Hexane (2 mL) was layered on a top of the formed solution. Crystals were formed within 2 weeks. Some crystals were taken out for the X-ray diffraction studies. The mother liquor was decanted. The remaining crystals were washed with hexane and dried under vacuum. The total yield was 259 mg (0.21 mmol, 42.3%).

Anal. found (calcd for $C_{67}H_{115}Mg_2O_{16}$): C, 65.89 (65.68); H, 9.66 (9.46).

Complex **6** demonstrates dynamic behavior in the solution. Solubility of **6** in benzene-d_6 and in toluene-d_8 is very low, ^1H NMR spectrum of **6** in this solvents contains broadened signals of low intensity. Dissolution of **6** in THF-d_8, $CDCl_3$ and CD_2Cl_2 results in fast decomposition with a formation of $(BHT)_2Mg(THF)_2$ and unidentifiable products.

S1.7. Synthesis of $[(BHT)(OCH_2CH_2CH_2CONMe_2)Mg]_2$ (7)

A solution of $HO(CH_2)_3CONMe_2$ (338 mg, 2.58 mmol) in THF (1 mL) was added dropwise to a stirred solution of $[(BHT)Mg(Bu)(THF)_2]$ (1.148 g, 2.58 mmol) in THF (7 mL). The stirring was stopped after 30 min, when microcrystals started to appear. The solution was decanted from the formed crystals 5 h later. The precipitate was washed with hexane (2×10 mL), dried under dynamic vacuum till the constant weight, yielding 537 mg (0.655 mmol, 50.8%) of microcrystalline powder.

Anal. found (calcd for solvate with one THF molecule $C_{46}H_{78}Mg_2N_2O_7$): C, 67.23 (67.40); H, 9.67 (9.59); N, 3.22 (3.42). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.95 (d, 4H, m-$\underline{H}_{(BHT)}$), 3.75-3.85 (br. m, 6H, $OC\underline{H}_{2(THF)}$ + $OC\underline{H}_2CH_2CH_2N$), 3.08 (s, 6H, $NC\underline{H}_3$), 3.01 (s, 6H, $NC\underline{H}_3$), 2.47 (br. s, 4H, $OCH_2CH_2C\underline{H}_2N$), 2.25 (s, 6H, $C\underline{H}_{3(BHT)}$), 1.87 (m, 2H, $C\underline{H}_{2(THF)}$), 1.71 (br. s, 4H, $OCH_2C\underline{H}_2CH_2N$), 1.44 (s, 36H, $(C\underline{H}_3)_3C_{(BHT)}$). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 177.6; 161.5; 137.7; 125.4; 119.8; 68.4; 64.6; 38.3; 37.2; 35.0; 33.3; 30.7; 29.4; 26.2; 21.4.

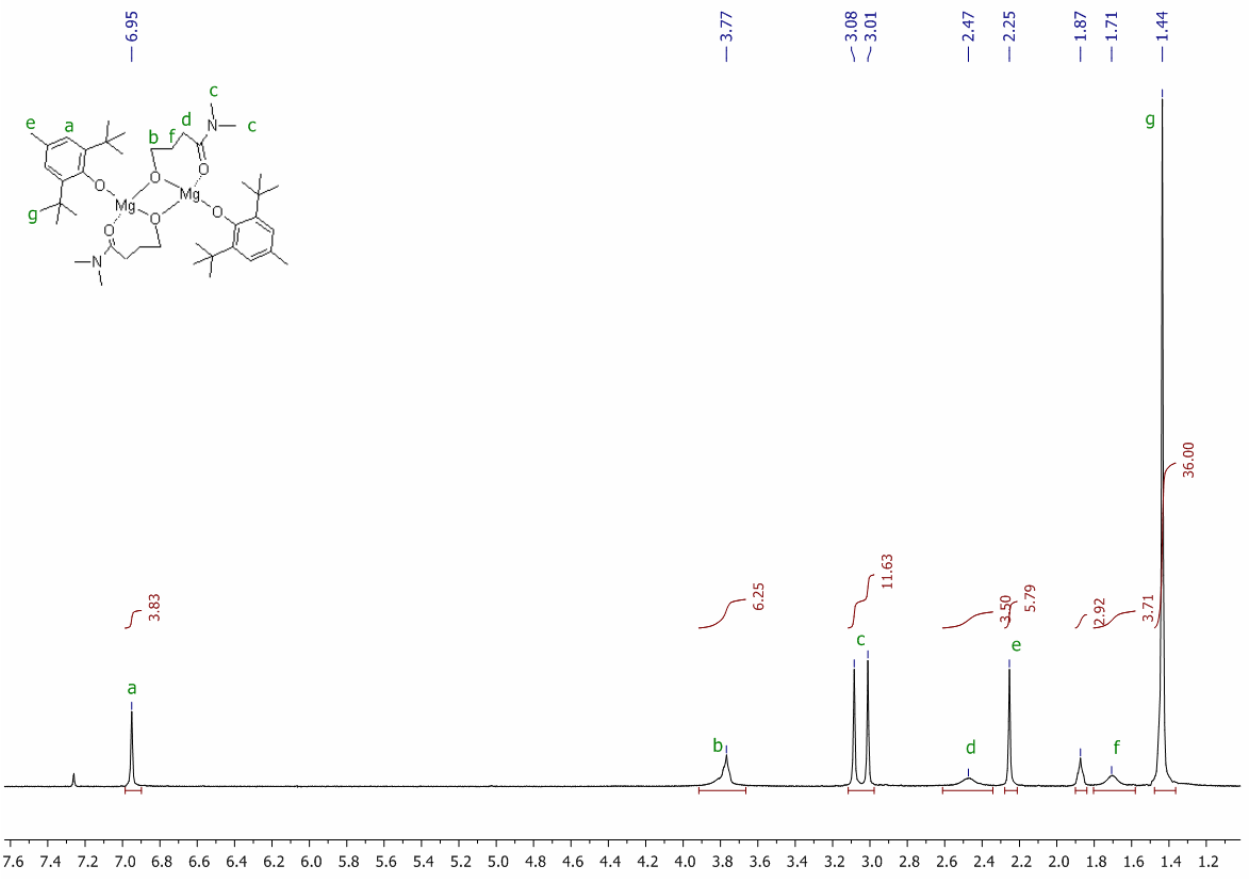

Fig. S9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of $[(BHT)(O(CH_2)_3CONMe_2)Mg]_2$ (**7**)

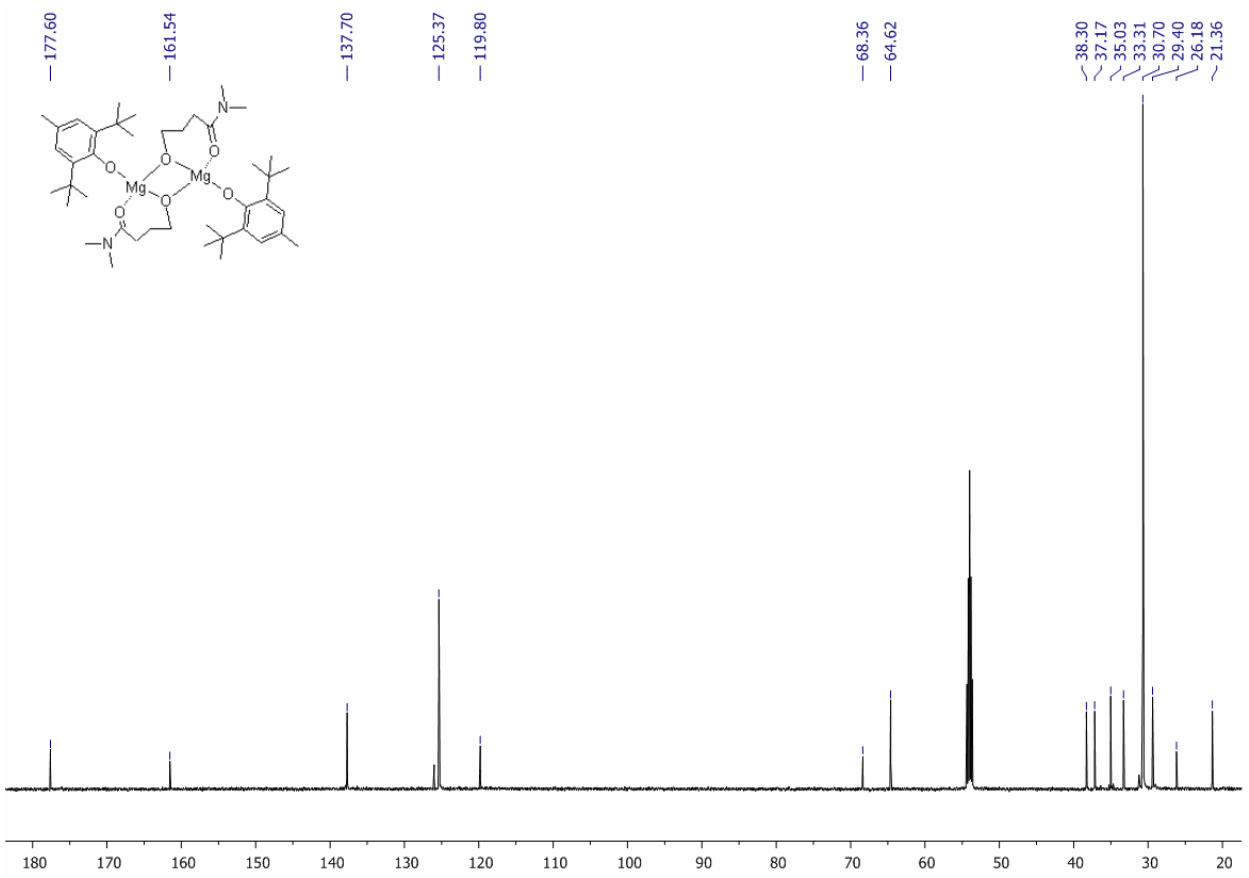

Fig. S10. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, CD_2Cl_2, 20 °C) of $[(BHT)(O(CH_2)_3CONMe_2)Mg]_2$ (**7**)

Crystal growth of $[(BHT)(OCH_2CH_2CH_2CONMe_2)Mg]_2(THF)_3$ *(7-*THF_3*).* A solution of $HO(CH_2)_3CONMe_2$ (66 mg, 0.5 mmol) in a hexane (1 mL) / THF (0.5 mL) mixture was added to a stirred solution of $[(BHT)Mg(Bu)]_2$ (150 mg, 0.25 mmol) in a hexane (4 mL) / THF (0.5 mL) mixture. After 2 days, precipitated crystals were taken for X-ray diffraction studies. Crystals of **7-**$\mathbf{THF_3}$ readily loose some non-coordinating THF molecules upon vacuum drying or recrystallization from aromatic solvents (toluene, benzene).

Crystal growth of $[(BHT)(OCH_2CH_2CH_2CONMe_2)Mg]_2$ *(7).* A solution of $HO(CH_2)_3CONMe_2$ (66 mg, 0.5 mmol) in hexane (1 mL) / toluene (5 mL) mixture was layered on top of a solution of $[(BHT)Mg(Bu)]_2$ (150 mg, 0.25 mmol) in a hexane (1 mL) / toluene (5 mL) mixture. After 2 days, precipitated crystals were taken for X-ray diffraction studies and elemental analysis.

S1.8. Synthesis $[(BHT)_2Mg(DMSO)_2]$ (8)

Method I. From **1**. A solution of DMSO (195 mg, 2.50 mmol) in toluene (1 mL) was added to a stirred solution of $[(BHT)Mg(\mu\text{-}OBn)(THF)]_2$ (106 mg, 0.125 mmol) in toluene (4 mL). After 3 minutes, stirring was stopped. Next day, some precipitated crystals were taken for X-ray

diffraction studies. The remaining crystals were washed with hexane and dried under vacuum. The total yield was 75 mg (121 mmol, 97% based on BHT and 48% based on Mg).

Method II. From **2**. A solution of DMSO (781 mg, 10.0 mmol) in toluene (4 mL) was added to a stirred solution of $[(BHT)_2Mg(THF)_2]$ (607 mg, 1.00 mmol) in toluene (16 mL). After 3 minutes, stirring was stopped. After 2 days, the mother liquor was decanted. Precipitated crystals were washed with hexane (2×5 mL) and dried under dynamic vacuum, yielding 616 mg (0.995 mmol, 99.5%) of colorless needles.

Anal. found (calcd for $C_{34}H_{58}MgO_4S_2$): C, 66.01 (65.94); H, 6.50 (9.44). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ 6.77 (s, 4H, m-H_{BHT}); 2.52 (s, 12H, S-CH_3); 2.12 (s, 6H, $CH_{3\ BHT}$); 1.35 (s, 36H, $(CH_3)_3C_{\ BHT}$). $^{13}C\{^1H\}$ NMR (151 MHz, CD_2Cl_2, 20 °C): δ 161.4 (ipso-C-O_{BHT}); 137.7; 125.4; 119.2; 41.6 (DMSO); 35.3 ($(CH_3)_3C_{BHT}$); 31.3 ($(CH_3)_3C_{BHT}$); 21.3 (CH_3-$_{BHT}$).

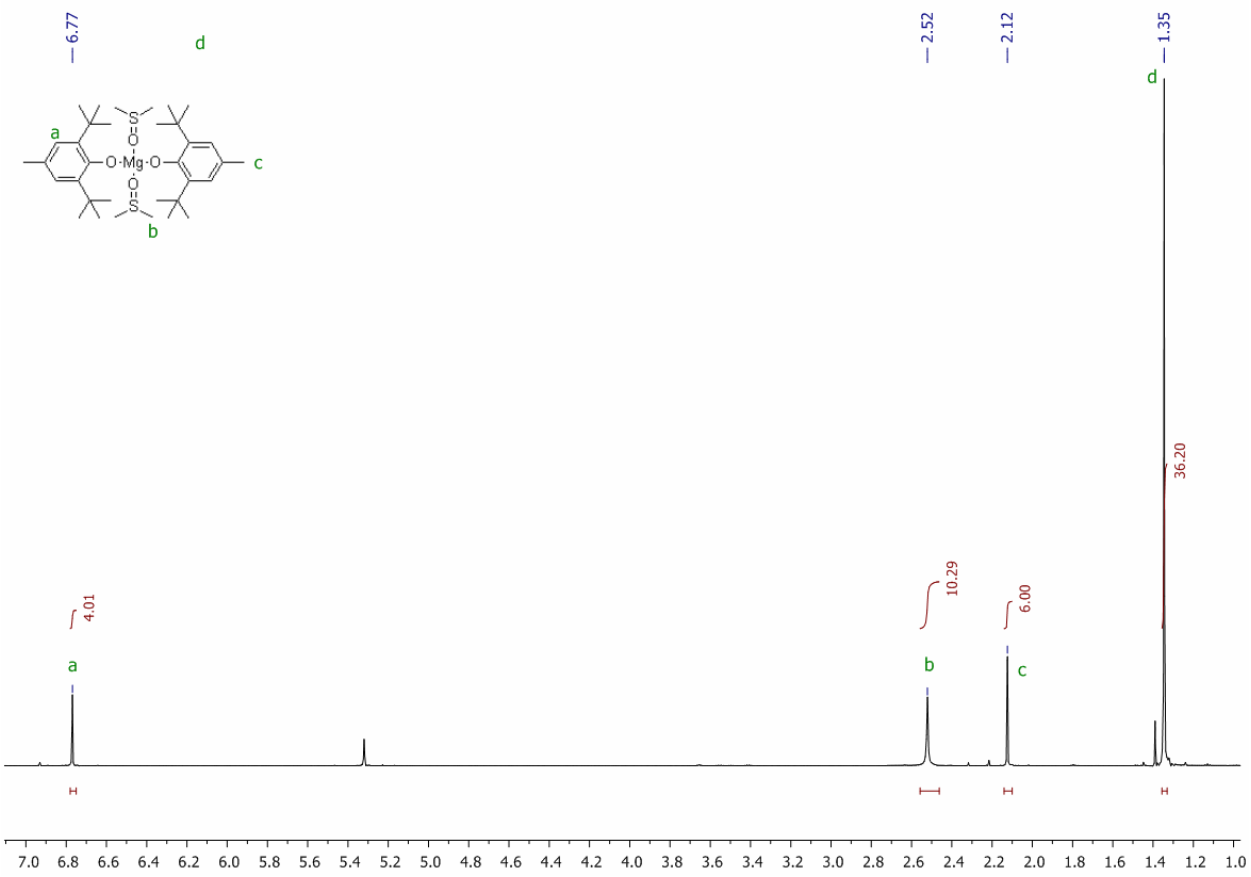

Fig. S11. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2, 20 °C) of $(BHT)_2Mg(DMSO)_2$ (**8**)

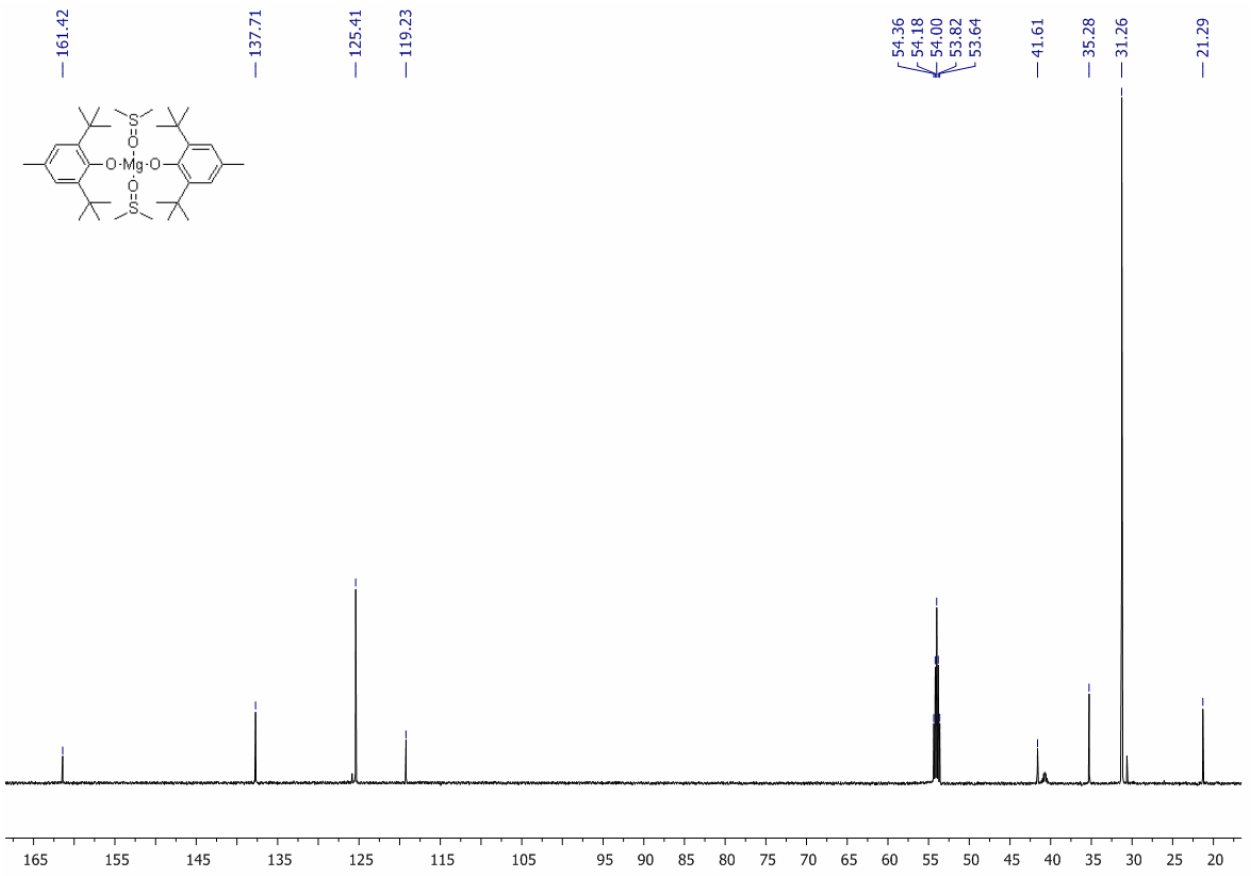

Fig. S12. $^{13}C\{^{1}H\}$ NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of $(BHT)_2Mg(DMSO)_2$ (**8**)

References

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2. I. E. Nifant'ev, A. V. Shlyakhtin, A. N. Tavtorkin, P. V. Ivchenko, R. S. Borisov and A. V. Churakov, *Catal. Commun.*, 2016, **87**, 106-111.

S2. X-ray diffraction studies

S2.1. General remarks and crystal data for compounds 1, 3–8

X-ray diffraction data were collected on a SMART APEX II area-detector diffractometer (graphite monochromator, ω-scan technique) using Mo-*K*α radiation. The intensity data were integrated by the SAINT program[1] and were corrected for absorption, using SADABS.[2] All structures were solved by direct methods and refined by full-matrix least squares on F^2.[3,4] All non-hydrogen atoms (except minor components of disordered fragments) were refined with anisotropic displacement parameters. All hydrogen atoms in [(BHT)Mg(OC_6H_4-4-^{tert}Bu)(THF)]$_2$ (**4**) were found from difference Fourier map and refined isotropically. In all other cases hydrogen atoms were placed in calculated positions (C-H distance = 0.95 Å for aromatic, 0.98 Å for methyl, 0.99 Å for methylene, 1.00 Å for tertiary hydrogen atoms) and refined using a riding model with isotropic displacement parameters taken as U_{iso}(H)=1.5U_{eq}(C) for methyl and 1.2U_{eq}(C) for other hydrogen atoms. A rotating group model was applied for methyl groups. The structures [(BHT)Mg(OBn)(THF)]$_2$ (**3**), [(BHT)Mg(OCH_2COOEt)(THF)]$_2$ (**5**), [(BHT)Mg(OCH(CH_3)$COOCH_2COO^tBu$)(THF)]$_2$ (**6**) and [BHT_2Mg(DMSO)$_2$] (**8**) contain conformationally disordered THF or DMSO ligands. The structure [BHT_2Mg(THF)$_2$] (**1**) contains a rotationally disordered *tert*-Bu fragment.

The structure **5** contains two highly disordered solvent molecules in the crystal channels, presumably THF and hexane, which were removed from the model by the SQUEEZE method.[5] See supplementary material for additional details on crystallographic models. SHELXTL[3] was used for molecular graphics. Crystal data, data collection and structure refinement details are summarized in Table S1.

Table S1. X-ray experimental details for the studied compounds.

	1	**3**	**4**	**5**
Empirical formula	$C_{38}H_{62}MgO_4$	$C_{52}H_{76}Mg_2O_6$	$C_{58}H_{88}Mg_2O_6$	$C_{56}H_{98}Mg_2O_{11}$
Formula weight	607.19	845.75	929.90	995.96
Temperature (K)	150(2)	180(2)	150(2)	150(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	$P2_1$	*P*nma	$P2_1/n$	$P2_1/c$
Unit Cell Dimensions				
a (Å)	10.4071(12)	20.396(3)	11.3771(6)	22.1915(12)
b (Å)	15.6408(18)	44.791(7)	11.1182(5)	9.8778(6)
c (Å)	11.4503(13)	11.0745(18)	23.0252(11)	26.2892(15)
β (º)	100.837(2)	90.00	101.382(1)	91.322(1)
Volume (Å^3)	1830.6(4)	10117(3)	2855.2(2)	5761.1(6)
Z	2	8	2	4
D_{calcd} (g/cm^3)	1.102	1.111	1.082	1.148
μ (mm^{-1})	0.084	0.093	0.087	0.097
$F(000)$	668	3680	1016	2184
Θ Range (º)	2.23-27.00	2.14-25.50	2.57-29.00	0.92-26.00
Index Ranges	-13≤h≤13 -19≤k≤19 -14≤l≤14	-24≤h≤24 -54≤k≤54 -13≤l≤13	-15≤h≤15 -15≤k≤15 -31≤l≤31	-27≤h≤27 -12≤k≤12 -32≤l≤32
Reflections collected	17740	84710	31112	49247
Reflections unique [R_{int}]	4143 [0.0355]	9556 [0.0567]	7595 [0.0236]	11320 [0.0315]
Reflections with $I > 2\sigma(I)$	3706	7271	6050	8362
Variables / restraints	433 / 1	555 / 40	474 / 0	557 / 51
Goodness-of-fit on F^2	1.027	1.030	1.021	1.042
Final R_1, wR_2 Indices with [$I>2\sigma(I)$]	0.0360, 0.0864	0.0628, 0.1644	0.0393, 0.1009	0.0594, 0.1627
R_1, wR_2 Indices (all data)	0.0422, 0.0904	0.0832, 0.1802	0.0534, 0.1106	0.0800, 0.1757
Largest difference in peak / hole (e/Å^3)	0.236 / -0.198	0.831 / -0.692	0.341 / -0.180	0.606 / -0.328
CCDC number	1545645	1463808	1545646	1545650

Table S1 (*continued*). X-ray experimental details for the studied compounds.

	6	**7**	**7'**	**8**
Empirical formula	$C_{67}H_{115}Mg_2O_{16}$	$C_{42}H_{70}Mg_2N_2O_6$	$C_{54}H_{94}Mg_2N_2O_9$	$C_{34}H_{58}MgO_4S_2$
Formula weight	1225.21	747.62	963.93	619.23
Temperature (K)	150(2)	150(2)	150(2)	150(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$C2/c$	$P2_1/n$
Unit Cell Dimensions				
a (Å)	15.7519(16)	10.4550(5)	23.5726(12)	14.3828(7)
b (Å)	26.940(3)	11.6723(6)	15.9574(8)	16.4536(8)
c (Å)	17.4774(18)	17.9485(9)	16.2479(8)	15.7807(8)
β (º)	104.308(2)	93.7360(7)	112.1687(7)	102.6563(8)
Volume ($Å^3$)	7186.6(13)	2185.67(19)	5660.0(5)	3643.7(3)
Z	4	2	4	4
D_{calcd} (g/cm^3)	1.132	1.136	1.131	1.129
μ (mm^{-1})	0.094	0.100	0.095	0.196
$F(000)$	2676	816	2112	1352
Θ Range (º)	2.02- 26.00	2.27-30.00	2.30-28.00	1.74-27.00
Index Ranges	-19≤h≤19 -33≤k≤33 -21≤l≤21	-14≤h≤14 -16≤k≤16 -25≤l≤25	-31≤h≤31 -21≤k≤21 -21≤l≤21	-18≤h≤18 -21≤k≤21 -20≤l≤20
Reflections collected	64794	25816	27031	35284
Reflections unique [R_{int}]	14129 [0.0366]	6366 [0.0225]	6804 [0.0278]	7948 [0.0236]
Reflections with $I > 2\sigma(I)$	10497	5278	5256	6730
Variables / restraints	774 / 32	276 / 0	312 / 30	422 / 34
Goodness-of-fit on F^2	1.029	1.033	1.047	1.032
Final R_1, wR_2 Indices with [$I>2\sigma(I)$]	0.0737, 0.2035	0.0419, 0.1147	0.0582, 0.1679	0.0447, 0.1145
R_1, wR_2 Indices (all data)	0.0980, 0.2233	0.0517, 0.1224	0.0749, 0.1837	0.0540, 0.1221
Largest difference in peak / hole ($e/Å^3$)	0.850 / -0.576	0.376 / -0.225	0.762 / -0.416	0.830 / -0.626
CCDC number	1545642	1545643	1545641	1545648

S2.2. Molecular structure of $(BHT)_2Mg(THF)_2$ (1)

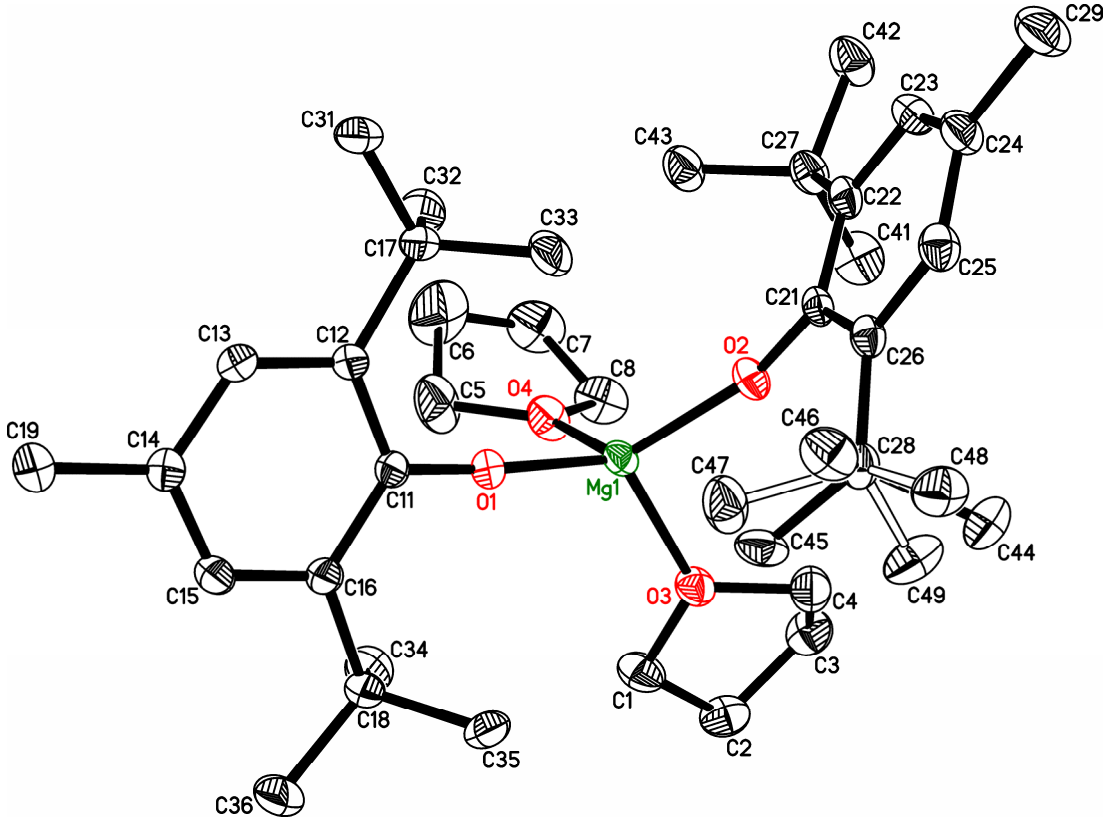

Fig. S13. Molecular structure of $(BHT)_2Mg(THF)_2$ (**1**). Disordered *tert*-Bu fragment is shown with open solid lines. H-atoms are omitted. Thermal ellipsoids are set to the 50% probability level

Mg-atom (c.n.=4) adopts distorted tetrahedral environment (Fig. S13). The lowest value of O-Mg-O angles corresponds the O_{THF}-Mg-O_{THF} angle. Mg-O_{BHT} bond lengths are slightly shorter than Mg-O_{THF}. One of ^{t}Bu-group of the BHT ligand in $(BHT)_2Mg(THF)_2$ is disordered over two positions.

Table S2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2$ $x10^3$) for $(BHT)_2Mg(THF)_2$ (**1**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U(eq)
Mg(1)	5084(1)	5308(1)	2684(1)	24(1)
O(1)	6288(1)	4671(1)	3727(1)	28(1)
O(2)	3456(1)	4904(1)	1939(1)	27(1)
O(3)	4543(2)	6535(1)	2984(1)	31(1)
O(4)	6327(2)	5776(1)	1633(1)	37(1)
C(1)	5399(3)	7233(2)	3494(2)	39(1)
C(2)	4637(3)	8052(2)	3158(2)	41(1)
C(3)	3563(3)	7785(2)	2131(2)	44(1)
C(4)	3268(3)	6889(2)	2486(3)	41(1)
C(5)	7710(3)	5608(3)	1746(3)	56(1)
C(6)	7882(4)	5501(3)	487(3)	79(1)
C(7)	6925(3)	6130(2)	-207(3)	61(1)
C(8)	5992(3)	6339(2)	613(2)	48(1)
C(11)	7085(2)	4148(2)	4441(2)	25(1)
C(12)	7241(2)	3280(2)	4124(2)	30(1)

C(13)	8137(2)	2771(2)	4876(2)	33(1)
C(14)	8863(2)	3060(2)	5941(2)	31(1)
C(15)	8668(2)	3901(2)	6255(2)	30(1)
C(16)	7810(2)	4454(1)	5549(2)	26(1)
C(17)	6474(3)	2888(2)	2964(2)	45(1)
C(18)	7681(2)	5379(2)	5961(2)	29(1)
C(19)	9842(2)	2488(2)	6702(2)	39(1)
C(21)	2532(2)	4314(1)	1625(2)	23(1)
C(22)	2228(2)	4027(1)	424(2)	26(1)
C(23)	1310(2)	3379(2)	116(2)	32(1)
C(24)	657(2)	3002(2)	931(2)	33(1)
C(25)	914(2)	3314(2)	2083(2)	29(1)
C(26)	1818(2)	3966(1)	2461(2)	25(1)
C(27)	2847(2)	4449(2)	-553(2)	32(1)
C(28)	1905(2)	4289(2)	3745(2)	27(1)
C(29)	-326(3)	2296(2)	562(3)	45(1)
C(31)	6760(4)	1927(2)	2877(3)	76(1)
C(32)	6863(3)	3343(3)	1889(2)	63(1)
C(33)	4994(3)	2956(2)	2922(3)	48(1)
C(34)	8114(3)	6010(2)	5083(3)	41(1)
C(35)	6263(2)	5560(2)	6095(2)	35(1)
C(36)	8547(3)	5562(2)	7183(2)	46(1)
C(41)	2501(3)	5401(2)	-604(2)	46(1)
C(42)	2320(3)	4079(2)	-1799(2)	44(1)
C(43)	4329(2)	4306(2)	-329(2)	39(1)
C(44)	660(5)	4770(3)	3772(5)	47(1)
C(45)	3089(4)	4826(3)	4268(4)	36(1)
C(46)	1963(5)	3498(3)	4570(4)	39(1)
C(47)	3253(6)	4143(6)	4536(5)	44(2)
C(48)	930(6)	3884(4)	4462(5)	38(2)
C(49)	1567(7)	5269(4)	3745(6)	46(2)

Table S3. Anisotropic displacement parameters ($Å^2$ x10^3) for $(BHT)_2Mg(THF)_2$ (**1**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	22(1)	27(1)	23(1)	-2(1)	3(1)	-5(1)
O(1)	22(1)	33(1)	29(1)	-4(1)	1(1)	3(1)
O(2)	24(1)	27(1)	30(1)	3(1)	0(1)	-6(1)
O(3)	31(1)	25(1)	37(1)	-3(1)	2(1)	-4(1)
O(4)	31(1)	53(1)	29(1)	1(1)	10(1)	-11(1)
C(1)	46(1)	31(1)	39(1)	-5(1)	1(1)	-9(1)
C(2)	52(2)	27(1)	46(2)	-2(1)	16(1)	-5(1)
C(3)	50(2)	40(1)	41(1)	5(1)	10(1)	7(1)
C(4)	33(1)	37(1)	52(2)	-3(1)	3(1)	2(1)
C(5)	30(1)	87(2)	53(2)	3(2)	13(1)	-14(1)
C(6)	67(2)	112(3)	69(2)	7(2)	44(2)	2(2)
C(7)	68(2)	78(2)	43(2)	3(2)	27(2)	-17(2)
C(8)	57(2)	49(2)	40(1)	4(1)	17(1)	-14(1)
C(11)	17(1)	34(1)	25(1)	-6(1)	5(1)	1(1)
C(12)	22(1)	37(1)	29(1)	-12(1)	1(1)	4(1)

C(13)	27(1)	32(1)	37(1)	-13(1)	2(1)	6(1)
C(14)	24(1)	36(1)	31(1)	-5(1)	2(1)	5(1)
C(15)	24(1)	39(1)	26(1)	-9(1)	2(1)	-1(1)
C(16)	20(1)	32(1)	27(1)	-7(1)	6(1)	-1(1)
C(17)	39(1)	46(2)	41(1)	-24(1)	-13(1)	17(1)
C(18)	27(1)	29(1)	30(1)	-9(1)	2(1)	-2(1)
C(19)	32(1)	41(1)	37(1)	-5(1)	-4(1)	7(1)
C(21)	18(1)	21(1)	28(1)	2(1)	-2(1)	0(1)
C(22)	21(1)	27(1)	26(1)	4(1)	-2(1)	1(1)
C(23)	30(1)	33(1)	29(1)	-4(1)	-1(1)	-4(1)
C(24)	28(1)	32(1)	38(1)	-4(1)	1(1)	-7(1)
C(25)	25(1)	28(1)	35(1)	4(1)	6(1)	-4(1)
C(26)	21(1)	24(1)	29(1)	4(1)	1(1)	1(1)
C(27)	30(1)	38(1)	26(1)	5(1)	0(1)	-3(1)
C(28)	23(1)	31(1)	29(1)	4(1)	8(1)	-1(1)
C(29)	41(1)	45(1)	47(2)	-11(1)	6(1)	-17(1)
C(31)	66(2)	62(2)	79(2)	-50(2)	-38(2)	35(2)
C(32)	51(2)	100(3)	33(1)	-28(2)	-6(1)	27(2)
C(33)	35(1)	30(1)	68(2)	-17(1)	-18(1)	2(1)
C(34)	39(1)	36(1)	49(2)	-4(1)	7(1)	-9(1)
C(35)	34(1)	33(1)	40(1)	-13(1)	11(1)	3(1)
C(36)	49(2)	40(1)	43(2)	-19(1)	-8(1)	2(1)
C(41)	54(2)	43(2)	39(1)	18(1)	6(1)	0(1)
C(42)	37(1)	67(2)	25(1)	1(1)	1(1)	-7(1)
C(43)	30(1)	60(2)	29(1)	-5(1)	6(1)	-7(1)
C(44)	37(2)	50(3)	56(3)	-8(2)	12(2)	15(2)
C(45)	40(2)	44(3)	26(2)	-12(2)	13(2)	-14(2)
C(46)	45(3)	45(3)	28(2)	4(2)	7(2)	-7(2)
C(47)	28(3)	73(5)	32(3)	2(3)	8(2)	-2(3)
C(48)	43(4)	40(3)	36(3)	-1(3)	18(3)	-8(3)
C(49)	59(4)	32(3)	55(4)	-2(3)	29(3)	6(3)

Table S4. Bond lengths for non-hydrogen atoms (Å) for $(BHT)_2Mg(THF)_2$ (**1**)

Atoms	Bond length	Atoms	Bond length	Atoms	Bond length
Mg(1)-O(1)	1.8514(16)	C(11)-C(16)	1.431(3)	C(22)-C(23)	1.392(3)
Mg(1)-O(2)	1.8589(16)	C(12)-C(13)	1.394(3)	C(22)-C(27)	1.540(3)
Mg(1)-O(3)	2.0464(18)	C(12)-C(17)	1.542(3)	C(23)-C(24)	1.386(3)
Mg(1)-O(4)	2.0603(17)	C(13)-C(14)	1.384(3)	C(24)-C(25)	1.384(3)
O(1)-C(11)	1.330(3)	C(14)-C(15)	1.389(3)	C(24)-C(29)	1.511(3)
O(2)-C(21)	1.333(2)	C(14)-C(19)	1.505(3)	C(25)-C(26)	1.400(3)
O(3)-C(4)	1.452(3)	C(15)-C(16)	1.388(3)	C(26)-C(28)	1.541(3)
O(3)-C(1)	1.459(3)	C(16)-C(18)	1.535(3)	C(27)-C(41)	1.531(4)
O(4)-C(5)	1.445(3)	C(17)-C(33)	1.536(4)	C(27)-C(43)	1.532(3)
O(4)-C(8)	1.451(3)	C(17)-C(31)	1.539(4)	C(27)-C(42)	1.542(3)
C(1)-C(2)	1.517(4)	C(17)-C(32)	1.541(5)	C(28)-C(44)	1.504(5)
C(2)-C(3)	1.520(4)	C(18)-C(34)	1.536(4)	C(28)-C(45)	1.519(5)
C(3)-C(4)	1.507(4)	C(18)-C(35)	1.539(3)	C(28)-C(47)	1.537(6)
C(5)-C(6)	1.495(5)	C(18)-C(36)	1.542(3)	C(28)-C(46)	1.550(5)
C(6)-C(7)	1.515(5)	C(21)-C(26)	1.425(3)	C(28)-C(48)	1.554(6)
C(7)-C(8)	1.509(4)	C(21)-C(22)	1.425(3)	C(28)-C(49)	1.573(7)
C(11)-C(12)	1.423(3)				

Table S5. Bond angles for non-hydrogen atoms (°) for $(BHT)_2Mg(THF)_2$ (**1**)

Atoms	Bond angles	Atoms	Bond angles
O(1)-Mg(1)-O(2)	124.11(8)	C(31)-C(17)-C(12)	111.7(2)
O(1)-Mg(1)-O(3)	124.82(7)	C(32)-C(17)-C(12)	109.5(2)
O(2)-Mg(1)-O(3)	98.06(7)	C(16)-C(18)-C(34)	110.54(19)
O(1)-Mg(1)-O(4)	98.33(7)	C(16)-C(18)-C(35)	110.21(18)
O(2)-Mg(1)-O(4)	118.10(7)	C(34)-C(18)-C(35)	110.6(2)
O(3)-Mg(1)-O(4)	89.29(8)	C(16)-C(18)-C(36)	112.6(2)
C(11)-O(1)-Mg(1)	174.60(15)	C(34)-C(18)-C(36)	106.3(2)
C(21)-O(2)-Mg(1)	155.31(14)	C(35)-C(18)-C(36)	106.49(19)
C(4)-O(3)-C(1)	108.43(18)	O(2)-C(21)-C(26)	121.61(18)
C(4)-O(3)-Mg(1)	123.46(14)	O(2)-C(21)-C(22)	119.73(18)
C(1)-O(3)-Mg(1)	127.00(14)	C(26)-C(21)-C(22)	118.66(18)
C(5)-O(4)-C(8)	105.5(2)	C(23)-C(22)-C(21)	119.4(2)
C(5)-O(4)-Mg(1)	127.39(17)	C(23)-C(22)-C(27)	119.31(19)
C(8)-O(4)-Mg(1)	127.11(16)	C(21)-C(22)-C(27)	121.28(18)
O(3)-C(1)-C(2)	106.21(19)	C(24)-C(23)-C(22)	122.7(2)
C(1)-C(2)-C(3)	103.8(2)	C(25)-C(24)-C(23)	117.4(2)
C(4)-C(3)-C(2)	101.8(2)	C(25)-C(24)-C(29)	121.6(2)
O(3)-C(4)-C(3)	104.0(2)	C(23)-C(24)-C(29)	121.0(2)
O(4)-C(5)-C(6)	103.4(2)	C(24)-C(25)-C(26)	123.4(2)
C(5)-C(6)-C(7)	104.3(3)	C(25)-C(26)-C(21)	118.4(2)
C(8)-C(7)-C(6)	104.5(2)	C(25)-C(26)-C(28)	116.71(19)
O(4)-C(8)-C(7)	106.5(3)	C(21)-C(26)-C(28)	124.82(18)
O(1)-C(11)-C(12)	121.17(18)	C(41)-C(27)-C(43)	111.8(2)
O(1)-C(11)-C(16)	120.25(19)	C(41)-C(27)-C(22)	108.5(2)
C(12)-C(11)-C(16)	118.58(19)	C(43)-C(27)-C(22)	111.20(18)
C(13)-C(12)-C(11)	118.86(19)	C(41)-C(27)-C(42)	106.8(2)
C(13)-C(12)-C(17)	118.8(2)	C(43)-C(27)-C(42)	105.8(2)
C(11)-C(12)-C(17)	122.3(2)	C(22)-C(27)-C(42)	112.71(19)
C(14)-C(13)-C(12)	123.3(2)	C(44)-C(28)-C(45)	110.7(3)
C(13)-C(14)-C(15)	117.1(2)	C(44)-C(28)-C(26)	106.7(2)
C(13)-C(14)-C(19)	121.0(2)	C(45)-C(28)-C(26)	117.1(2)
C(15)-C(14)-C(19)	121.9(2)	C(47)-C(28)-C(26)	113.4(3)
C(16)-C(15)-C(14)	123.2(2)	C(44)-C(28)-C(46)	108.8(3)
C(15)-C(16)-C(11)	118.87(19)	C(45)-C(28)-C(46)	105.4(3)
C(15)-C(16)-C(18)	119.44(19)	C(26)-C(28)-C(46)	107.9(2)
C(11)-C(16)-C(18)	121.68(19)	C(47)-C(28)-C(48)	104.0(4)
C(33)-C(17)-C(31)	105.7(3)	C(26)-C(28)-C(48)	116.3(3)
C(33)-C(17)-C(32)	110.8(2)	C(47)-C(28)-C(49)	108.9(5)
C(31)-C(17)-C(32)	108.5(3)	C(26)-C(28)-C(49)	110.3(3)
C(33)-C(17)-C(12)	110.7(2)	C(48)-C(28)-C(49)	103.3(4)

Table S6. Torsion angles (°) for $(BHT)_2Mg(THF)_2$ (**1**)

Atoms	Torsion angles	Atoms	Torsion angles
O(1)-Mg(1)-O(2)-C(21)	-8.1(4)	C(13)-C(12)-C(17)-C(31)	5.0(4)
O(3)-Mg(1)-O(2)-C(21)	-150.6(3)	C(11)-C(12)-C(17)-C(31)	-176.4(3)
O(4)-Mg(1)-O(2)-C(21)	115.9(3)	C(13)-C(12)-C(17)-C(32)	-115.1(3)
O(1)-Mg(1)-O(3)-C(4)	-151.42(17)	C(11)-C(12)-C(17)-C(32)	63.5(3)
O(2)-Mg(1)-O(3)-C(4)	-9.38(19)	C(15)-C(16)-C(18)-C(34)	117.2(2)
O(4)-Mg(1)-O(3)-C(4)	108.91(18)	C(11)-C(16)-C(18)-C(34)	-61.5(3)
O(1)-Mg(1)-O(3)-C(1)	42.0(2)	C(15)-C(16)-C(18)-C(35)	-120.2(2)
O(2)-Mg(1)-O(3)-C(1)	-175.93(18)	C(11)-C(16)-C(18)-C(35)	61.0(3)
O(4)-Mg(1)-O(3)-C(1)	-57.64(19)	C(15)-C(16)-C(18)-C(36)	-1.5(3)
O(1)-Mg(1)-O(4)-C(5)	0.6(2)	C(11)-C(16)-C(18)-C(36)	179.7(2)
O(2)-Mg(1)-O(4)-C(5)	-135.5(2)	Mg(1)-O(2)-C(21)-C(26)	72.1(4)
O(3)-Mg(1)-O(4)-C(5)	125.7(2)	Mg(1)-O(2)-C(21)-C(22)	-108.8(3)
O(1)-Mg(1)-O(4)-C(8)	180.0(2)	O(2)-C(21)-C(22)-C(23)	176.7(2)
O(2)-Mg(1)-O(4)-C(8)	43.9(2)	C(26)-C(21)-C(22)-C(23)	-4.2(3)
O(3)-Mg(1)-O(4)-C(8)	-54.9(2)	O(2)-C(21)-C(22)-C(27)	-6.2(3)
C(4)-O(3)-C(1)-C(2)	-6.6(3)	C(26)-C(21)-C(22)-C(27)	172.92(19)
Mg(1)-O(3)-C(1)-C(2)	161.64(16)	C(21)-C(22)-C(23)-C(24)	1.0(3)
O(3)-C(1)-C(2)-C(3)	-18.3(3)	C(27)-C(22)-C(23)-C(24)	-176.3(2)
C(1)-C(2)-C(3)-C(4)	35.0(3)	C(22)-C(23)-C(24)-C(25)	2.1(4)
C(1)-O(3)-C(4)-C(3)	29.1(3)	C(22)-C(23)-C(24)-C(29)	-179.6(2)
Mg(1)-O(3)-C(4)-C(3)	-139.63(17)	C(23)-C(24)-C(25)-C(26)	-1.9(3)
C(2)-C(3)-C(4)-O(3)	-39.4(3)	C(29)-C(24)-C(25)-C(26)	179.8(2)
C(8)-O(4)-C(5)-C(6)	-40.3(3)	C(24)-C(25)-C(26)-C(21)	-1.3(3)
Mg(1)-O(4)-C(5)-C(6)	139.2(3)	C(24)-C(25)-C(26)-C(28)	175.1(2)
O(4)-C(5)-C(6)-C(7)	35.5(4)	O(2)-C(21)-C(26)-C(25)	-176.53(19)
C(5)-C(6)-C(7)-C(8)	-17.5(4)	C(22)-C(21)-C(26)-C(25)	4.4(3)
C(5)-O(4)-C(8)-C(7)	29.2(3)	O(2)-C(21)-C(26)-C(28)	7.3(3)
Mg(1)-O(4)-C(8)-C(7)	-150.26(19)	C(22)-C(21)-C(26)-C(28)	-171.79(18)
C(6)-C(7)-C(8)-O(4)	-6.5(3)	C(23)-C(22)-C(27)-C(41)	118.8(2)
O(1)-C(11)-C(12)-C(13)	176.8(2)	C(21)-C(22)-C(27)-C(41)	-58.3(3)
C(16)-C(11)-C(12)-C(13)	-3.0(3)	C(23)-C(22)-C(27)-C(43)	-117.9(2)
O(1)-C(11)-C(12)-C(17)	-1.8(3)	C(21)-C(22)-C(27)-C(43)	65.0(3)
C(16)-C(11)-C(12)-C(17)	178.4(2)	C(23)-C(22)-C(27)-C(42)	0.7(3)
C(11)-C(12)-C(13)-C(14)	2.0(4)	C(21)-C(22)-C(27)-C(42)	-176.4(2)
C(17)-C(12)-C(13)-C(14)	-179.4(2)	C(25)-C(26)-C(28)-C(44)	-70.2(3)
C(12)-C(13)-C(14)-C(15)	0.1(4)	C(21)-C(26)-C(28)-C(44)	106.1(3)
C(12)-C(13)-C(14)-C(19)	-178.5(2)	C(25)-C(26)-C(28)-C(45)	165.2(3)
C(13)-C(14)-C(15)-C(16)	-1.1(3)	C(21)-C(26)-C(28)-C(45)	-18.5(4)
C(19)-C(14)-C(15)-C(16)	177.4(2)	C(25)-C(26)-C(28)-C(47)	117.8(4)
C(14)-C(15)-C(16)-C(11)	0.0(3)	C(21)-C(26)-C(28)-C(47)	-66.0(4)
C(14)-C(15)-C(16)-C(18)	-178.8(2)	C(25)-C(26)-C(28)-C(46)	46.7(3)
O(1)-C(11)-C(16)-C(15)	-177.75(19)	C(21)-C(26)-C(28)-C(46)	-137.1(3)
C(12)-C(11)-C(16)-C(15)	2.1(3)	C(25)-C(26)-C(28)-C(48)	-2.7(4)
O(1)-C(11)-C(16)-C(18)	1.0(3)	C(21)-C(26)-C(28)-C(48)	173.5(3)
C(12)-C(11)-C(16)-C(18)	-179.1(2)	C(25)-C(26)-C(28)-C(49)	-119.8(3)
C(13)-C(12)-C(17)-C(33)	122.5(3)	C(21)-C(26)-C(28)-C(49)	56.4(4)
C(11)-C(12)-C(17)-C(33)	-58.9(3)		

S2.3. Molecular structure of [(BHT)Mg(μ-OBn)(THF)]$_2$ (3)

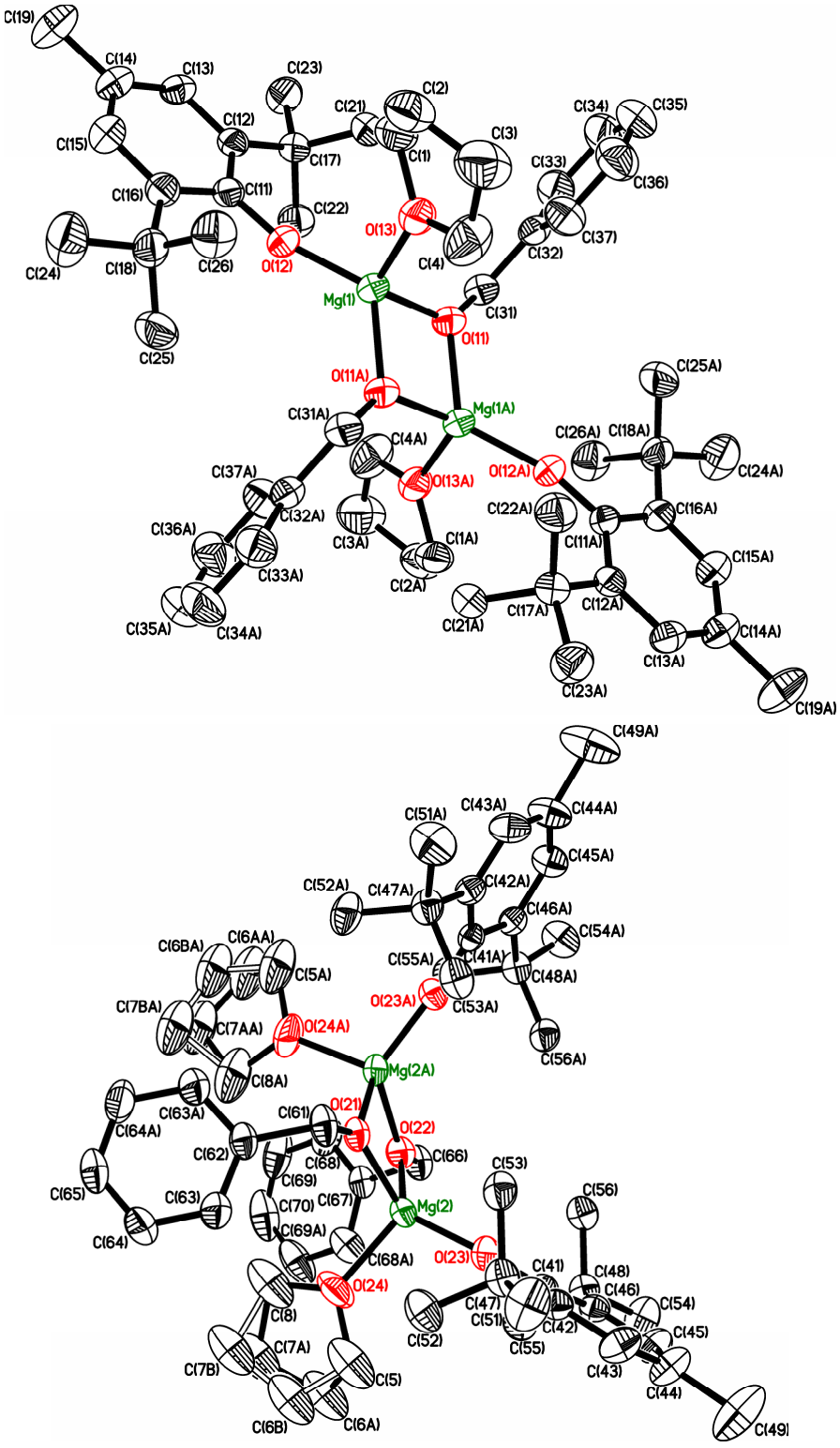

Fig. S14. Two independent molecules of [(BHT)Mg(μ-OBn)(THF)]$_2$ (**3**) with BHT (or THF) ligands being in *trans* (top) and *cis* (bottom) positions about the Mg_2O_2 rhomboid core in **3**. Disordered THF molecules are shown with open solid lines. H-atoms are omitted. Thermal ellipsoids are set to the 50% probability level. Symmetry codes (A) to generate equivalent atoms: -x+1, -y+1, -z+2 for the upper molecule; x, -y+3/2, z for the lower molecule.

[(BHT)(THF)Mg(μ-κ^1O:κ^1O-OBn)$_2$Mg(THF)(BHT)] contains two crystallographically independent dimeric molecules of geometric isomers (Fig. S14) with a 1:1 ratio. In the both molecules, Mg-atom is in distorted tetrahedral environment (c.n.=4). Two bridging benzyl groups connect two Mg-atoms, forming a Mg_2O_2 rhomboid core. The first molecule (Fig. S14, top) is located at an inversion center. The half of the molecule is crystallographicaly unique, the Mg_2O_2 core is flat, and BHT ligands are in the trans-position about the core as well as THF ligands. The other molecule (Fig. S14, bottom) possesses a nearly flat Mg_2O_2 core with folding angle of 16.8° between Mg2-O21-O22 and Mg2A-O21-O22 planes. The half of the molecule is unique. The other half is generated by a 2-fold screw axis. THF molecules are disordered over two positions. The THF and BHT ligands are in the cis-positions with respect to the Mg_2O_2 core. The both molecules exhibit the shortest distances for Mg-O_{BHT} bonds, and the longest – for Mg-O_{THF}.

Table S7. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^2 x10^3) for [(BHT)Mg(THF)(μ-OBn)]$_2$ (**3**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U(eq)
Mg(1)	4730(1)	5171(1)	8984(1)	39(1)
O(11)	4884(1)	4753(1)	9426(2)	43(1)
O(12)	3967(1)	5348(1)	8429(2)	42(1)
O(13)	5388(1)	5312(1)	7742(2)	47(1)
C(1)	5235(2)	5411(1)	6521(3)	54(1)
C(2)	5760(2)	5630(1)	6215(3)	63(1)
C(3)	6347(2)	5503(1)	6862(4)	81(1)
C(4)	6072(2)	5377(1)	7996(4)	70(1)
C(11)	3515(1)	5481(1)	7748(2)	36(1)
C(12)	3127(1)	5309(1)	6927(2)	35(1)
C(13)	2682(1)	5458(1)	6180(2)	38(1)
C(14)	2581(1)	5764(1)	6230(2)	42(1)
C(15)	2945(1)	5924(1)	7065(3)	44(1)
C(16)	3407(1)	5794(1)	7825(2)	39(1)
C(17)	3184(1)	4968(1)	6874(2)	39(1)
C(18)	3792(1)	5990(1)	8726(3)	48(1)
C(19)	2082(2)	5914(1)	5432(3)	63(1)
C(21)	3868(1)	4873(1)	6433(3)	47(1)
C(22)	3038(2)	4831(1)	8120(3)	49(1)
C(23)	2686(2)	4828(1)	5990(3)	51(1)
C(24)	3559(2)	6315(1)	8724(4)	74(1)
C(25)	3706(2)	5871(1)	10016(3)	63(1)
C(26)	4520(1)	5993(1)	8376(3)	57(1)
C(31)	4734(1)	4477(1)	8880(2)	43(1)
C(32)	5132(1)	4403(1)	7770(2)	39(1)
C(33)	4937(2)	4170(1)	7031(3)	53(1)
C(34)	5299(2)	4095(1)	6020(3)	71(1)
C(35)	5856(2)	4246(1)	5725(3)	70(1)
C(36)	6053(2)	4475(1)	6445(3)	65(1)
C(37)	5695(2)	4553(1)	7466(3)	53(1)
Mg(2)	4595(1)	7181(1)	4321(1)	40(1)

O(21)	4676(1)	7500	5508(2)	43(1)
O(22)	4316(1)	7500	3239(2)	44(1)
O(23)	5276(1)	6925(1)	3967(2)	43(1)
O(24)	3823(1)	6927(1)	4734(2)	75(1)
C(5)	3823(2)	6605(1)	4680(5)	108(1)
C(6A)	3206(2)	6524(1)	4026(6)	108(1)
C(7A)	2763(2)	6739(1)	4715(7)	108(1)
C(6B)	3106(4)	6521(2)	4801(16)	108(1)
C(7B)	2818(4)	6771(2)	5550(13)	108(1)
C(8)	3168(2)	7026(1)	4944(5)	108(1)
C(41)	5742(1)	6726(1)	3739(2)	37(1)
C(42)	6134(1)	6610(1)	4693(2)	42(1)
C(43)	6600(2)	6395(1)	4425(3)	57(1)
C(44)	6711(2)	6292(1)	3270(3)	63(1)
C(45)	6341(2)	6413(1)	2345(3)	52(1)
C(46)	5858(1)	6626(1)	2535(2)	39(1)
C(47)	6067(2)	6724(1)	5999(2)	48(1)
C(48)	5467(1)	6751(1)	1462(2)	44(1)
C(49)	7217(3)	6052(1)	3033(4)	107(2)
C(51)	6541(2)	6564(1)	6874(3)	75(1)
C(52)	5374(2)	6664(1)	6487(3)	64(1)
C(53)	6234(2)	7057(1)	6042(3)	53(1)
C(54)	5677(2)	6605(1)	257(3)	66(1)
C(55)	4731(2)	6684(1)	1608(3)	57(1)
C(56)	5586(2)	7086(1)	1339(3)	50(1)
C(61)	4804(2)	7500	6774(4)	54(1)
C(62)	4191(2)	7500	7515(3)	46(1)
C(63)	3895(2)	7238(1)	7867(3)	64(1)
C(64)	3316(2)	7237(1)	8530(3)	74(1)
C(65)	3032(3)	7500	8845(4)	68(1)
C(66)	4076(2)	7500	2029(4)	50(1)
C(67)	3336(2)	7500	1962(3)	43(1)
C(68)	2993(2)	7765(1)	1916(3)	61(1)
C(69)	2307(2)	7765(1)	1845(3)	81(1)
C(70)	1980(3)	7500	1806(5)	86(2)

Table S8. Anisotropic displacement parameters ($Å^2$ x10^3) for [(BHT)Mg(THF)(μ-OBn)]$_2$ (**3**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	38(1)	49(1)	30(1)	-3(1)	-7(1)	9(1)
O(11)	47(1)	49(1)	32(1)	-7(1)	-10(1)	9(1)
O(12)	38(1)	53(1)	34(1)	-3(1)	-8(1)	11(1)
O(13)	35(1)	62(1)	43(1)	1(1)	-4(1)	5(1)
C(1)	49(2)	77(2)	36(2)	-3(1)	1(1)	5(2)
C(2)	66(2)	77(2)	47(2)	0(2)	9(2)	-4(2)
C(3)	52(2)	127(4)	63(2)	-3(2)	5(2)	-12(2)
C(4)	41(2)	86(3)	82(3)	14(2)	-10(2)	-6(2)
C(11)	30(1)	49(2)	29(1)	1(1)	1(1)	5(1)
C(12)	32(1)	45(1)	27(1)	2(1)	4(1)	3(1)
C(13)	36(1)	46(2)	31(1)	4(1)	-4(1)	-4(1)
C(14)	40(1)	46(2)	40(2)	10(1)	-8(1)	-3(1)
C(15)	42(2)	42(2)	47(2)	4(1)	-5(1)	0(1)
C(16)	34(1)	47(2)	37(1)	-3(1)	-3(1)	2(1)

C(17)	41(1)	43(2)	32(1)	-2(1)	-1(1)	5(1)
C(18)	45(2)	49(2)	49(2)	-12(1)	-13(1)	8(1)
C(19)	69(2)	49(2)	70(2)	21(2)	-31(2)	-7(2)
C(21)	48(2)	56(2)	37(1)	-6(1)	0(1)	12(1)
C(22)	54(2)	50(2)	44(2)	5(1)	5(1)	1(1)
C(23)	56(2)	44(2)	54(2)	-4(1)	-12(2)	1(1)
C(24)	74(2)	56(2)	93(3)	-28(2)	-34(2)	13(2)
C(25)	60(2)	84(2)	45(2)	-21(2)	-7(2)	12(2)
C(26)	46(2)	57(2)	67(2)	-8(2)	-11(2)	-8(1)
C(31)	43(2)	49(2)	36(1)	-1(1)	-5(1)	2(1)
C(32)	45(2)	39(1)	33(1)	2(1)	-7(1)	7(1)
C(33)	54(2)	47(2)	57(2)	-10(1)	-6(2)	0(1)
C(34)	80(3)	71(2)	61(2)	-33(2)	-6(2)	12(2)
C(35)	76(2)	88(3)	46(2)	-11(2)	9(2)	20(2)
C(36)	64(2)	70(2)	60(2)	2(2)	17(2)	1(2)
C(37)	57(2)	52(2)	51(2)	-7(1)	4(2)	-4(1)
Mg(2)	33(1)	48(1)	40(1)	1(1)	3(1)	-4(1)
O(21)	42(1)	54(2)	33(1)	0	9(1)	0
O(22)	31(1)	55(2)	46(2)	0	-9(1)	0
O(23)	41(1)	53(1)	35(1)	-1(1)	0(1)	4(1)
O(24)	55(1)	79(2)	90(2)	6(1)	13(1)	-31(1)
C(5)	80(2)	142(3)	103(2)	29(2)	3(2)	-43(2)
C(6A)	80(2)	142(3)	103(2)	29(2)	3(2)	-43(2)
C(7A)	80(2)	142(3)	103(2)	29(2)	3(2)	-43(2)
C(6B)	80(2)	142(3)	103(2)	29(2)	3(2)	-43(2)
C(7B)	80(2)	142(3)	103(2)	29(2)	3(2)	-43(2)
C(8)	80(2)	142(3)	103(2)	29(2)	3(2)	-43(2)
C(41)	37(1)	35(1)	38(1)	0(1)	0(1)	-6(1)
C(42)	49(2)	40(2)	36(1)	3(1)	-2(1)	-3(1)
C(43)	71(2)	48(2)	51(2)	0(1)	-17(2)	11(2)
C(44)	77(2)	52(2)	60(2)	-14(2)	-14(2)	22(2)
C(45)	62(2)	51(2)	43(2)	-14(1)	-7(1)	7(1)
C(46)	41(1)	37(1)	38(1)	-2(1)	-3(1)	-6(1)
C(47)	50(2)	61(2)	34(1)	5(1)	-2(1)	1(1)
C(48)	45(2)	56(2)	32(1)	-6(1)	-6(1)	-3(1)
C(49)	137(4)	97(3)	86(3)	-28(2)	-31(3)	65(3)
C(51)	88(3)	99(3)	39(2)	4(2)	-13(2)	23(2)
C(52)	70(2)	81(2)	41(2)	16(2)	8(2)	-9(2)
C(53)	49(2)	69(2)	41(2)	-15(1)	-1(1)	-3(2)
C(54)	73(2)	85(2)	39(2)	-13(2)	-11(2)	13(2)
C(55)	48(2)	71(2)	53(2)	-8(2)	-13(1)	-6(2)
C(56)	51(2)	61(2)	38(2)	10(1)	-2(1)	1(1)
C(61)	45(2)	82(3)	35(2)	0	9(2)	0
C(62)	45(2)	61(3)	32(2)	0	6(2)	0
C(63)	74(2)	58(2)	62(2)	-2(2)	26(2)	2(2)
C(64)	81(3)	71(2)	69(2)	0(2)	33(2)	-19(2)
C(65)	61(3)	93(4)	51(3)	0	24(2)	0
C(66)	36(2)	73(3)	42(2)	0	-5(2)	0
C(67)	35(2)	63(3)	32(2)	0	-4(2)	0
C(68)	56(2)	81(2)	46(2)	-11(2)	-9(2)	16(2)
C(69)	58(2)	137(3)	49(2)	-13(2)	-7(2)	39(2)
C(70)	41(3)	170(6)	45(3)	0	-6(2)	0

Table S9. Bond lengths for non-hydrogen atoms (Å) for [(BHT)Mg(THF)(μ-OBn)]$_2$ (**3**)

Atoms	Bond length	Atoms	Bond length	Atoms	Bond length
Mg(1)-O(12)	1.8509(19)	C(18)-C(26)	1.535(4)	C(41)-C(46)	1.426(4)
Mg(1)-O(11)#1	1.9582(19)	C(31)-C(32)	1.510(4)	C(42)-C(43)	1.384(4)
Mg(1)-O(11)	1.960(2)	C(32)-C(37)	1.371(4)	C(42)-C(47)	1.540(4)
Mg(1)-O(13)	2.022(2)	C(32)-C(33)	1.386(4)	C(43)-C(44)	1.379(5)
Mg(1)-Mg(1)#1	2.9371(17)	C(33)-C(34)	1.382(5)	C(43)-H(43)	0.9500
O(11)-C(31)	1.411(3)	C(34)-C(35)	1.361(5)	C(44)-C(45)	1.382(4)
O(11)-Mg(1)#1	1.9582(19)	C(35)-C(36)	1.362(5)	C(44)-C(49)	1.515(5)
O(12)-C(11)	1.332(3)	C(36)-C(37)	1.391(4)	C(45)-C(46)	1.388(4)
O(13)-C(4)	1.452(4)	Mg(2)-O(23)	1.844(2)	C(46)-C(48)	1.535(4)
O(13)-C(1)	1.458(3)	Mg(2)-O(21)	1.947(2)	C(47)-C(53)	1.531(4)
C(1)-C(2)	1.493(5)	Mg(2)-O(22)	1.949(2)	C(47)-C(52)	1.538(4)
C(2)-C(3)	1.507(5)	Mg(2)-O(24)	1.996(2)	C(47)-C(51)	1.546(4)
C(3)-C(4)	1.486(5)	Mg(2)-Mg(2)#2	2.8548(19)	C(48)-C(56)	1.529(4)
C(11)-C(16)	1.424(4)	O(21)-C(61)	1.426(5)	C(48)-C(55)	1.539(4)
C(11)-C(12)	1.429(4)	O(21)-Mg(2)#2	1.947(2)	C(48)-C(54)	1.546(4)
C(12)-C(13)	1.398(4)	O(22)-C(66)	1.426(5)	C(61)-C(62)	1.496(5)
C(12)-C(17)	1.535(4)	O(22)-Mg(2)#2	1.949(2)	C(62)-C(63)	1.376(4)
C(13)-C(14)	1.386(4)	O(23)-C(41)	1.327(3)	C(62)-C(63)#2	1.376(4)
C(14)-C(15)	1.387(4)	O(24)-C(8)	1.428(4)	C(63)-C(64)	1.389(5)
C(14)-C(19)	1.506(4)	O(24)-C(5)	1.446(4)	C(64)-C(65)	1.359(4)
C(15)-C(16)	1.391(4)	C(5)-C(6A)	1.496(5)	C(65)-C(64)#2	1.360(5)
C(16)-C(18)	1.542(4)	C(5)-C(6B)	1.515(5)	C(66)-C(67)	1.511(5)
C(17)-C(21)	1.536(4)	C(6A)-C(7A)	1.527(5)	C(67)-C(68)	1.377(4)
C(17)-C(22)	1.539(4)	C(7A)-C(8)	1.547(5)	C(67)-C(68)#2	1.377(4)
C(17)-C(23)	1.544(4)	C(6B)-C(7B)	1.512(6)	C(68)-C(69)	1.402(5)
C(18)-C(24)	1.533(4)	C(7B)-C(8)	1.505(5)	C(69)-C(70)	1.361(5)
C(18)-C(25)	1.534(5)	C(41)-C(42)	1.423(4)	C(70)-C(69)#2	1.361(5)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+2; #2 x,-y+3/2,z

Table S10. Bond angles for non-hydrogen atoms (°) for [(BHT)Mg(THF)(μ-OBn)]$_2$ (**3**)

Atoms	Bond angles	Atoms	Bond angles
O(12)-Mg(1)-O(11)#1	124.24(9)	O(23)-Mg(2)-Mg(2)#2	128.59(7)
O(12)-Mg(1)-O(11)	128.70(10)	O(21)-Mg(2)-Mg(2)#2	42.86(6)
O(11)#1-Mg(1)-O(11)	82.89(9)	O(22)-Mg(2)-Mg(2)#2	42.91(6)
O(12)-Mg(1)-O(13)	101.48(9)	O(24)-Mg(2)-Mg(2)#2	124.77(8)
O(11)#1-Mg(1)-O(13)	106.90(9)	C(61)-O(21)-Mg(2)	132.76(6)
O(11)-Mg(1)-O(13)	111.23(9)	C(61)-O(21)-Mg(2)#2	132.76(6)
O(12)-Mg(1)-Mg(1)#1	142.41(8)	Mg(2)-O(21)-Mg(2)#2	94.28(12)
O(11)#1-Mg(1)-Mg(1)#1	41.47(6)	C(66)-O(22)-Mg(2)	132.68(7)
O(11)-Mg(1)-Mg(1)#1	41.42(6)	C(66)-O(22)-Mg(2)#2	132.68(7)
O(13)-Mg(1)-Mg(1)#1	115.81(7)	Mg(2)-O(22)-Mg(2)#2	94.17(12)
C(31)-O(11)-Mg(1)#1	128.66(16)	C(41)-O(23)-Mg(2)	176.45(18)
C(31)-O(11)-Mg(1)	134.06(16)	C(8)-O(24)-C(5)	108.4(3)
Mg(1)#1-O(11)-Mg(1)	97.11(9)	C(8)-O(24)-Mg(2)	126.8(2)
C(11)-O(12)-Mg(1)	164.00(17)	C(5)-O(24)-Mg(2)	124.1(2)
C(4)-O(13)-C(1)	108.9(2)	O(24)-C(5)-C(6A)	105.3(4)
C(4)-O(13)-Mg(1)	124.7(2)	O(24)-C(5)-C(6B)	104.2(4)
C(1)-O(13)-Mg(1)	125.70(17)	C(5)-C(6A)-C(7A)	95.8(4)
O(13)-C(1)-C(2)	104.8(2)	C(6A)-C(7A)-C(8)	106.9(3)
C(1)-C(2)-C(3)	102.3(3)	C(7B)-C(6B)-C(5)	103.8(5)

C(4)-C(3)-C(2)	104.2(3)	C(8)-C(7B)-C(6B)	97.8(5)
O(13)-C(4)-C(3)	106.0(3)	O(24)-C(8)-C(7B)	106.3(4)
O(12)-C(11)-C(16)	121.0(2)	O(24)-C(8)-C(7A)	102.5(3)
O(12)-C(11)-C(12)	120.1(2)	O(23)-C(41)-C(42)	120.4(2)
C(16)-C(11)-C(12)	118.9(2)	O(23)-C(41)-C(46)	120.4(2)
C(13)-C(12)-C(11)	118.6(2)	C(42)-C(41)-C(46)	119.2(2)
C(13)-C(12)-C(17)	120.1(2)	C(43)-C(42)-C(41)	118.7(3)
C(11)-C(12)-C(17)	121.2(2)	C(43)-C(42)-C(47)	119.5(3)
C(14)-C(13)-C(12)	123.0(2)	C(41)-C(42)-C(47)	121.8(2)
C(13)-C(14)-C(15)	117.3(2)	C(44)-C(43)-C(42)	122.9(3)
C(13)-C(14)-C(19)	121.2(3)	C(43)-C(44)-C(45)	117.8(3)
C(15)-C(14)-C(19)	121.4(3)	C(43)-C(44)-C(49)	120.6(3)
C(14)-C(15)-C(16)	123.3(3)	C(45)-C(44)-C(49)	121.5(3)
C(15)-C(16)-C(11)	118.8(2)	C(44)-C(45)-C(46)	123.0(3)
C(15)-C(16)-C(18)	119.9(2)	C(45)-C(46)-C(41)	118.3(2)
C(11)-C(16)-C(18)	121.3(2)	C(45)-C(46)-C(48)	120.0(2)
C(12)-C(17)-C(21)	110.8(2)	C(41)-C(46)-C(48)	121.7(2)
C(12)-C(17)-C(22)	110.3(2)	C(53)-C(47)-C(52)	111.3(3)
C(21)-C(17)-C(22)	110.7(2)	C(53)-C(47)-C(42)	109.4(2)
C(12)-C(17)-C(23)	112.2(2)	C(52)-C(47)-C(42)	110.7(3)
C(21)-C(17)-C(23)	106.5(2)	C(53)-C(47)-C(51)	107.0(3)
C(22)-C(17)-C(23)	106.2(2)	C(52)-C(47)-C(51)	105.9(3)
C(24)-C(18)-C(25)	107.2(3)	C(42)-C(47)-C(51)	112.4(3)
C(24)-C(18)-C(26)	106.8(3)	C(56)-C(48)-C(46)	110.0(2)
C(25)-C(18)-C(26)	110.4(3)	C(56)-C(48)-C(55)	110.9(3)
C(24)-C(18)-C(16)	112.4(2)	C(46)-C(48)-C(55)	110.8(2)
C(25)-C(18)-C(16)	110.4(3)	C(56)-C(48)-C(54)	107.1(3)
C(26)-C(18)-C(16)	109.6(2)	C(46)-C(48)-C(54)	111.8(2)
O(11)-C(31)-C(32)	115.1(2)	C(55)-C(48)-C(54)	106.2(2)
C(37)-C(32)-C(33)	117.7(3)	O(21)-C(61)-C(62)	112.8(3)
C(37)-C(32)-C(31)	122.9(2)	C(63)-C(62)-C(63)#2	117.1(4)
C(33)-C(32)-C(31)	119.4(3)	C(63)-C(62)-C(61)	121.5(2)
C(34)-C(33)-C(32)	120.5(3)	C(63)#2-C(62)-C(61)	121.5(2)
C(35)-C(34)-C(33)	121.4(3)	C(62)-C(63)-C(64)	121.7(3)
C(34)-C(35)-C(36)	118.7(3)	C(65)-C(64)-C(63)	119.6(4)
C(35)-C(36)-C(37)	120.7(3)	C(64)-C(65)-C(64)#2	120.3(5)
C(32)-C(37)-C(36)	121.1(3)	O(22)-C(66)-C(67)	112.9(3)
O(23)-Mg(2)-O(21)	122.49(10)	C(68)-C(67)-C(68)#2	118.8(4)
O(23)-Mg(2)-O(22)	123.11(11)	C(68)-C(67)-C(66)	120.6(2)
O(21)-Mg(2)-O(22)	84.42(9)	C(68)#2-C(67)-C(66)	120.6(2)
O(23)-Mg(2)-O(24)	106.64(11)	C(67)-C(68)-C(69)	120.6(4)
O(21)-Mg(2)-O(24)	109.24(11)	C(70)-C(69)-C(68)	119.3(4)
O(22)-Mg(2)-O(24)	109.15(11)	C(69)#2-C(70)-C(69)	121.2(5)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+2; #2 x,-y+3/2,z

S2.4. Molecular structure of [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (4)

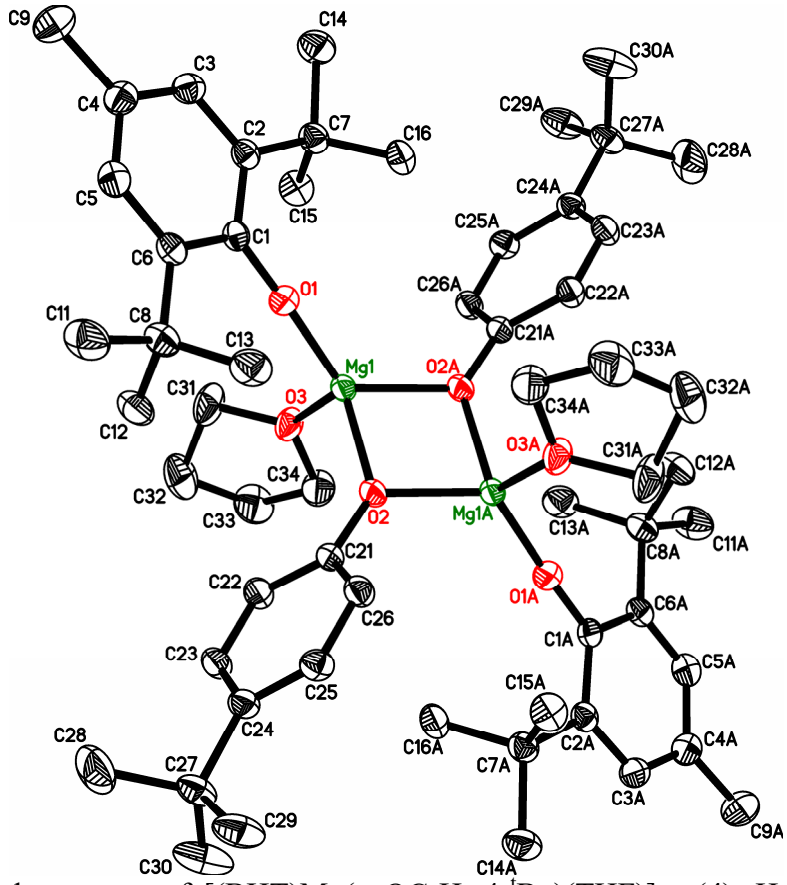

Figure S15. Crystal structure of [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**). H-atoms are omitted. Thermal ellipsoids are set to the 50% probability level. Symmetry code: -x+1, -y+1, -z+1.

Dimeric compound [(BHT)(THF)Mg(μ-κ^1O:κ^1O-OC_6H_4-4-^{t}Bu)$_2$Mg(THF)(BHT)] (Fig. S15) has a flat Mg_2O_2 rhomboid core and BHT (or THF) ligands being in the trans-position. The molecule is located at an inversion center.

Table S11. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^2 x10^3) for [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U(eq)
Mg(1)	5487(1)	6229(1)	5085(1)	20(1)
O(1)	6746(1)	7069(1)	5515(1)	26(1)
C(1)	7628(1)	7728(1)	5824(1)	21(1)
C(2)	8624(1)	8079(1)	5573(1)	22(1)
C(3)	9477(1)	8853(1)	5895(1)	25(1)
C(4)	9406(1)	9285(1)	6452(1)	27(1)
C(5)	8471(1)	8876(1)	6706(1)	27(1)
C(6)	7587(1)	8098(1)	6415(1)	23(1)
C(7)	8763(1)	7627(1)	4959(1)	25(1)
C(8)	6583(1)	7663(1)	6725(1)	28(1)
C(9)	10309(1)	10174(1)	6771(1)	38(1)
C(11)	6762(1)	8115(2)	7368(1)	41(1)
C(12)	5362(1)	8149(1)	6401(1)	34(1)
C(13)	6558(1)	6282(1)	6751(1)	36(1)

C(14)	9950(1)	8033(1)	4794(1)	36(1)
C(15)	7749(1)	8141(1)	4479(1)	32(1)
C(16)	8781(1)	6247(1)	4946(1)	29(1)
O(2)	4405(1)	5180(1)	5417(1)	23(1)
C(21)	3690(1)	5295(1)	5826(1)	22(1)
C(22)	2890(1)	6252(1)	5801(1)	25(1)
C(23)	2114(1)	6319(1)	6195(1)	26(1)
C(24)	2101(1)	5438(1)	6628(1)	23(1)
C(25)	2927(1)	4507(1)	6656(1)	25(1)
C(26)	3717(1)	4437(1)	6266(1)	24(1)
C(27)	1185(1)	5509(1)	7033(1)	30(1)
C(28)	1395(2)	6676(2)	7400(1)	53(1)
C(29)	1295(1)	4454(2)	7463(1)	40(1)
C(30)	-78(1)	5511(2)	6654(1)	52(1)
O(3)	4395(1)	7372(1)	4559(1)	30(1)
C(31)	4397(1)	8674(1)	4621(1)	41(1)
C(32)	3100(2)	9026(1)	4458(1)	47(1)
C(33)	2625(1)	8155(2)	3965(1)	46(1)
C(34)	3291(1)	7002(1)	4158(1)	36(1)

Table S12. Anisotropic displacement parameters ($Å^2$ x10^3) for [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U_{11}$ + ... + 2 h k a* b* U_{12}]

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	20(1)	17(1)	25(1)	1(1)	8(1)	1(1)
O(1)	25(1)	25(1)	28(1)	-4(1)	6(1)	-2(1)
C(1)	22(1)	18(1)	25(1)	1(1)	4(1)	3(1)
C(2)	24(1)	20(1)	24(1)	3(1)	5(1)	4(1)
C(3)	22(1)	24(1)	30(1)	4(1)	4(1)	1(1)
C(4)	25(1)	26(1)	28(1)	1(1)	-1(1)	1(1)
C(5)	28(1)	28(1)	24(1)	-1(1)	2(1)	5(1)
C(6)	23(1)	23(1)	24(1)	2(1)	6(1)	5(1)
C(7)	26(1)	26(1)	25(1)	1(1)	9(1)	1(1)
C(8)	26(1)	34(1)	26(1)	0(1)	9(1)	3(1)
C(9)	33(1)	43(1)	36(1)	-4(1)	-3(1)	-7(1)
C(11)	38(1)	62(1)	27(1)	-6(1)	13(1)	-2(1)
C(12)	26(1)	42(1)	35(1)	-5(1)	10(1)	6(1)
C(13)	37(1)	36(1)	38(1)	9(1)	15(1)	1(1)
C(14)	34(1)	42(1)	35(1)	0(1)	16(1)	-3(1)
C(15)	36(1)	33(1)	27(1)	5(1)	6(1)	3(1)
C(16)	32(1)	27(1)	30(1)	-3(1)	10(1)	5(1)
O(2)	25(1)	21(1)	27(1)	-2(1)	14(1)	0(1)
C(21)	22(1)	21(1)	24(1)	-3(1)	10(1)	-1(1)
C(22)	30(1)	20(1)	27(1)	4(1)	12(1)	3(1)
C(23)	26(1)	24(1)	30(1)	2(1)	12(1)	5(1)
C(24)	22(1)	26(1)	22(1)	-1(1)	8(1)	-1(1)
C(25)	25(1)	25(1)	24(1)	5(1)	7(1)	0(1)
C(26)	24(1)	22(1)	28(1)	2(1)	8(1)	4(1)
C(27)	27(1)	38(1)	29(1)	5(1)	16(1)	4(1)
C(28)	71(1)	49(1)	49(1)	-8(1)	39(1)	3(1)
C(29)	32(1)	54(1)	39(1)	17(1)	18(1)	3(1)
C(30)	25(1)	83(1)	49(1)	22(1)	14(1)	8(1)
O(3)	29(1)	18(1)	38(1)	0(1)	-2(1)	3(1)
C(31)	48(1)	18(1)	51(1)	3(1)	-5(1)	4(1)

C(32)	56(1)	34(1)	51(1)	6(1)	14(1)	20(1)
C(33)	36(1)	48(1)	49(1)	6(1)	-3(1)	13(1)
C(34)	31(1)	34(1)	39(1)	-4(1)	-4(1)	3(1)

Table S13. Bond lengths for non-hydrogen atoms (Å) for [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**)

Atoms	Bond length	Atoms	Bond length	Atoms	Bond length
Mg(1)-O(1)	1.8284(9)	C(5)-C(6)	1.3939(16)	C(23)-C(24)	1.3992(15)
Mg(1)-O(2)	1.9565(8)	C(6)-C(8)	1.5391(16)	C(24)-C(25)	1.3908(15)
Mg(1)-O(2)#1	1.9652(8)	C(7)-C(16)	1.5357(16)	C(24)-C(27)	1.5318(15)
Mg(1)-O(3)	2.0082(9)	C(7)-C(14)	1.5403(17)	C(25)-C(26)	1.3925(15)
Mg(1)-Mg(1)#1	2.9460(7)	C(7)-C(15)	1.5412(16)	C(27)-C(29)	1.5241(18)
O(1)-C(1)	1.3305(13)	C(8)-C(13)	1.5374(18)	C(27)-C(30)	1.5254(19)
C(1)-C(2)	1.4254(15)	C(8)-C(11)	1.5381(18)	C(27)-C(28)	1.541(2)
C(1)-C(6)	1.4292(15)	C(8)-C(12)	1.5385(17)	O(3)-C(31)	1.4545(14)
C(2)-C(3)	1.3962(16)	O(2)-C(21)	1.3666(12)	O(3)-C(34)	1.4636(15)
C(2)-C(7)	1.5370(15)	O(2)-Mg(1)#1	1.9652(8)	C(31)-C(32)	1.501(2)
C(3)-C(4)	1.3867(17)	C(21)-C(26)	1.3880(15)	C(32)-C(33)	1.509(2)
C(4)-C(5)	1.3869(17)	C(21)-C(22)	1.3933(15)	C(33)-C(34)	1.510(2)
C(4)-C(9)	1.5081(17)	C(22)-C(23)	1.3881(15)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1

Table S14. Bond angles for non-hydrogen atoms (°) for [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**)

Atoms	Bond angles	Atoms	Bond angles
O(1)-Mg(1)-O(2)	125.39(4)	C(13)-C(8)-C(12)	110.36(11)
O(1)-Mg(1)-O(2)#1	126.30(4)	C(11)-C(8)-C(12)	106.62(10)
O(2)-Mg(1)-O(2)#1	82.61(3)	C(13)-C(8)-C(6)	110.68(10)
O(1)-Mg(1)-O(3)	109.18(4)	C(11)-C(8)-C(6)	112.01(11)
O(2)-Mg(1)-O(3)	104.54(4)	C(12)-C(8)-C(6)	110.31(10)
O(2)#1-Mg(1)-O(3)	104.64(4)	C(21)-O(2)-Mg(1)	135.94(7)
O(1)-Mg(1)-Mg(1)#1	141.22(3)	C(21)-O(2)-Mg(1)#1	126.52(7)
O(2)-Mg(1)-Mg(1)#1	41.42(2)	Mg(1)-O(2)-Mg(1)#1	97.39(3)
O(2)#1-Mg(1)-Mg(1)#1	41.19(2)	O(2)-C(21)-C(26)	120.56(9)
O(3)-Mg(1)-Mg(1)#1	109.59(3)	O(2)-C(21)-C(22)	121.05(10)
C(1)-O(1)-Mg(1)	177.14(7)	C(26)-C(21)-C(22)	118.35(10)
O(1)-C(1)-C(2)	120.60(9)	C(23)-C(22)-C(21)	120.60(10)
O(1)-C(1)-C(6)	120.34(9)	C(22)-C(23)-C(24)	121.66(10)
C(2)-C(1)-C(6)	119.06(10)	C(25)-C(24)-C(23)	116.93(10)
C(3)-C(2)-C(1)	118.51(10)	C(25)-C(24)-C(27)	122.97(10)
C(3)-C(2)-C(7)	120.24(10)	C(23)-C(24)-C(27)	120.08(10)
C(1)-C(2)-C(7)	121.25(10)	C(24)-C(25)-C(26)	121.82(10)
C(4)-C(3)-C(2)	122.97(11)	C(21)-C(26)-C(25)	120.57(10)
C(3)-C(4)-C(5)	117.70(11)	C(29)-C(27)-C(30)	108.65(12)
C(3)-C(4)-C(9)	121.26(11)	C(29)-C(27)-C(24)	112.16(10)
C(5)-C(4)-C(9)	121.04(11)	C(30)-C(27)-C(24)	109.26(10)
C(4)-C(5)-C(6)	122.82(11)	C(29)-C(27)-C(28)	107.91(12)
C(5)-C(6)-C(1)	118.66(10)	C(30)-C(27)-C(28)	109.77(14)
C(5)-C(6)-C(8)	120.21(10)	C(24)-C(27)-C(28)	109.06(11)
C(1)-C(6)-C(8)	121.13(10)	C(31)-O(3)-C(34)	109.05(9)
C(16)-C(7)-C(2)	110.41(9)	C(31)-O(3)-Mg(1)	125.58(8)
C(16)-C(7)-C(14)	105.79(10)	C(34)-O(3)-Mg(1)	123.66(7)

C(2)-C(7)-C(14)	112.64(10)	O(3)-C(31)-C(32)	104.62(12)
C(16)-C(7)-C(15)	111.54(10)	C(31)-C(32)-C(33)	102.10(12)
C(2)-C(7)-C(15)	109.90(9)	C(32)-C(33)-C(34)	103.79(11)
C(14)-C(7)-C(15)	106.46(10)	O(3)-C(34)-C(33)	105.38(11)
C(13)-C(8)-C(11)	106.73(11)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1

Table S15. Torsion angles (°) for [(BHT)Mg(μ-OC_6H_4-4-^{t}Bu)(THF)]$_2$ (**4**)

Atoms	Torsion angles	Atoms	Torsion angles
O(1)-C(1)-C(2)-C(3)	174.76(9)	Mg(1)-O(2)-C(21)-C(26)	-132.51(10)
C(6)-C(1)-C(2)-C(3)	-5.12(15)	Mg(1)#1-O(2)-C(21)-C(26)	53.06(13)
O(1)-C(1)-C(2)-C(7)	-4.85(15)	Mg(1)-O(2)-C(21)-C(22)	49.61(15)
C(6)-C(1)-C(2)-C(7)	175.27(9)	Mg(1)#1-O(2)-C(21)-C(22)	-124.82(10)
C(1)-C(2)-C(3)-C(4)	0. 75(16)	O(2)-C(21)-C(22)-C(23)	175.85(10)
C(7)-C(2)-C(3)-C(4)	-179.63(10)	C(26)-C(21)-C(22)-C(23)	-2.08(17)
C(2)-C(3)-C(4)-C(5)	3.17(17)	C(21)-C(22)-C(23)-C(24)	-0.17(18)
C(2)-C(3)-C(4)-C(9)	-176.56(11)	C(22)-C(23)-C(24)-C(25)	1.82(17)
C(3)-C(4)-C(5)-C(6)	-2.74(17)	C(22)-C(23)-C(24)-C(27)	-176.70(11)
C(9)-C(4)-C(5)-C(6)	177.00(11)	C(23)-C(24)-C(25)-C(26)	-1.25(17)
C(4)-C(5)-C(6)-C(1)	-1.59(16)	C(27)-C(24)-C(25)-C(26)	177.23(11)
C(4)-C(5)-C(6)-C(8)	179.13(10)	O(2)-C(21)-C(26)-C(25)	-175.30(10)
O(1)-C(1)-C(6)-C(5)	-174.35(10)	C(22)-C(21)-C(26)-C(25)	2.64(17)
C(2)-C(1)-C(6)-C(5)	5.53(15)	C(24)-C(25)-C(26)-C(21)	-0.98(18)
O(1)-C(1)-C(6)-C(8)	4.93(15)	C(25)-C(24)-C(27)-C(29)	0.19(17)
C(2)-C(1)-C(6)-C(8)	-175.19(10)	C(23)-C(24)-C(27)-C(29)	178.62(12)
C(3)-C(2)-C(7)-C(16)	122.96(11)	C(25)-C(24)-C(27)-C(30)	-120.34(14)
C(1)-C(2)-C(7)-C(16)	-57.43(13)	C(23)-C(24)-C(27)-C(30)	58.09(16)
C(3)-C(2)-C(7)-C(14)	4.95(15)	C(25)-C(24)-C(27)-C(28)	119.67(14)
C(1)-C(2)-C(7)-C(14)	-175.45(10)	C(23)-C(24)-C(27)-C(28)	-61.90(15)
C(3)-C(2)-C(7)-C(15)	-113.58(11)	O(1)-Mg(1)-O(3)-C(31)	-16.00(12)
C(1)-C(2)-C(7)-C(15)	66.02(13)	O(2)-Mg(1)-O(3)-C(31)	120.36(11)
C(5)-C(6)-C(8)-C(13)	-123.03(12)	O(2)#1-Mg(1)-O(3)-C(31)	-153.63(11)
C(1)-C(6)-C(8)-C(13)	57.70(14)	Mg(1)#1-Mg(1)-O(3)-C(31)	163.47(11)
C(5)-C(6)-C(8)-C(11)	-4.05(16)	O(1)-Mg(1)-O(3)-C(34)	-179.46(9)
C(1)-C(6)-C(8)-C(11)	176.68(11)	O(2)-Mg(1)-O(3)-C(34)	-43.09(10)
C(5)-C(6)-C(8)-C(12)	114.54(12)	O(2)#1-Mg(1)-O(3)-C(34)	42.92(10)
C(1)-C(6)-C(8)-C(12)	-64.73(14)	Mg(1)#1-Mg(1)-O(3)-C(34)	0.02(10)
O(1)-Mg(1)-O(2)-C(21)	54.71(11)	C(34)-O(3)-C(31)-C(32)	22.29(16)
O(2)#1-Mg(1)-O(2)-C(21)	-175.49(12)	Mg(1)-O(3)-C(31)-C(32)	-143.19(10)
O(3)-Mg(1)-O(2)-C(21)	-72.21(10)	O(3)-C(31)-C(32)-C(33)	-36.65(16)
Mg(1)#1-Mg(1)-O(2)-C(21)	-175.49(12)	C(31)-C(32)-C(33)-C(34)	37.26(17)
O(1)-Mg(1)-O(2)-Mg(1)#1	-129.81(5)	C(31)-O(3)-C(34)-C(33)	1.38(16)
O(2)#1-Mg(1)-O(2)-Mg(1)#1	0.0	Mg(1)-O(3)-C(34)-C(33)	167.19(10)
O(3)-Mg(1)-O(2)-Mg(1)#1	103.28(4)	C(32)-C(33)-C(34)-O(3)	-24.28(17)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1

S2.5. Molecular structure of [(BHT)Mg(THF)(μ-OCH_2COOEt)]$_2$(THF)(hexane) (5)

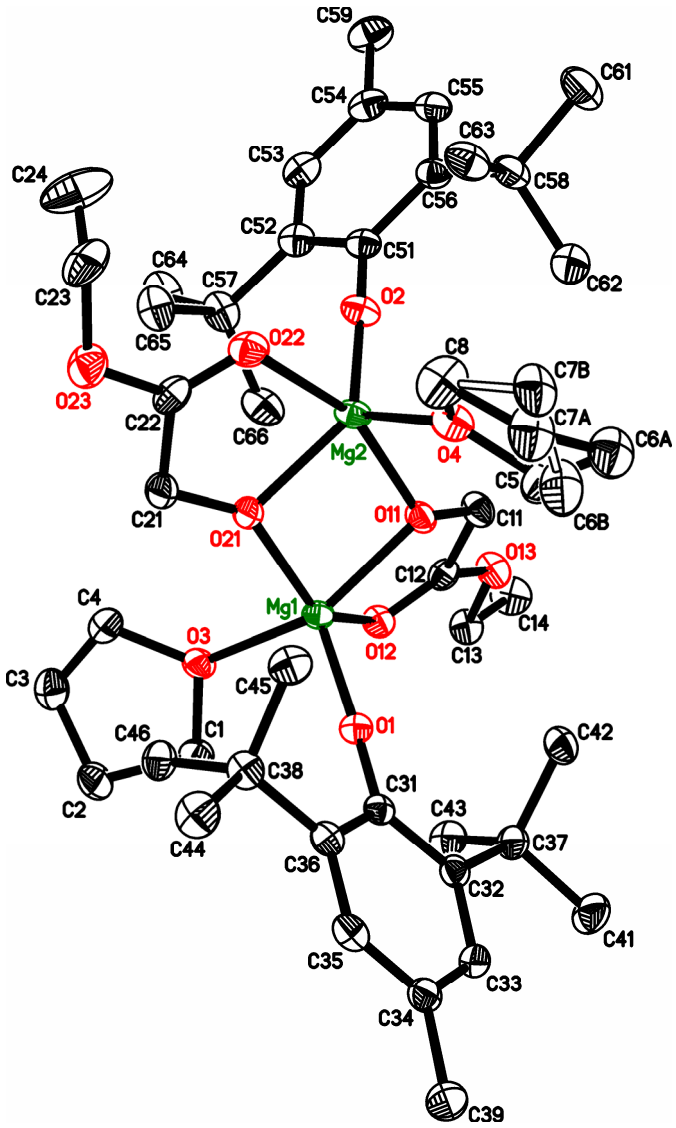

Fig. S16. Molecular structures of [(BHT)Mg(THF)(μ-OCH_2COOEt)]$_2$ (**5**). Hydrogen atoms are omitted. Thermal ellipsoids are set to the 50% probability level. The disordered THF molecule is shown with open solid lines.

Complex [(BHT)Mg(THF)(μ-κ^1O:κ^2O,O'-OCH_2COOEt)]$_2$(THF)(hexane) has two highly disordered non-coordinating solvent molecules in crystal channels. The non-coordinating solvent molecules have been deleted from the crystallographic model by the SQUEEZE procedure. According to NMR ^{1}H and ^{13}C{^{1}H} studies, these molecules are THF and hexane with an approximate molar ratio of 1:1. The main residue **4** (Fig. S16) possesses a dimeric structure, the Mg_2O_2 central rhomboid core, and c.n.=5. Folding angles of the Mg_2O_2 core are 0.6° between two O-Mg-O planes and 0.8° between Mg-O-Mg planes. One THF molecule is disordered over 2 positions. Lactate anions exhibit the μ-κ^1:κ^2-semi-bridging coordination mode: oxygen atom of hydroxyl group is bound to the both Mg-atoms, the O-atom of the carboxyl group is coordinated to only one of the magnesium atoms. The shortest Mg-O bond distances are Mg-O_{BHT} bonds, the longest are Mg-$O_{C=O}$.

Table S16. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2$ $x10^3$) for $[(BHT)Mg(\mu\text{-}OCH_2COOEt)(THF)]_2$ (**5**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Mg(1)	6818(1)	4860(1)	5828(1)	
Mg(2)	8162(1)	5349(1)	6011(1)	
O(1)	6224(1)	6146(1)	5998(1)	
O(2)	8712(1)	3915(2)	6089(1)	
O(3)	6395(1)	3980(2)	5188(1)	
C(1)	5749(1)	3783(3)	5166(1)	
C(2)	5572(1)	3758(3)	4604(1)	
C(3)	6128(1)	3187(3)	4372(1)	
C(4)	6625(1)	3772(3)	4681(1)	
O(4)	8253(1)	7042(2)	6476(1)	
C(5)	7912(1)	7213(3)	6937(1)	
C(6A)	8185(2)	8376(5)	7220(2)	
C(7A)	8380(3)	9249(7)	6784(3)	
C(6B)	8011(6)	8767(13)	6956(5)	
C(7B)	8624(6)	9220(20)	6803(7)	
C(8)	8592(2)	8261(3)	6383(1)	
O(11)	7451(1)	4755(2)	6386(1)	
O(12)	6572(1)	3018(2)	6203(1)	
O(13)	6797(1)	1774(2)	6896(1)	
O(21)	7540(1)	5443(2)	5450(1)	
O(22)	8645(1)	6438(2)	5451(1)	
O(23)	8580(1)	6993(2)	4630(1)	
C(11)	7400(1)	3695(2)	6735(1)	
C(12)	6874(1)	2807(2)	6576(1)	
C(13)	6300(1)	866(2)	6776(1)	
C(14)	6388(1)	-385(3)	7088(1)	
C(21)	7730(1)	5993(3)	4995(1)	
C(22)	8368(1)	6497(2)	5055(1)	
C(23)	9223(1)	7352(3)	4634(1)	
C(24)	9587(2)	6142(4)	4588(2)	
C(31)	5830(1)	7110(2)	6093(1)	
C(32)	5408(1)	6974(2)	6492(1)	
C(33)	4979(1)	7978(2)	6560(1)	
C(34)	4944(1)	9137(2)	6264(1)	
C(35)	5365(1)	9287(2)	5889(1)	
C(36)	5812(1)	8326(2)	5796(1)	
C(37)	5421(1)	5729(2)	6848(1)	
C(38)	6272(1)	8587(2)	5381(1)	
C(39)	4460(1)	10196(3)	6340(1)	
C(41)	4958(1)	5836(3)	7272(1)	
C(42)	6044(1)	5597(3)	7112(1)	
C(43)	5268(1)	4436(2)	6546(1)	
C(44)	6190(1)	9987(3)	5129(1)	
C(45)	6916(1)	8575(3)	5612(1)	
C(46)	6196(1)	7524(2)	4954(1)	
C(51)	9081(1)	2871(2)	6132(1)	
C(52)	9037(1)	1761(2)	5786(1)	
C(53)	9446(1)	700(2)	5839(1)	
C(54)	9888(1)	647(2)	6219(1)	

C(55)	9924(1)	1730(2)	6553(1)
C(56)	9541(1)	2845(2)	6520(1)
C(57)	8549(1)	1736(2)	5360(1)
C(58)	9614(1)	4042(3)	6897(1)
C(59)	10316(1)	-540(3)	6266(1)
C(61)	10140(1)	3819(3)	7282(1)
C(62)	9042(1)	4208(3)	7209(1)
C(63)	9748(1)	5357(3)	6613(1)
C(64)	8567(2)	443(3)	5038(1)
C(65)	8650(1)	2925(3)	4990(1)
C(66)	7920(1)	1818(3)	5586(1)

Table S17. Anisotropic displacement parameters ($Å^2$ x10^3) for [(BHT)Mg(μ-OCH_2COOEt)(THF)]$_2$ (**5**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	24(1)	31(1)	35(1)	0(1)	-1(1)	-4(1)
Mg(2)	24(1)	31(1)	45(1)	7(1)	-2(1)	-6(1)
O(1)	30(1)	28(1)	35(1)	2(1)	2(1)	-2(1)
O(2)	32(1)	29(1)	52(1)	0(1)	-7(1)	-1(1)
O(3)	30(1)	40(1)	39(1)	-6(1)	-6(1)	-4(1)
C(1)	33(1)	49(1)	45(1)	-5(1)	-1(1)	-7(1)
C(2)	42(1)	74(2)	44(1)	-8(1)	-11(1)	-11(1)
C(3)	64(2)	54(2)	42(1)	-5(1)	-1(1)	0(1)
C(4)	43(1)	70(2)	42(1)	-7(1)	7(1)	4(1)
O(4)	41(1)	32(1)	57(1)	0(1)	-5(1)	-10(1)
C(5)	57(2)	67(2)	68(2)	-22(2)	17(2)	-14(2)
C(6A)	69(3)	65(3)	63(3)	-9(2)	1(2)	-21(2)
C(7A)	86(4)	44(2)	62(3)	-13(2)	1(3)	-28(3)
C(6B)	76(6)	80(5)	51(5)	0(4)	3(5)	-40(5)
C(7B)	65(6)	59(5)	53(5)	-9(4)	-5(5)	-35(5)
C(8)	74(2)	42(2)	79(2)	-5(1)	14(2)	-22(1)
O(11)	31(1)	44(1)	30(1)	9(1)	-3(1)	-4(1)
O(12)	35(1)	35(1)	38(1)	2(1)	-1(1)	-6(1)
O(13)	46(1)	42(1)	44(1)	9(1)	-4(1)	-13(1)
O(21)	30(1)	53(1)	30(1)	9(1)	2(1)	-2(1)
O(22)	33(1)	41(1)	51(1)	8(1)	4(1)	-8(1)
O(23)	55(1)	57(1)	48(1)	8(1)	8(1)	-11(1)
C(11)	39(1)	44(1)	36(1)	10(1)	-5(1)	-10(1)
C(12)	35(1)	31(1)	35(1)	1(1)	8(1)	-5(1)
C(13)	44(1)	34(1)	44(1)	1(1)	0(1)	-12(1)
C(14)	60(2)	41(2)	71(2)	7(1)	1(2)	-8(1)
C(21)	39(1)	50(1)	34(1)	8(1)	2(1)	-3(1)
C(22)	42(1)	31(1)	44(1)	3(1)	15(1)	-8(1)
C(23)	60(2)	64(2)	66(2)	2(2)	29(2)	-25(2)
C(24)	57(2)	96(3)	162(4)	-3(3)	48(3)	-21(2)
C(31)	27(1)	28(1)	30(1)	-4(1)	-4(1)	-5(1)
C(32)	32(1)	35(1)	29(1)	-2(1)	-3(1)	-2(1)
C(33)	35(1)	46(1)	31(1)	-6(1)	0(1)	3(1)
C(34)	41(1)	37(1)	36(1)	-7(1)	-6(1)	7(1)
C(35)	43(1)	27(1)	40(1)	0(1)	-10(1)	0(1)

C(36)	34(1)	28(1)	34(1)	-2(1)	-5(1)	-6(1)
C(37)	40(1)	44(1)	34(1)	9(1)	6(1)	2(1)
C(38)	40(1)	29(1)	41(1)	5(1)	1(1)	-7(1)
C(39)	60(2)	55(2)	51(2)	-7(1)	-1(1)	21(1)
C(41)	61(2)	65(2)	44(2)	15(1)	18(1)	9(1)
C(42)	52(2)	51(2)	36(1)	7(1)	-5(1)	6(1)
C(43)	43(1)	40(1)	47(1)	11(1)	7(1)	-5(1)
C(44)	60(2)	38(1)	55(2)	12(1)	8(1)	-6(1)
C(45)	39(1)	38(1)	56(2)	2(1)	6(1)	-13(1)
C(46)	46(1)	41(1)	36(1)	5(1)	5(1)	-4(1)
C(51)	29(1)	29(1)	44(1)	6(1)	2(1)	-5(1)
C(52)	38(1)	27(1)	48(1)	7(1)	4(1)	-9(1)
C(53)	46(1)	27(1)	54(2)	4(1)	12(1)	-7(1)
C(54)	39(1)	33(1)	57(2)	12(1)	13(1)	1(1)
C(55)	31(1)	43(1)	50(1)	11(1)	1(1)	1(1)
C(56)	32(1)	36(1)	43(1)	6(1)	1(1)	-1(1)
C(57)	56(2)	31(1)	49(1)	1(1)	-7(1)	-13(1)
C(58)	38(1)	49(1)	48(1)	-3(1)	-11(1)	3(1)
C(59)	52(2)	44(2)	78(2)	11(1)	13(2)	13(1)
C(61)	61(2)	72(2)	60(2)	-8(2)	-24(2)	9(2)
C(62)	57(2)	70(2)	51(2)	-4(1)	0(1)	8(2)
C(63)	48(2)	40(1)	67(2)	-10(1)	-13(1)	-7(1)
C(64)	93(2)	37(2)	63(2)	-7(1)	-12(2)	-13(2)
C(65)	71(2)	42(1)	48(2)	4(1)	-6(1)	-8(1)
C(66)	48(2)	43(1)	67(2)	5(1)	-13(1)	-19(1)

Table S18. Bond lengths for non-hydrogen atoms (Å) for [(BHT)Mg(μ-OCH_2COOEt)(THF)]$_2$ (**5**).

Bonds	Bond lengths	Bonds	Bond lengths	Bonds	Bond lengths
Mg(1)-O(1)	1.8899(16)	C(6B)-C(7B)	1.495(15)	C(36)-C(38)	1.533(3)
Mg(1)-O(21)	1.9903(16)	C(7B)-C(8)	1.451(16)	C(37)-C(41)	1.535(3)
Mg(1)-O(11)	2.0101(16)	O(11)-C(11)	1.398(3)	C(37)-C(43)	1.538(4)
Mg(1)-O(3)	2.0952(16)	O(12)-C(12)	1.191(3)	C(37)-C(42)	1.539(3)
Mg(1)-O(12)	2.1467(17)	O(13)-C(12)	1.335(3)	C(38)-C(45)	1.539(3)
Mg(2)-O(2)	1.8777(17)	O(13)-C(13)	1.453(3)	C(38)-C(44)	1.542(3)
Mg(2)-O(11)	1.9695(16)	O(21)-C(21)	1.388(3)	C(38)-C(46)	1.545(3)
Mg(2)-O(21)	1.9994(16)	O(22)-C(22)	1.199(3)	C(51)-C(52)	1.426(3)
Mg(2)-O(4)	2.0792(18)	O(23)-C(22)	1.317(3)	C(51)-C(56)	1.427(3)
Mg(2)-O(22)	2.1309(17)	O(23)-C(23)	1.469(3)	C(52)-C(53)	1.391(3)
O(1)-C(31)	1.321(2)	C(11)-C(12)	1.512(3)	C(52)-C(57)	1.541(3)
O(2)-C(51)	1.321(3)	C(13)-C(14)	1.494(4)	C(53)-C(54)	1.384(4)
O(3)-C(1)	1.448(3)	C(21)-C(22)	1.507(3)	C(54)-C(55)	1.385(4)
O(3)-C(4)	1.453(3)	C(23)-C(24)	1.449(5)	C(54)-C(59)	1.512(3)
C(1)-C(2)	1.520(3)	C(31)-C(32)	1.429(3)	C(55)-C(56)	1.393(3)
C(2)-C(3)	1.500(4)	C(31)-C(36)	1.433(3)	C(56)-C(58)	1.547(3)
C(3)-C(4)	1.472(4)	C(32)-C(33)	1.390(3)	C(57)-C(66)	1.533(4)
O(4)-C(8)	1.444(3)	C(32)-C(37)	1.546(3)	C(57)-C(64)	1.534(4)
O(4)-C(5)	1.452(3)	C(33)-C(34)	1.385(3)	C(57)-C(65)	1.544(3)
C(5)-C(6A)	1.489(5)	C(34)-C(35)	1.380(3)	C(58)-C(63)	1.530(4)
C(5)-C(6B)	1.551(12)	C(34)-C(39)	1.516(3)	C(58)-C(62)	1.537(4)
C(6A)-C(7A)	1.506(8)	C(35)-C(36)	1.399(3)	C(58)-C(61)	1.544(4)
C(7A)-C(8)	1.518(7)				

Table S19. Bond angles for non-hydrogen atoms (°) for [(BHT)Mg(μ-OCH_2COOEt)(THF)]$_2$ (**5**).

Atoms	Bond angles	Atoms	Bond angles
O(1)-Mg(1)-O(21)	119.76(7)	O(22)-C(22)-O(23)	124.7(2)
O(1)-Mg(1)-O(11)	109.94(7)	O(22)-C(22)-C(21)	122.4(2)
O(21)-Mg(1)-O(11)	79.74(6)	O(23)-C(22)-C(21)	112.9(2)
O(1)-Mg(1)-O(3)	99.65(7)	C(24)-C(23)-O(23)	110.1(3)
O(21)-Mg(1)-O(3)	93.98(7)	O(1)-C(31)-C(32)	121.29(19)
O(11)-Mg(1)-O(3)	148.92(7)	O(1)-C(31)-C(36)	120.78(19)
O(1)-Mg(1)-O(12)	106.00(7)	C(32)-C(31)-C(36)	117.94(19)
O(21)-Mg(1)-O(12)	133.70(7)	C(33)-C(32)-C(31)	119.3(2)
O(11)-Mg(1)-O(12)	78.52(6)	C(33)-C(32)-C(37)	119.5(2)
O(3)-Mg(1)-O(12)	84.52(7)	C(31)-C(32)-C(37)	121.15(19)
O(2)-Mg(2)-O(11)	104.26(7)	C(34)-C(33)-C(32)	123.2(2)
O(2)-Mg(2)-O(21)	123.48(8)	C(35)-C(34)-C(33)	117.4(2)
O(11)-Mg(2)-O(21)	80.50(6)	C(35)-C(34)-C(39)	120.8(2)
O(2)-Mg(2)-O(4)	119.24(8)	C(33)-C(34)-C(39)	121.8(2)
O(11)-Mg(2)-O(4)	90.76(7)	C(34)-C(35)-C(36)	123.1(2)
O(21)-Mg(2)-O(4)	116.93(8)	C(35)-C(36)-C(31)	119.0(2)
O(2)-Mg(2)-O(22)	96.93(7)	C(35)-C(36)-C(38)	119.9(2)
O(11)-Mg(2)-O(22)	156.53(7)	C(31)-C(36)-C(38)	121.16(19)
O(21)-Mg(2)-O(22)	79.45(7)	C(41)-C(37)-C(43)	106.8(2)
O(4)-Mg(2)-O(22)	87.55(7)	C(41)-C(37)-C(42)	106.7(2)
C(31)-O(1)-Mg(1)	175.64(14)	C(43)-C(37)-C(42)	110.4(2)
C(51)-O(2)-Mg(2)	177.44(15)	C(41)-C(37)-C(32)	112.4(2)
C(1)-O(3)-C(4)	108.32(17)	C(43)-C(37)-C(32)	110.32(18)
C(1)-O(3)-Mg(1)	120.74(13)	C(42)-C(37)-C(32)	110.06(19)
C(4)-O(3)-Mg(1)	129.45(14)	C(36)-C(38)-C(45)	110.29(19)
O(3)-C(1)-C(2)	105.80(19)	C(36)-C(38)-C(44)	112.4(2)
C(3)-C(2)-C(1)	101.9(2)	C(45)-C(38)-C(44)	106.05(19)
C(4)-C(3)-C(2)	103.9(2)	C(36)-C(38)-C(46)	109.82(18)
O(3)-C(4)-C(3)	106.7(2)	C(45)-C(38)-C(46)	111.5(2)
C(8)-O(4)-C(5)	109.1(2)	C(44)-C(38)-C(46)	106.7(2)
C(8)-O(4)-Mg(2)	127.93(17)	O(2)-C(51)-C(52)	120.8(2)
C(5)-O(4)-Mg(2)	122.66(15)	O(2)-C(51)-C(56)	120.5(2)
O(4)-C(5)-C(6A)	107.0(3)	C(52)-C(51)-C(56)	118.7(2)
O(4)-C(5)-C(6B)	93.8(5)	C(53)-C(52)-C(51)	118.7(2)
C(5)-C(6A)-C(7A)	100.6(4)	C(53)-C(52)-C(57)	120.4(2)
C(6A)-C(7A)-C(8)	105.0(5)	C(51)-C(52)-C(57)	120.9(2)
C(7B)-C(6B)-C(5)	114.4(12)	C(54)-C(53)-C(52)	123.4(2)
C(8)-C(7B)-C(6B)	89.0(9)	C(53)-C(54)-C(55)	117.2(2)
O(4)-C(8)-C(7B)	115.5(8)	C(53)-C(54)-C(59)	121.5(2)
O(4)-C(8)-C(7A)	104.4(3)	C(55)-C(54)-C(59)	121.3(2)
C(11)-O(11)-Mg(2)	128.98(14)	C(54)-C(55)-C(56)	123.1(2)
C(11)-O(11)-Mg(1)	116.87(13)	C(55)-C(56)-C(51)	118.9(2)
Mg(2)-O(11)-Mg(1)	100.05(7)	C(55)-C(56)-C(58)	120.7(2)
C(12)-O(12)-Mg(1)	112.52(14)	C(51)-C(56)-C(58)	120.4(2)
C(12)-O(13)-C(13)	116.16(18)	C(66)-C(57)-C(64)	107.1(2)
C(21)-O(21)-Mg(1)	143.88(14)	C(66)-C(57)-C(52)	110.4(2)
C(21)-O(21)-Mg(2)	115.81(13)	C(64)-C(57)-C(52)	112.9(2)
Mg(1)-O(21)-Mg(2)	99.71(7)	C(66)-C(57)-C(65)	110.5(2)
C(22)-O(22)-Mg(2)	111.67(14)	C(64)-C(57)-C(65)	106.3(2)
C(22)-O(23)-C(23)	116.8(2)	C(52)-C(57)-C(65)	109.66(19)
O(11)-C(11)-C(12)	109.06(18)	C(63)-C(58)-C(62)	110.0(2)

O(12)-C(12)-O(13)	125.1(2)	C(63)-C(58)-C(61)	106.8(2)
O(12)-C(12)-C(11)	122.7(2)	C(62)-C(58)-C(61)	106.6(2)
O(13)-C(12)-C(11)	112.17(19)	C(63)-C(58)-C(56)	110.8(2)
O(13)-C(13)-C(14)	107.5(2)	C(62)-C(58)-C(56)	110.4(2)
O(21)-C(21)-C(22)	110.06(19)	C(61)-C(58)-C(56)	112.2(2)

Table S20. Torsion angles (°) for [(BHT)Mg(μ-OCH_2COOEt)(THF)]$_2$ (**5**).

Atoms	Torsion angles	Atoms	Torsion angles
C(4)-O(3)-C(1)-C(2)	-12.5(3)	C(32)-C(33)-C(34)-C(39)	178.5(2)
Mg(1)-O(3)-C(1)-C(2)	154.80(17)	C(33)-C(34)-C(35)-C(36)	0.7(3)
O(3)-C(1)-C(2)-C(3)	30.2(3)	C(39)-C(34)-C(35)-C(36)	-178.4(2)
C(1)-C(2)-C(3)-C(4)	-36.4(3)	C(34)-C(35)-C(36)-C(31)	1.4(3)
C(1)-O(3)-C(4)-C(3)	-10.8(3)	C(34)-C(35)-C(36)-C(38)	-178.4(2)
Mg(1)-O(3)-C(4)-C(3)	-176.64(16)	O(1)-C(31)-C(36)-C(35)	176.28(18)
C(2)-C(3)-C(4)-O(3)	29.9(3)	C(32)-C(31)-C(36)-C(35)	-3.4(3)
C(8)-O(4)-C(5)-C(6A)	-17.4(4)	O(1)-C(31)-C(36)-C(38)	-3.9(3)
Mg(2)-O(4)-C(5)-C(6A)	168.5(3)	C(32)-C(31)-C(36)-C(38)	176.38(19)
C(8)-O(4)-C(5)-C(6B)	13.8(6)	C(33)-C(32)-C(37)-C(41)	-4.2(3)
Mg(2)-O(4)-C(5)-C(6B)	-160.2(6)	C(31)-C(32)-C(37)-C(41)	176.0(2)
O(4)-C(5)-C(6A)-C(7A)	33.3(5)	C(33)-C(32)-C(37)-C(43)	114.9(2)
C(5)-C(6A)-C(7A)-C(8)	-36.7(5)	C(31)-C(32)-C(37)-C(43)	-64.9(3)
O(4)-C(5)-C(6B)-C(7B)	-38.4(12)	C(33)-C(32)-C(37)-C(42)	-123.0(2)
C(5)-C(6B)-C(7B)-C(8)	43.1(15)	C(31)-C(32)-C(37)-C(42)	57.2(3)
C(5)-O(4)-C(8)-C(7B)	12.6(9)	C(35)-C(36)-C(38)-C(45)	121.0(2)
Mg(2)-O(4)-C(8)-C(7B)	-173.7(9)	C(31)-C(36)-C(38)-C(45)	-58.8(3)
C(5)-O(4)-C(8)-C(7A)	-6.3(4)	C(35)-C(36)-C(38)-C(44)	2.9(3)
Mg(2)-O(4)-C(8)-C(7A)	167.3(3)	C(31)-C(36)-C(38)-C(44)	-176.9(2)
C(6B)-C(7B)-C(8)-O(4)	-31.9(14)	C(35)-C(36)-C(38)-C(46)	-115.7(2)
C(6A)-C(7A)-C(8)-O(4)	27.3(5)	C(31)-C(36)-C(38)-C(46)	64.5(3)
Mg(2)-O(11)-C(11)-C(12)	-128.02(17)	O(2)-C(51)-C(52)-C(53)	178.5(2)
Mg(1)-O(11)-C(11)-C(12)	3.4(2)	C(56)-C(51)-C(52)-C(53)	-0.4(3)
Mg(1)-O(12)-C(12)-O(13)	176.25(17)	O(2)-C(51)-C(52)-C(57)	-1.2(3)
Mg(1)-O(12)-C(12)-C(11)	-4.6(3)	C(56)-C(51)-C(52)-C(57)	179.9(2)
C(13)-O(13)-C(12)-O(12)	-1.0(3)	C(51)-C(52)-C(53)-C(54)	1.5(3)
C(13)-O(13)-C(12)-C(11)	179.8(2)	C(57)-C(52)-C(53)-C(54)	-178.8(2)
C(13)-O(13)-C(12)-Mg(1)	13.3(9)	C(52)-C(53)-C(54)-C(55)	-1.3(3)
O(11)-C(11)-C(12)-O(12)	1.1(3)	C(52)-C(53)-C(54)-C(59)	179.0(2)
O(11)-C(11)-C(12)-O(13)	-179.66(18)	C(53)-C(54)-C(55)-C(56)	0.0(3)
O(11)-C(11)-C(12)-Mg(1)	-2.20(16)	C(59)-C(54)-C(55)-C(56)	179.6(2)
C(12)-O(13)-C(13)-C(14)	165.4(2)	C(54)-C(55)-C(56)-C(51)	1.1(3)
Mg(1)-O(21)-C(21)-C(22)	164.11(19)	C(54)-C(55)-C(56)-C(58)	-178.4(2)
Mg(2)-O(21)-C(21)-C(22)	-4.5(3)	O(2)-C(51)-C(56)-C(55)	-179.7(2)
Mg(2)-O(22)-C(22)-O(23)	-173.21(19)	C(52)-C(51)-C(56)-C(55)	-0.9(3)
Mg(2)-O(22)-C(22)-C(21)	6.6(3)	O(2)-C(51)-C(56)-C(58)	-0.2(3)
C(23)-O(23)-C(22)-O(22)	7.3(4)	C(52)-C(51)-C(56)-C(58)	178.7(2)
C(23)-O(23)-C(22)-C(21)	-172.6(2)	C(53)-C(52)-C(57)-C(66)	121.5(2)
C(23)-O(23)-C(22)-Mg(2)	-17.3(10)	C(51)-C(52)-C(57)-C(66)	-58.8(3)
O(21)-C(21)-C(22)-O(22)	-1.8(3)	C(53)-C(52)-C(57)-C(64)	1.8(3)
O(21)-C(21)-C(22)-O(23)	178.0(2)	C(51)-C(52)-C(57)-C(64)	-178.6(2)
O(21)-C(21)-C(22)-Mg(2)	2.96(17)	C(53)-C(52)-C(57)-C(65)	-116.5(2)
C(22)-O(23)-C(23)-C(24)	77.5(4)	C(51)-C(52)-C(57)-C(65)	63.2(3)
O(1)-C(31)-C(32)-C(33)	-176.23(19)	C(55)-C(56)-C(58)-C(63)	119.4(2)

C(36)-C(31)-C(32)-C(33)	3.5(3)	C(51)-C(56)-C(58)-C(63)	-60.2(3)
O(1)-C(31)-C(32)-C(37)	3.5(3)	C(55)-C(56)-C(58)-C(62)	-118.5(2)
C(36)-C(31)-C(32)-C(37)	-176.76(19)	C(51)-C(56)-C(58)-C(62)	61.9(3)
C(31)-C(32)-C(33)-C(34)	-1.5(3)	C(55)-C(56)-C(58)-C(61)	0.1(3)
C(37)-C(32)-C(33)-C(34)	178.7(2)	C(51)-C(56)-C(58)-C(61)	-179.4(2)
C(32)-C(33)-C(34)-C(35)	-0.6(3)		

S2.6. Molecular structure of [(BHT)Mg(THF)(μ-OCH(CH$_3$)COOCH$_2$COO^{t}Bu)]$_2$ (6)

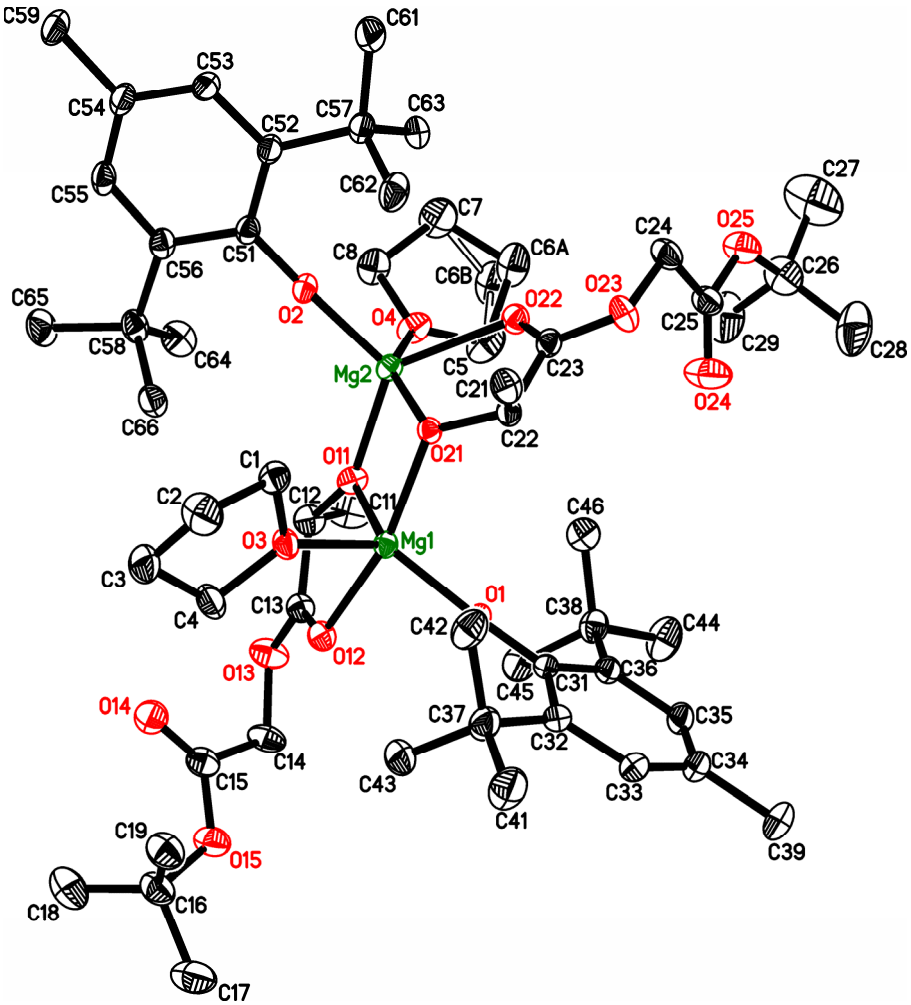

Fig. S17. Molecular structures of [(BHT)Mg(THF)(μ-OCH(CH$_3$)COOCH$_2$COO^{t}Bu)]$_2$ (**6**). Non-coordinating solvent molecules and hydrogen atoms are omitted. Thermal ellipsoids are set to the 50% probability level. The disordered THF molecule is shown with open solid lines

Compound [(BHT)Mg(THF)(μ-κ^{1}O:κ^{2}O,O'-OCH(CH$_3$)COOCH$_2$COO^{t}Bu)]$_2$(THF)$_2$(C$_6$H$_{14}$)$_{0.5}$ has two non-coordinating solvent molecules in crystal channels. The main residue **6** (Fig. S17) possesses a dimeric structure, has the Mg$_2$O$_2$ central rhomboid core, c.n.=5. Folding angles are 3.1° between O-Mg-O planes and 3.6° between Mg-O-Mg planes. A carbon atom (C6) of one coordinated THF molecule is disordered over two positions. Lactate anions exhibit μ-κ^1:κ^2-semi-bridging coordination mode: oxygen atom of hydroxyl group is bound to the both Mg-atoms; the O-atom of the nearest carboxyl group is coordinated to only one of the magnesium atoms. The shortest Mg-O bond distances are Mg-O$_{BHT}$ bonds, the longest are Mg-O$_{C=O}$.

Table S21. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2$ $x10^3$) for [(BHT)Mg(μ-OCH(CH_3)$COOCH_2COO^tBu$)(THF)]$_2$ (**5**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U(eq)
Mg(1)	7092(1)	6566(1)	3383(1)	27(1)
Mg(2)	5134(1)	6373(1)	2842(1)	29(1)
O(1)	7895(1)	6596(1)	2748(1)	34(1)
O(2)	4346(1)	6574(1)	3440(1)	32(1)
O(3)	7208(1)	7038(1)	4332(1)	34(1)
C(1)	6686(2)	7484(1)	4314(2)	39(1)
C(2)	7130(3)	7769(1)	5037(2)	62(1)
C(3)	7480(3)	7359(2)	5623(2)	56(1)
C(4)	7762(2)	6976(1)	5124(2)	49(1)
O(4)	4421(1)	5734(1)	2372(1)	45(1)
C(5)	4500(3)	5482(2)	1664(3)	66(1)
C(6A)	3591(5)	5466(4)	1159(5)	68(2)
C(6B)	3670(5)	5185(6)	1357(8)	68(2)
C(7)	3022(3)	5447(2)	1756(3)	75(1)
C(8)	3629(2)	5551(1)	2552(2)	52(1)
O(11)	6220(1)	6037(1)	3435(1)	34(1)
O(12)	7895(1)	6034(1)	4136(1)	35(1)
O(13)	7877(2)	5265(1)	4604(2)	50(1)
O(14)	8670(2)	5837(1)	5906(1)	54(1)
O(15)	9997(2)	5689(1)	5660(1)	51(1)
O(21)	6022(1)	6898(1)	2746(1)	27(1)
O(22)	4728(1)	6612(1)	1596(1)	36(1)
O(23)	4961(2)	7208(1)	768(1)	42(1)
O(24)	5283(2)	6434(1)	-94(2)	75(1)
O(25)	3890(2)	6407(1)	-798(1)	52(1)
C(11)	6271(3)	5139(1)	3439(3)	63(1)
C(12)	6511(2)	5618(1)	3892(2)	41(1)
C(13)	7492(2)	5665(1)	4221(2)	36(1)
C(14)	8820(2)	5285(1)	4858(2)	48(1)
C(15)	9131(2)	5641(1)	5540(2)	44(1)
C(16)	10513(2)	6019(1)	6280(2)	52(1)
C(17)	11432(3)	5959(2)	6172(3)	72(1)
C(18)	10460(3)	5839(2)	7084(2)	75(1)
C(19)	10194(3)	6544(1)	6117(2)	57(1)
C(21)	5902(2)	7722(1)	2139(2)	40(1)
C(22)	5943(2)	7161(1)	2047(2)	31(1)
C(23)	5149(2)	6966(1)	1452(2)	32(1)
C(24)	4250(2)	7023(1)	153(2)	43(1)
C(25)	4554(2)	6586(1)	-245(2)	41(1)
C(26)	4007(3)	5971(1)	-1284(2)	63(1)
C(27)	3120(4)	5920(2)	-1836(4)	123(2)
C(28)	4670(4)	6088(2)	-1756(3)	94(2)
C(29)	4269(4)	5530(2)	-758(3)	87(1)
C(31)	8428(2)	6655(1)	2277(2)	32(1)
C(32)	9045(2)	7053(1)	2402(2)	36(1)
C(33)	9571(2)	7114(1)	1871(2)	43(1)
C(34)	9527(2)	6801(1)	1235(2)	45(1)
C(35)	8949(2)	6407(1)	1138(2)	43(1)
C(36)	8402(2)	6316(1)	1644(2)	35(1)

C(37)	9150(2)	7403(1)	3115(2)	44(1)
C(38)	7818(2)	5851(1)	1534(2)	42(1)
C(39)	10121(3)	6882(2)	681(2)	62(1)
C(41)	9859(3)	7795(2)	3153(2)	64(1)
C(42)	8291(2)	7686(1)	3062(2)	50(1)
C(43)	9406(2)	7103(2)	3879(2)	56(1)
C(44)	7897(3)	5543(2)	816(3)	67(1)
C(45)	8117(3)	5519(1)	2266(2)	56(1)
C(46)	6851(2)	5981(1)	1405(2)	47(1)
C(51)	3782(2)	6737(1)	3831(2)	30(1)
C(52)	3097(2)	7073(1)	3471(2)	33(1)
C(53)	2508(2)	7230(1)	3900(2)	39(1)
C(54)	2549(2)	7077(1)	4661(2)	41(1)
C(55)	3217(2)	6759(1)	5008(2)	40(1)
C(56)	3842(2)	6586(1)	4628(2)	34(1)
C(57)	2989(2)	7266(1)	2627(2)	42(1)
C(58)	4572(2)	6233(1)	5068(2)	41(1)
C(59)	1890(2)	7263(2)	5094(2)	60(1)
C(61)	2226(3)	7633(2)	2385(2)	67(1)
C(62)	3821(2)	7539(1)	2568(2)	50(1)
C(63)	2798(2)	6828(1)	2041(2)	48(1)
C(64)	4495(3)	5725(1)	4656(2)	53(1)
C(65)	4529(3)	6140(2)	5931(2)	56(1)
C(66)	5477(2)	6462(1)	5109(2)	42(1)
O(7)	3343(3)	4175(2)	2334(3)	140(2)
C(71)	2944(5)	3937(3)	1588(4)	119(2)
C(72)	2040(4)	4068(2)	1409(4)	96(2)
C(73)	1845(4)	4134(2)	2186(4)	105(2)
C(74)	2709(5)	4111(3)	2787(4)	122(2)
O(81)	9531(4)	4559(2)	6378(3)	71(2)
C(81)	9062(8)	4666(4)	6955(7)	122(4)
C(82)	8982(10)	4199(4)	7378(8)	129(5)
C(83)	8827(11)	3882(8)	6629(11)	207(10)
C(84)	9625(5)	4029(2)	6321(5)	59(2)
O(82)	9109(9)	4322(5)	5939(7)	135(4)
C(85)	8284(12)	4413(10)	6104(11)	205(11)
C(86)	8419(8)	4184(5)	6900(8)	92(4)
C(87)	9174(6)	3831(3)	6928(6)	55(2)
C(88)	9753(10)	4225(8)	6656(10)	161(8)
C(91)	8841(9)	4095(5)	548(8)	249(6)
C(92)	9137(7)	4460(4)	24(7)	199(4)
C(93)	9913(7)	4797(3)	261(5)	178(4)

Table S22. Anisotropic displacement parameters ($Å^2$ x10^3) for [(BHT)Mg(μ-OCH(CH_3)COOCH_2COO^{t}Bu)(THF)]$_2$ (**5**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	30(1)	25(1)	26(1)	2(1)	9(1)	1(1)
Mg(2)	30(1)	28(1)	33(1)	-2(1)	11(1)	-3(1)
O(1)	34(1)	39(1)	32(1)	0(1)	14(1)	1(1)
O(2)	37(1)	33(1)	29(1)	1(1)	14(1)	1(1)

O(3)	41(1)	34(1)	26(1)	-2(1)	6(1)	7(1)
C(1)	44(2)	34(2)	39(2)	-4(1)	12(1)	8(1)
C(2)	72(3)	50(2)	58(2)	-23(2)	6(2)	7(2)
C(3)	55(2)	75(3)	38(2)	-17(2)	11(2)	-8(2)
C(4)	53(2)	60(2)	29(2)	-2(1)	0(1)	11(2)
O(4)	41(1)	37(1)	59(1)	-15(1)	18(1)	-11(1)
C(5)	73(3)	53(2)	79(3)	-32(2)	34(2)	-14(2)
C(6A)	83(4)	70(5)	56(4)	-20(4)	25(3)	-33(4)
C(6B)	83(4)	70(5)	56(4)	-20(4)	25(3)	-33(4)
C(7)	59(2)	94(3)	70(3)	-29(2)	15(2)	-30(2)
C(8)	55(2)	47(2)	56(2)	-5(2)	19(2)	-22(2)
O(11)	34(1)	24(1)	45(1)	5(1)	13(1)	-1(1)
O(12)	39(1)	31(1)	35(1)	3(1)	7(1)	2(1)
O(13)	45(1)	31(1)	67(2)	8(1)	0(1)	4(1)
O(14)	51(1)	60(2)	51(1)	7(1)	13(1)	10(1)
O(15)	42(1)	50(1)	56(1)	-10(1)	2(1)	7(1)
O(21)	29(1)	27(1)	24(1)	3(1)	6(1)	-2(1)
O(22)	36(1)	40(1)	31(1)	-6(1)	7(1)	-5(1)
O(23)	52(1)	41(1)	29(1)	0(1)	-1(1)	-4(1)
O(24)	47(2)	85(2)	82(2)	-30(2)	-4(1)	19(1)
O(25)	49(1)	49(1)	51(1)	-20(1)	-1(1)	5(1)
C(11)	52(2)	31(2)	96(3)	0(2)	-2(2)	-6(2)
C(12)	45(2)	28(2)	49(2)	10(1)	13(1)	0(1)
C(13)	40(2)	32(2)	36(2)	1(1)	8(1)	4(1)
C(14)	40(2)	35(2)	61(2)	3(2)	-3(2)	11(1)
C(15)	45(2)	37(2)	48(2)	10(1)	5(2)	10(1)
C(16)	48(2)	53(2)	46(2)	-11(2)	-2(2)	4(2)
C(17)	45(2)	79(3)	83(3)	-28(2)	-1(2)	5(2)
C(18)	79(3)	81(3)	54(2)	10(2)	-3(2)	8(2)
C(19)	57(2)	53(2)	55(2)	-5(2)	4(2)	1(2)
C(21)	46(2)	34(2)	37(2)	3(1)	8(1)	-3(1)
C(22)	34(1)	34(2)	26(1)	3(1)	8(1)	-1(1)
C(23)	37(2)	33(2)	28(1)	-3(1)	11(1)	4(1)
C(24)	45(2)	45(2)	33(2)	-6(1)	-2(1)	3(1)
C(25)	37(2)	45(2)	37(2)	-2(1)	2(1)	3(1)
C(26)	79(3)	45(2)	59(2)	-20(2)	7(2)	9(2)
C(27)	132(4)	93(4)	115(4)	-60(3)	-22(4)	8(3)
C(28)	158(4)	68(3)	72(3)	-11(2)	59(3)	15(3)
C(29)	141(4)	47(2)	82(3)	-11(2)	46(3)	6(2)
C(31)	27(1)	42(2)	28(1)	6(1)	8(1)	8(1)
C(32)	28(1)	48(2)	33(2)	1(1)	8(1)	3(1)
C(33)	33(2)	57(2)	38(2)	5(1)	11(1)	-2(1)
C(34)	40(2)	62(2)	38(2)	8(2)	18(1)	7(2)
C(35)	45(2)	53(2)	33(2)	3(1)	16(1)	12(2)
C(36)	36(2)	39(2)	31(1)	3(1)	9(1)	8(1)
C(37)	39(2)	57(2)	39(2)	-8(2)	14(1)	-13(2)
C(38)	52(2)	37(2)	41(2)	-4(1)	17(1)	4(1)
C(39)	58(2)	87(3)	51(2)	4(2)	34(2)	-1(2)
C(41)	60(2)	80(3)	57(2)	-22(2)	23(2)	-31(2)
C(42)	55(2)	44(2)	56(2)	-10(2)	26(2)	-8(2)
C(43)	50(2)	83(3)	34(2)	-9(2)	6(2)	-11(2)
C(44)	90(3)	54(2)	67(3)	-23(2)	38(2)	-10(2)
C(45)	69(2)	39(2)	65(2)	9(2)	27(2)	14(2)
C(46)	48(2)	41(2)	50(2)	-7(2)	11(2)	-7(1)

C(51)	31(1)	34(1)	27(1)	-2(1)	10(1)	-7(1)
C(52)	34(2)	40(2)	28(1)	-3(1)	11(1)	-3(1)
C(53)	31(2)	55(2)	34(2)	-8(1)	10(1)	1(1)
C(54)	35(2)	62(2)	32(2)	-13(1)	15(1)	-12(1)
C(55)	41(2)	55(2)	27(1)	-3(1)	14(1)	-18(1)
C(56)	36(2)	37(2)	30(1)	0(1)	10(1)	-12(1)
C(57)	47(2)	51(2)	33(2)	8(1)	18(1)	14(1)
C(58)	48(2)	41(2)	32(2)	7(1)	9(1)	-9(1)
C(59)	41(2)	105(3)	40(2)	-13(2)	21(2)	-3(2)
C(61)	75(3)	88(3)	42(2)	19(2)	23(2)	41(2)
C(62)	69(2)	41(2)	47(2)	12(2)	32(2)	9(2)
C(63)	47(2)	70(2)	26(2)	1(2)	9(1)	9(2)
C(64)	63(2)	36(2)	57(2)	12(2)	12(2)	-6(2)
C(65)	62(2)	66(2)	41(2)	21(2)	14(2)	-7(2)
C(66)	43(2)	48(2)	33(2)	5(1)	6(1)	-6(1)
O(7)	92(3)	185(5)	136(4)	-11(4)	12(3)	7(3)
C(71)	127(6)	134(6)	97(5)	3(4)	28(4)	11(5)
C(72)	101(4)	88(4)	94(4)	3(3)	12(3)	6(3)
C(73)	105(4)	82(4)	141(6)	0(4)	56(4)	10(3)
C(74)	144(6)	139(6)	83(4)	15(4)	28(4)	16(5)

Table S23. Bond lengths for non-hydrogen atoms (Å) for [(BHT)Mg(μ-$OCH(CH_3)COOCH_2COO^tBu$)(THF)]$_2$ (**5**)

Bonds	Bond lengths	Bonds	Bond lengths	Bonds	Bond lengths
Mg(1)-O(1)	1.879(2)	O(23)-C(23)	1.330(3)	C(51)-C(56)	1.433(4)
Mg(1)-O(21)	1.989(2)	O(23)-C(24)	1.437(4)	C(52)-C(53)	1.394(4)
Mg(1)-O(11)	1.997(2)	O(24)-C(25)	1.185(4)	C(52)-C(57)	1.533(4)
Mg(1)-O(3)	2.061(2)	O(25)-C(25)	1.327(4)	C(53)-C(54)	1.379(4)
Mg(1)-O(12)	2.137(2)	O(25)-C(26)	1.489(4)	C(54)-C(55)	1.376(5)
Mg(2)-O(2)	1.889(2)	C(11)-C(12)	1.513(5)	C(54)-C(59)	1.514(4)
Mg(2)-O(11)	1.986(2)	C(12)-C(13)	1.515(4)	C(55)-C(56)	1.396(4)
Mg(2)-O(21)	2.0245(19)	C(14)-C(15)	1.513(5)	C(56)-C(58)	1.542(4)
Mg(2)-O(4)	2.107(2)	C(16)-C(19)	1.504(5)	C(57)-C(62)	1.528(5)
Mg(2)-O(22)	2.208(2)	C(16)-C(18)	1.510(6)	C(57)-C(61)	1.533(5)
O(1)-C(31)	1.323(3)	C(16)-C(17)	1.513(5)	C(57)-C(63)	1.541(5)
O(2)-C(51)	1.322(3)	C(21)-C(22)	1.523(4)	C(58)-C(64)	1.536(5)
O(3)-C(1)	1.452(3)	C(22)-C(23)	1.509(4)	C(58)-C(66)	1.539(4)
O(3)-C(4)	1.452(4)	C(24)-C(25)	1.504(4)	C(58)-C(65)	1.546(4)
C(1)-C(2)	1.497(5)	C(26)-C(27)	1.495(7)	O(7)-C(74)	1.430(8)
C(2)-C(3)	1.515(6)	C(26)-C(29)	1.497(6)	O(7)-C(71)	1.449(8)
C(3)-C(4)	1.488(5)	C(26)-C(28)	1.515(7)	C(71)-C(72)	1.426(8)
O(4)-C(5)	1.443(4)	C(31)-C(32)	1.426(4)	C(72)-C(73)	1.476(8)
O(4)-C(8)	1.447(4)	C(31)-C(36)	1.427(4)	C(73)-C(74)	1.501(9)
C(5)-C(6A)	1.486(9)	C(32)-C(33)	1.398(4)	O(81)-C(81)	1.421(8)
C(5)-C(6B)	1.514(10)	C(32)-C(37)	1.539(4)	O(81)-C(84)	1.439(7)
C(6A)-C(7)	1.534(9)	C(33)-C(34)	1.384(5)	C(81)-C(82)	1.480(9)
C(6B)-C(7)	1.542(10)	C(34)-C(35)	1.382(5)	C(82)-C(83)	1.532(10)
C(7)-C(8)	1.508(5)	C(34)-C(39)	1.518(4)	C(83)-C(84)	1.537(9)
O(11)-C(12)	1.393(3)	C(35)-C(36)	1.400(4)	O(82)-C(85)	1.420(10)
O(12)-C(13)	1.208(4)	C(36)-C(38)	1.538(4)	O(82)-C(88)	1.427(10)
O(13)-C(13)	1.332(4)	C(37)-C(41)	1.527(5)	C(85)-C(86)	1.489(10)

O(13)-C(14)	1.443(4)	C(37)-C(43)	1.528(5)	C(86)-C(87)	1.514(9)
O(14)-C(15)	1.202(4)	C(37)-C(42)	1.536(5)	C(87)-C(88)	1.549(10)
O(15)-C(15)	1.333(4)	C(38)-C(46)	1.525(5)	C(91)-C(92)	1.495(9)
O(15)-C(16)	1.480(4)	C(38)-C(44)	1.535(5)	C(92)-C(93)	1.496(8)
O(21)-C(22)	1.391(3)	C(38)-C(45)	1.537(5)	C(93)-C(93)#1	1.494(9)
O(22)-C(23)	1.223(3)	C(51)-C(52)	1.430(4)		

Symmetry transformations used to generate equivalent atoms: #1 -x+2, -y+1, -z.

Table S24. Bond angles for non-hydrogen atoms (°) for [(BHT)Mg(μ-$OCH(CH_3)COOCH_2COO^tBu$)(THF)]$_2$ (**5**)

Atoms	Bond angles	Atoms	Bond angles
O(1)-Mg(1)-O(21)	104.59(9)	O(25)-C(25)-C(24)	109.6(3)
O(1)-Mg(1)-O(11)	128.93(9)	O(25)-C(26)-C(27)	102.3(3)
O(21)-Mg(1)-O(11)	81.26(8)	O(25)-C(26)-C(29)	109.2(3)
O(1)-Mg(1)-O(3)	120.67(9)	C(27)-C(26)-C(29)	113.3(5)
O(21)-Mg(1)-O(3)	93.88(8)	O(25)-C(26)-C(28)	110.3(3)
O(11)-Mg(1)-O(3)	109.17(9)	C(27)-C(26)-C(28)	109.2(5)
O(1)-Mg(1)-O(12)	90.59(9)	C(29)-C(26)-C(28)	112.1(4)
O(21)-Mg(1)-O(12)	159.60(9)	O(1)-C(31)-C(32)	120.5(3)
O(11)-Mg(1)-O(12)	78.57(8)	O(1)-C(31)-C(36)	120.3(3)
O(3)-Mg(1)-O(12)	89.83(8)	C(32)-C(31)-C(36)	119.1(3)
O(2)-Mg(2)-O(11)	116.18(9)	C(33)-C(32)-C(31)	118.7(3)
O(2)-Mg(2)-O(21)	113.99(9)	C(33)-C(32)-C(37)	120.0(3)
O(11)-Mg(2)-O(21)	80.64(8)	C(31)-C(32)-C(37)	121.2(2)
O(2)-Mg(2)-O(4)	95.22(9)	C(34)-C(33)-C(32)	122.8(3)
O(11)-Mg(2)-O(4)	97.98(9)	C(35)-C(34)-C(33)	117.9(3)
O(21)-Mg(2)-O(4)	148.26(9)	C(35)-C(34)-C(39)	121.6(3)
O(2)-Mg(2)-O(22)	113.12(9)	C(33)-C(34)-C(39)	120.6(3)
O(11)-Mg(2)-O(22)	130.48(9)	C(34)-C(35)-C(36)	123.1(3)
O(21)-Mg(2)-O(22)	75.66(8)	C(35)-C(36)-C(31)	118.3(3)
O(4)-Mg(2)-O(22)	81.79(9)	C(35)-C(36)-C(38)	120.4(3)
C(31)-O(1)-Mg(1)	174.91(19)	C(31)-C(36)-C(38)	121.3(3)
C(51)-O(2)-Mg(2)	176.71(19)	C(41)-C(37)-C(43)	107.2(3)
C(1)-O(3)-C(4)	108.6(2)	C(41)-C(37)-C(42)	106.5(3)
C(1)-O(3)-Mg(1)	123.74(17)	C(43)-C(37)-C(42)	110.6(3)
C(4)-O(3)-Mg(1)	127.56(18)	C(41)-C(37)-C(32)	113.0(3)
O(3)-C(1)-C(2)	105.2(3)	C(43)-C(37)-C(32)	109.6(3)
C(1)-C(2)-C(3)	102.3(3)	C(42)-C(37)-C(32)	109.8(3)
C(4)-C(3)-C(2)	102.7(3)	C(46)-C(38)-C(44)	106.5(3)
O(3)-C(4)-C(3)	106.5(3)	C(46)-C(38)-C(45)	110.3(3)
C(5)-O(4)-C(8)	106.8(3)	C(44)-C(38)-C(45)	107.1(3)
C(5)-O(4)-Mg(2)	124.6(2)	C(46)-C(38)-C(36)	112.1(3)
C(8)-O(4)-Mg(2)	126.7(2)	C(44)-C(38)-C(36)	112.1(3)
O(4)-C(5)-C(6A)	104.4(4)	C(45)-C(38)-C(36)	108.7(3)
O(4)-C(5)-C(6B)	107.7(5)	O(2)-C(51)-C(52)	120.9(2)
C(5)-C(6A)-C(7)	103.6(5)	O(2)-C(51)-C(56)	121.2(3)
C(5)-C(6B)-C(7)	101.9(8)	C(52)-C(51)-C(56)	118.0(2)
C(8)-C(7)-C(6A)	106.2(4)	C(53)-C(52)-C(51)	119.0(3)
C(8)-C(7)-C(6B)	99.4(5)	C(53)-C(52)-C(57)	119.0(3)
O(4)-C(8)-C(7)	104.3(3)	C(51)-C(52)-C(57)	122.0(2)
C(12)-O(11)-Mg(2)	141.88(18)	C(54)-C(53)-C(52)	123.3(3)

C(12)-O(11)-Mg(1)	118.17(18)	C(55)-C(54)-C(53)	117.3(3)
Mg(2)-O(11)-Mg(1)	99.50(9)	C(55)-C(54)-C(59)	122.1(3)
C(13)-O(12)-Mg(1)	112.25(19)	C(53)-C(54)-C(59)	120.6(3)
C(13)-O(13)-C(14)	115.5(2)	C(54)-C(55)-C(56)	123.5(3)
C(15)-O(15)-C(16)	122.0(3)	C(55)-C(56)-C(51)	118.8(3)
C(22)-O(21)-Mg(1)	126.85(16)	C(55)-C(56)-C(58)	119.7(3)
C(22)-O(21)-Mg(2)	121.00(16)	C(51)-C(56)-C(58)	121.4(3)
Mg(1)-O(21)-Mg(2)	98.50(8)	C(62)-C(57)-C(61)	107.3(3)
C(23)-O(22)-Mg(2)	112.99(18)	C(62)-C(57)-C(52)	109.6(3)
C(23)-O(23)-C(24)	117.5(2)	C(61)-C(57)-C(52)	112.1(2)
C(25)-O(25)-C(26)	121.1(3)	C(62)-C(57)-C(63)	110.7(3)
O(11)-C(12)-C(11)	112.7(3)	C(61)-C(57)-C(63)	107.4(3)
O(11)-C(12)-C(13)	108.1(2)	C(52)-C(57)-C(63)	109.7(3)
C(11)-C(12)-C(13)	111.6(3)	C(64)-C(58)-C(66)	110.0(3)
O(12)-C(13)-O(13)	122.6(3)	C(64)-C(58)-C(56)	110.6(3)
O(12)-C(13)-C(12)	122.7(3)	C(66)-C(58)-C(56)	110.2(2)
O(13)-C(13)-C(12)	114.8(3)	C(64)-C(58)-C(65)	107.2(3)
O(13)-C(14)-C(15)	112.0(3)	C(66)-C(58)-C(65)	106.4(3)
O(14)-C(15)-O(15)	127.0(3)	C(56)-C(58)-C(65)	112.2(3)
O(14)-C(15)-C(14)	125.2(3)	C(74)-O(7)-C(71)	103.8(5)
O(15)-C(15)-C(14)	107.8(3)	C(72)-C(71)-O(7)	106.0(6)
O(15)-C(16)-C(19)	109.2(3)	C(71)-C(72)-C(73)	104.6(5)
O(15)-C(16)-C(18)	109.9(3)	C(72)-C(73)-C(74)	106.3(5)
C(19)-C(16)-C(18)	112.7(3)	O(7)-C(74)-C(73)	104.2(5)
O(15)-C(16)-C(17)	102.4(3)	C(81)-O(81)-C(84)	109.3(7)
C(19)-C(16)-C(17)	111.3(4)	O(81)-C(81)-C(82)	107.8(9)
C(18)-C(16)-C(17)	110.9(4)	C(81)-C(82)-C(83)	93.6(12)
O(21)-C(22)-C(23)	107.8(2)	C(82)-C(83)-C(84)	100.6(10)
O(21)-C(22)-C(21)	114.2(2)	O(81)-C(84)-C(83)	97.2(9)
C(23)-C(22)-C(21)	111.7(2)	C(85)-O(82)-C(88)	109.9(14)
O(22)-C(23)-O(23)	123.8(3)	O(82)-C(85)-C(86)	101.1(12)
O(22)-C(23)-C(22)	121.9(2)	C(85)-C(86)-C(87)	102.7(11)
O(23)-C(23)-C(22)	114.3(2)	C(86)-C(87)-C(88)	94.4(11)
O(23)-C(24)-C(25)	109.8(3)	O(82)-C(88)-C(87)	93.0(10)
O(24)-C(25)-O(25)	125.6(3)	C(91)-C(92)-C(93)	125.9(10)
O(24)-C(25)-C(24)	124.8(3)	C(93)#1-C(93)-C(92)	122.5(11)

Symmetry transformations used to generate equivalent atoms: #1 -x+2, -y+1, -z

Table S25. Torsion angles (°) for [(BHT)Mg(μ-OCH(CH_3)COOCH_2COO^{t}Bu)(THF)]$_2$ (**5**)

Atoms	Torsion angles	Atoms	Torsion angles
O(1)-Mg(1)-O(3)-C(1)	100.4(2)	O(21)-Mg(1)-C(13)-C(12)	1.0(2)
O(21)-Mg(1)-O(3)-C(1)	-9.1(2)	O(11)-Mg(1)-C(13)-C(12)	-1.57(16)
O(11)-Mg(1)-O(3)-C(1)	-91.2(2)	O(3)-Mg(1)-C(13)-C(12)	105.89(18)
O(12)-Mg(1)-O(3)-C(1)	-169.1(2)	O(12)-Mg(1)-C(13)-C(12)	175.0(3)
O(1)-Mg(1)-O(3)-C(4)	-83.6(3)	C(13)-O(13)-C(14)-C(15)	71.9(4)
O(21)-Mg(1)-O(3)-C(4)	166.9(3)	C(16)-O(15)-C(15)-O(14)	-2.0(5)
O(11)-Mg(1)-O(3)-C(4)	84.8(3)	C(16)-O(15)-C(15)-C(14)	179.0(3)
O(12)-Mg(1)-O(3)-C(4)	7.0(3)	O(13)-C(14)-C(15)-O(14)	9.6(5)
C(4)-O(3)-C(1)-C(2)	16.8(4)	O(13)-C(14)-C(15)-O(15)	-171.3(3)
Mg(1)-O(3)-C(1)-C(2)	-166.5(2)	C(15)-O(15)-C(16)-C(19)	-60.6(4)
O(3)-C(1)-C(2)-C(3)	-33.8(4)	C(15)-O(15)-C(16)-C(18)	63.6(4)

C(1)-C(2)-C(3)-C(4)	37.7(4)
C(1)-O(3)-C(4)-C(3)	7.5(4)
Mg(1)-O(3)-C(4)-C(3)	-169.1(2)
C(2)-C(3)-C(4)-O(3)	-28.3(4)
O(2)-Mg(2)-O(4)-C(5)	159.0(3)
O(11)-Mg(2)-O(4)-C(5)	-83.6(3)
O(21)-Mg(2)-O(4)-C(5)	1.5(4)
O(22)-Mg(2)-O(4)-C(5)	46.4(3)
O(2)-Mg(2)-O(4)-C(8)	-3.1(3)
O(11)-Mg(2)-O(4)-C(8)	114.3(3)
O(21)-Mg(2)-O(4)-C(8)	-160.6(2)
O(22)-Mg(2)-O(4)-C(8)	-115.7(3)
C(8)-O(4)-C(5)-C(6A)	40.1(5)
Mg(2)-O(4)-C(5)-C(6A)	-125.0(5)
C(8)-O(4)-C(5)-C(6B)	6.8(8)
Mg(2)-O(4)-C(5)-C(6B)	-158.3(7)
O(4)-C(5)-C(6A)-C(7)	-30.1(7)
C(6B)-C(5)-C(6A)-C(7)	70.3(10)
O(4)-C(5)-C(6B)-C(7)	20.7(11)
C(6A)-C(5)-C(6B)-C(7)	-68.4(11)
C(5)-C(6A)-C(7)-C(8)	10.5(7)
C(5)-C(6A)-C(7)-C(6B)	-71.0(11)
C(5)-C(6B)-C(7)-C(8)	-38.5(10)
C(5)-C(6B)-C(7)-C(6A)	67.1(10)
C(5)-O(4)-C(8)-C(7)	-32.6(4)
Mg(2)-O(4)-C(8)-C(7)	132.1(3)
C(6A)-C(7)-C(8)-O(4)	12.8(6)
C(6B)-C(7)-C(8)-O(4)	44.1(7)
O(2)-Mg(2)-O(11)-C(12)	61.5(3)
O(21)-Mg(2)-O(11)-C(12)	173.7(3)
O(4)-Mg(2)-O(11)-C(12)	-38.4(3)
O(22)-Mg(2)-O(11)-C(12)	-124.4(3)
O(2)-Mg(2)-O(11)-Mg(1)	-109.83(10)
O(21)-Mg(2)-O(11)-Mg(1)	2.39(8)
O(4)-Mg(2)-O(11)-Mg(1)	150.30(9)
O(22)-Mg(2)-O(11)-Mg(1)	64.31(13)
O(1)-Mg(1)-O(11)-C(12)	81.9(2)
O(21)-Mg(1)-O(11)-C(12)	-176.3(2)
O(3)-Mg(1)-O(11)-C(12)	-85.2(2)
O(12)-Mg(1)-O(11)-C(12)	0.5(2)
O(1)-Mg(1)-O(11)-Mg(2)	-104.16(12)
O(21)-Mg(1)-O(11)-Mg(2)	-2.43(8)
O(3)-Mg(1)-O(11)-Mg(2)	88.66(10)
O(12)-Mg(1)-O(11)-Mg(2)	174.45(10)
O(1)-Mg(1)-O(12)-C(13)	-126.9(2)
O(21)-Mg(1)-O(12)-C(13)	11.7(4)
O(11)-Mg(1)-O(12)-C(13)	2.8(2)
O(3)-Mg(1)-O(12)-C(13)	112.4(2)
O(1)-Mg(1)-O(21)-C(22)	-9.2(2)
O(11)-Mg(1)-O(21)-C(22)	-137.3(2)
O(3)-Mg(1)-O(21)-C(22)	113.8(2)
O(12)-Mg(1)-O(21)-C(22)	-146.2(2)
O(1)-Mg(1)-O(21)-Mg(2)	130.47(9)
O(11)-Mg(1)-O(21)-Mg(2)	2.37(8)
C(15)-O(15)-C(16)-C(17)	-178.6(3)
Mg(1)-O(21)-C(22)-C(23)	129.98(19)
Mg(2)-O(21)-C(22)-C(23)	-1.8(3)
Mg(1)-O(21)-C(22)-C(21)	-105.3(2)
Mg(2)-O(21)-C(22)-C(21)	123.0(2)
Mg(2)-O(22)-C(23)-O(23)	-172.4(2)
Mg(2)-O(22)-C(23)-C(22)	8.3(3)
C(24)-O(23)-C(23)-O(22)	-3.5(4)
C(24)-O(23)-C(23)-C(22)	175.8(2)
O(21)-C(22)-C(23)-O(22)	-4.9(4)
C(21)-C(22)-C(23)-O(22)	-131.1(3)
O(21)-C(22)-C(23)-O(23)	175.8(2)
C(21)-C(22)-C(23)-O(23)	49.6(3)
C(23)-O(23)-C(24)-C(25)	-79.5(3)
C(26)-O(25)-C(25)-O(24)	1.6(6)
C(26)-O(25)-C(25)-C(24)	-179.8(3)
O(23)-C(24)-C(25)-O(24)	-3.2(5)
O(23)-C(24)-C(25)-O(25)	178.2(3)
C(25)-O(25)-C(26)-C(27)	-177.5(4)
C(25)-O(25)-C(26)-C(29)	62.2(5)
C(25)-O(25)-C(26)-C(28)	-61.5(5)
O(1)-C(31)-C(32)-C(33)	-177.4(3)
C(36)-C(31)-C(32)-C(33)	3.7(4)
O(1)-C(31)-C(32)-C(37)	3.8(4)
C(36)-C(31)-C(32)-C(37)	-175.1(3)
C(31)-C(32)-C(33)-C(34)	-0.9(5)
C(37)-C(32)-C(33)-C(34)	177.8(3)
C(32)-C(33)-C(34)-C(35)	-1.4(5)
C(32)-C(33)-C(34)-C(39)	-179.4(3)
C(33)-C(34)-C(35)-C(36)	1.1(5)
C(39)-C(34)-C(35)-C(36)	179.0(3)
C(34)-C(35)-C(36)-C(31)	1.6(5)
C(34)-C(35)-C(36)-C(38)	-176.0(3)
O(1)-C(31)-C(36)-C(35)	177.1(3)
C(32)-C(31)-C(36)-C(35)	-4.0(4)
O(1)-C(31)-C(36)-C(38)	-5.4(4)
C(32)-C(31)-C(36)-C(38)	173.6(3)
C(33)-C(32)-C(37)-C(41)	-0.2(5)
C(31)-C(32)-C(37)-C(41)	178.6(3)
C(33)-C(32)-C(37)-C(43)	-119.7(3)
C(31)-C(32)-C(37)-C(43)	59.1(4)
C(33)-C(32)-C(37)-C(42)	118.6(3)
C(31)-C(32)-C(37)-C(42)	-62.7(4)
C(35)-C(36)-C(38)-C(46)	-122.1(3)
C(31)-C(36)-C(38)-C(46)	60.4(4)
C(35)-C(36)-C(38)-C(44)	-2.4(4)
C(31)-C(36)-C(38)-C(44)	-180.0(3)
C(35)-C(36)-C(38)-C(45)	115.7(3)
C(31)-C(36)-C(38)-C(45)	-61.8(4)
O(2)-C(51)-C(52)-C(53)	179.0(3)
C(56)-C(51)-C(52)-C(53)	-1.4(4)
O(2)-C(51)-C(52)-C(57)	-0.9(4)
C(56)-C(51)-C(52)-C(57)	178.7(3)
C(51)-C(52)-C(53)-C(54)	-0.1(5)

O(3)-Mg(1)-O(21)-Mg(2)	-106.45(9)	C(57)-C(52)-C(53)-C(54)	179.8(3)
O(12)-Mg(1)-O(21)-Mg(2)	-6.5(3)	C(52)-C(53)-C(54)-C(55)	1.0(5)
O(2)-Mg(2)-O(21)-C(22)	-104.94(19)	C(52)-C(53)-C(54)-C(59)	179.8(3)
O(11)-Mg(2)-O(21)-C(22)	140.48(19)	C(53)-C(54)-C(55)-C(56)	-0.3(5)
O(4)-Mg(2)-O(21)-C(22)	50.4(3)	C(59)-C(54)-C(55)-C(56)	-179.1(3)
O(22)-Mg(2)-O(21)-C(22)	4.32(18)	C(54)-C(55)-C(56)-C(51)	-1.1(4)
O(2)-Mg(2)-O(21)-Mg(1)	112.19(10)	C(54)-C(55)-C(56)-C(58)	179.5(3)
O(11)-Mg(2)-O(21)-Mg(1)	-2.39(8)	O(2)-C(51)-C(56)-C(55)	-178.5(3)
O(4)-Mg(2)-O(21)-Mg(1)	-92.45(18)	C(52)-C(51)-C(56)-C(55)	1.9(4)
O(22)-Mg(2)-O(21)-Mg(1)	-138.55(9)	O(2)-C(51)-C(56)-C(58)	0.8(4)
O(2)-Mg(2)-O(22)-C(23)	103.6(2)	C(52)-C(51)-C(56)-C(58)	-178.7(3)
O(11)-Mg(2)-O(22)-C(23)	-70.7(2)	C(53)-C(52)-C(57)-C(62)	120.9(3)
O(21)-Mg(2)-O(22)-C(23)	-6.69(19)	C(51)-C(52)-C(57)-C(62)	-59.2(4)
O(4)-Mg(2)-O(22)-C(23)	-164.2(2)	C(53)-C(52)-C(57)-C(61)	1.9(5)
Mg(2)-O(11)-C(12)-C(11)	62.8(4)	C(51)-C(52)-C(57)-C(61)	-178.2(3)
Mg(1)-O(11)-C(12)-C(11)	-126.9(3)	C(53)-C(52)-C(57)-C(63)	-117.4(3)
Mg(2)-O(11)-C(12)-C(13)	-173.3(2)	C(51)-C(52)-C(57)-C(63)	62.6(4)
Mg(1)-O(11)-C(12)-C(13)	-3.1(3)	C(55)-C(56)-C(58)-C(64)	116.5(3)
Mg(1)-O(12)-C(13)-O(13)	173.4(2)	C(51)-C(56)-C(58)-C(64)	-62.8(4)
Mg(1)-O(12)-C(13)-C(12)	-5.8(4)	C(55)-C(56)-C(58)-C(66)	-121.6(3)
C(14)-O(13)-C(13)-O(12)	-4.7(4)	C(51)-C(56)-C(58)-C(66)	59.1(4)
C(14)-O(13)-C(13)-C(12)	174.5(3)	C(55)-C(56)-C(58)-C(65)	-3.2(4)
C(14)-O(13)-C(13)-Mg(1)	14.7(10)	C(51)-C(56)-C(58)-C(65)	177.4(3)
O(11)-C(12)-C(13)-O(12)	6.1(4)	C(74)-O(7)-C(71)-C(72)	40.4(7)
C(11)-C(12)-C(13)-O(12)	130.6(3)	O(7)-C(71)-C(72)-C(73)	-29.7(7)
O(11)-C(12)-C(13)-O(13)	-173.2(3)	C(71)-C(72)-C(73)-C(74)	8.7(7)
C(11)-C(12)-C(13)-O(13)	-48.7(4)	C(71)-O(7)-C(74)-C(73)	-33.4(7)
O(11)-C(12)-C(13)-Mg(1)	1.9(2)	C(72)-C(73)-C(74)-O(7)	15.5(8)
C(11)-C(12)-C(13)-Mg(1)	126.5(3)	C(84)-O(81)-C(81)-C(82)	9.7(13)
O(1)-Mg(1)-C(13)-O(12)	55.6(2)	O(81)-C(81)-C(82)-C(83)	-38.9(14)
O(21)-Mg(1)-C(13)-O(12)	-174.08(18)	C(81)-C(82)-C(83)-C(84)	53.4(15)
O(11)-Mg(1)-C(13)-O(12)	-176.6(2)	C(81)-O(81)-C(84)-C(83)	24.5(11)
O(3)-Mg(1)-C(13)-O(12)	-69.2(2)	C(82)-C(83)-C(84)-O(81)	-49.2(14)
O(1)-Mg(1)-C(13)-O(13)	32.1(9)	C(88)-O(82)-C(85)-C(86)	-20(2)
O(21)-Mg(1)-C(13)-O(13)	162.4(8)	O(82)-C(85)-C(86)-C(87)	-21(2)
O(11)-Mg(1)-C(13)-O(13)	159.8(9)	C(85)-C(86)-C(87)-C(88)	49.7(15)
O(3)-Mg(1)-C(13)-O(13)	-92.7(9)	C(85)-O(82)-C(88)-C(87)	50(2)
O(12)-Mg(1)-C(13)-O(13)	-23.5(8)	C(86)-C(87)-C(88)-O(82)	-57.9(14)
O(1)-Mg(1)-C(13)-C(12)	-129.33(18)	C(91)-C(92)-C(93)-C(93)#1	-170.5(13)

Symmetry transformation used to generate equivalent atoms: #1 -x+2, -y+1, -z.

S2.7. Molecular structure of {(BHT)Mg[μ-O(CH$_2$)$_3$CON(CH$_3$)$_2$]}$_2$ (7)

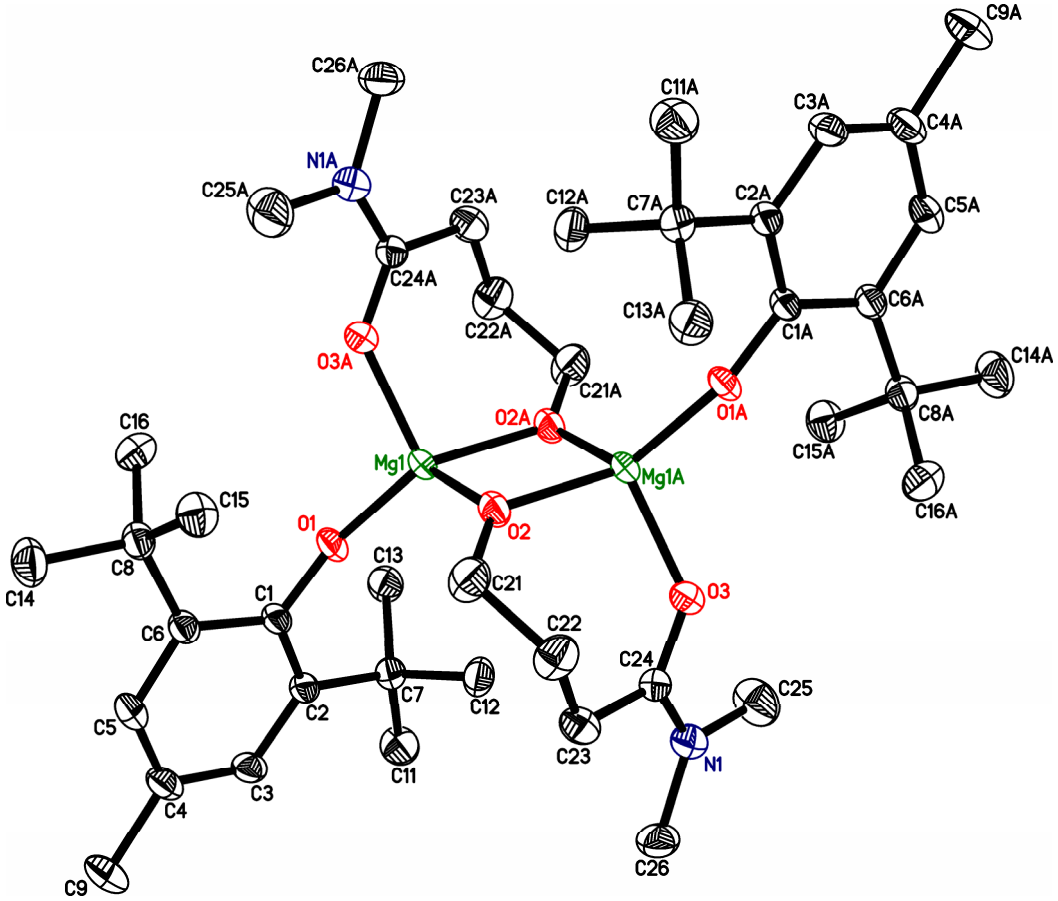

Fig. S18. Molecular structures of {(BHT)Mg[μ-O(CH$_2$)$_3$CON(CH$_3$)$_2$]}$_2$ (**7**). Hydrogen atoms are omitted. Thermal ellipsoids are set to the 50% probability level. Symmetry transformations used to generate equivalent atoms: (A) -x, -y+1, -z+1

Complex {(BHT)Mg[μ-κ^{1}O:κ^{2}O,O'-O(CH$_2$)$_3$CON(CH$_3$)$_2$]}$_2$ (**7**) was prepared in the absence of a σ-donor solvent. The complex is located at an inversion center, which makes a half of the dimer (Fig. S18) to be crystallographically unique. The Mg_2O_2 core folding angle is 0°. The hydroxylamide ligand, O(CH$_2$)$_3$CON(CH$_3$)$_2$, demonstrates the μ-κ^1:κ^2 semibridging coordination mode. The Mg coordination number is 4 (distorted tetrahedron).

Table S26. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for {(BHT)Mg[μ-$O(CH_2)_3CON(CH_3)_2$]}$_2$ (**7**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U(eq)
Mg(1)	142(1)	4473(1)	5737(1)	21(1)
N(1)	3315(1)	4752(1)	3543(1)	28(1)
O(1)	1354(1)	3728(1)	6364(1)	25(1)
O(2)	615(1)	5899(1)	5260(1)	24(1)
O(3)	1417(1)	5528(1)	3725(1)	28(1)
C(1)	2442(1)	3535(1)	6756(1)	20(1)
C(2)	3378(1)	2786(1)	6475(1)	21(1)
C(3)	4570(1)	2683(1)	6873(1)	25(1)
C(4)	4864(1)	3259(1)	7542(1)	28(1)
C(5)	3902(1)	3903(1)	7838(1)	26(1)
C(6)	2684(1)	4041(1)	7477(1)	22(1)
C(7)	3071(1)	2095(1)	5752(1)	24(1)
C(8)	1619(1)	4676(1)	7866(1)	24(1)
C(9)	6177(1)	3157(1)	7948(1)	39(1)
C(11)	4143(1)	1245(1)	5595(1)	34(1)
C(12)	2919(1)	2909(1)	5077(1)	30(1)
C(13)	1844(1)	1381(1)	5812(1)	31(1)
C(14)	2067(1)	5061(1)	8659(1)	38(1)
C(15)	1178(1)	5769(1)	7444(1)	32(1)
C(16)	469(1)	3869(1)	7940(1)	31(1)
C(21)	1523(1)	6747(1)	5467(1)	35(1)
C(22)	2323(1)	7119(1)	4829(1)	33(1)
C(23)	3188(1)	6185(1)	4539(1)	31(1)
C(24)	2591(1)	5458(1)	3912(1)	23(1)
C(25)	2725(2)	4063(1)	2937(1)	44(1)
C(26)	4682(1)	4553(1)	3709(1)	34(1)

Table S27. Anisotropic displacement parameters ($Å^2$ $x10^3$) for {(BHT)Mg[μ-$O(CH_2)_3CON(CH_3)_2$]}$_2$ (**7**). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}]

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	16(1)	29(1)	17(1)	2(1)	-3(1)	2(1)
N(1)	22(1)	33(1)	28(1)	0(1)	1(1)	3(1)
O(1)	20(1)	34(1)	21(1)	1(1)	-6(1)	6(1)
O(2)	23(1)	29(1)	20(1)	0(1)	-4(1)	-4(1)
O(3)	19(1)	43(1)	22(1)	-2(1)	-1(1)	2(1)
C(1)	18(1)	24(1)	19(1)	4(1)	-2(1)	1(1)
C(2)	19(1)	24(1)	20(1)	4(1)	-1(1)	0(1)
C(3)	19(1)	28(1)	28(1)	5(1)	0(1)	3(1)
C(4)	20(1)	32(1)	30(1)	5(1)	-7(1)	-1(1)
C(5)	25(1)	29(1)	23(1)	1(1)	-7(1)	-1(1)
C(6)	21(1)	24(1)	20(1)	2(1)	-2(1)	1(1)
C(7)	23(1)	26(1)	21(1)	1(1)	1(1)	1(1)
C(8)	25(1)	26(1)	21(1)	0(1)	-1(1)	3(1)
C(9)	24(1)	48(1)	42(1)	2(1)	-13(1)	2(1)
C(11)	33(1)	33(1)	35(1)	-5(1)	1(1)	6(1)

C(12)	35(1)	35(1)	21(1)	3(1)	3(1)	2(1)
C(13)	31(1)	33(1)	29(1)	-2(1)	0(1)	-8(1)
C(14)	43(1)	45(1)	25(1)	-8(1)	-4(1)	9(1)
C(15)	36(1)	26(1)	32(1)	2(1)	0(1)	5(1)
C(16)	31(1)	32(1)	32(1)	2(1)	9(1)	1(1)
C(21)	38(1)	41(1)	28(1)	-10(1)	5(1)	-16(1)
C(22)	38(1)	28(1)	33(1)	-4(1)	7(1)	-11(1)
C(23)	25(1)	38(1)	30(1)	-4(1)	-3(1)	-6(1)
C(24)	20(1)	29(1)	20(1)	4(1)	1(1)	-2(1)
C(25)	45(1)	48(1)	39(1)	-15(1)	-4(1)	8(1)
C(26)	22(1)	40(1)	41(1)	7(1)	4(1)	6(1)

Table S28. Bond lengths for non-hydrogen atoms (Å) for $\{(BHT)Mg[\mu\text{-}O(CH_2)_3CON(CH_3)_2]\}_2$ (**7**)

Atoms	Bond lengths	Atoms	Bond lengths	Atoms	Bond lengths
Mg(1)-O(1)	1.8546(8)	O(3)-C(24)	1.2541(13)	C(7)-C(11)	1.5367(16)
Mg(1)-O(3)#1	1.9485(9)	C(1)-C(2)	1.4293(14)	C(7)-C(13)	1.5396(15)
Mg(1)-O(2)	1.9497(9)	C(1)-C(6)	1.4294(14)	C(7)-C(12)	1.5400(15)
Mg(1)-O(2)#1	1.9579(8)	C(2)-C(3)	1.4006(13)	C(8)-C(14)	1.5367(16)
Mg(1)-Mg(1)#1	2.9147(7)	C(2)-C(7)	1.5437(14)	C(8)-C(15)	1.5387(16)
N(1)-C(24)	1.3252(14)	C(3)-C(4)	1.3919(16)	C(8)-C(16)	1.5399(16)
N(1)-C(25)	1.4573(17)	C(4)-C(5)	1.3880(16)	C(21)-C(22)	1.5243(17)
N(1)-C(26)	1.4595(14)	C(4)-C(9)	1.5164(15)	C(22)-C(23)	1.5296(18)
O(1)-C(1)	1.3178(11)	C(5)-C(6)	1.3998(14)	C(23)-C(24)	1.5116(16)
O(2)-C(21)	1.4044(14)	C(6)-C(8)	1.5426(15)		

Symmetry transformations used to generate equivalent atoms: #1 -x, -y+1, -z+1

Table S29. Bond angles for non-hydrogen atoms (°) for $\{(BHT)Mg[\mu\text{-}O(CH_2)_3CON(CH_3)_2]\}_2$ (**7**)

Atoms	Bond angles	Atoms	Bond angles
O(1)-Mg(1)-O(3)#1	105.03(4)	C(5)-C(4)-C(3)	117.78(9)
O(1)-Mg(1)-O(2)	118.93(4)	C(5)-C(4)-C(9)	120.96(11)
O(3)#1-Mg(1)-O(2)	117.49(4)	C(3)-C(4)-C(9)	121.23(11)
O(1)-Mg(1)-O(2)#1	132.07(4)	C(4)-C(5)-C(6)	123.05(10)
O(3)#1-Mg(1)-O(2)#1	98.74(4)	C(5)-C(6)-C(1)	118.24(9)
O(2)-Mg(1)-O(2)#1	83.53(4)	C(5)-C(6)-C(8)	120.51(9)
O(1)-Mg(1)-Mg(1)#1	140.69(3)	C(1)-C(6)-C(8)	121.19(9)
O(3)#1-Mg(1)-Mg(1)#1	114.26(3)	C(11)-C(7)-C(13)	106.52(9)
O(2)-Mg(1)-Mg(1)#1	41.87(2)	C(11)-C(7)-C(12)	107.07(9)
O(2)#1-Mg(1)-Mg(1)#1	41.66(2)	C(13)-C(7)-C(12)	110.22(9)
C(24)-N(1)-C(25)	119.27(10)	C(11)-C(7)-C(2)	112.14(9)
C(24)-N(1)-C(26)	125.48(10)	C(13)-C(7)-C(2)	110.65(8)
C(25)-N(1)-C(26)	115.19(11)	C(12)-C(7)-C(2)	110.12(9)
C(1)-O(1)-Mg(1)	159.42(8)	C(14)-C(8)-C(15)	106.09(10)
C(21)-O(2)-Mg(1)	132.21(8)	C(14)-C(8)-C(16)	107.00(10)
C(21)-O(2)-Mg(1)#1	128.59(7)	C(15)-C(8)-C(16)	109.82(9)
Mg(1)-O(2)-Mg(1)#1	96.47(4)	C(14)-C(8)-C(6)	112.00(9)
C(24)-O(3)-Mg(1)#1	134.71(7)	C(15)-C(8)-C(6)	112.18(9)
O(1)-C(1)-C(2)	120.20(9)	C(16)-C(8)-C(6)	109.58(9)
O(1)-C(1)-C(6)	120.60(9)	O(2)-C(21)-C(22)	113.39(10)
C(2)-C(1)-C(6)	119.17(9)	C(21)-C(22)-C(23)	114.68(11)

C(3)-C(2)-C(1)	118.61(9)	C(24)-C(23)-C(22)	115.42(10)
C(3)-C(2)-C(7)	120.94(9)	O(3)-C(24)-N(1)	119.18(10)
C(1)-C(2)-C(7)	120.45(8)	O(3)-C(24)-C(23)	120.80(10)
C(4)-C(3)-C(2)	122.55(10)	N(1)-C(24)-C(23)	120.01(10)

Symmetry transformations used to generate equivalent atoms: #1 -x, -y+1, -z+1

Table S30. Torsion angles (°) for $\{(BHT)Mg[\mu\text{-}O(CH_2)_3CON(CH_3)_2]\}_2$ (**7**)

Atoms	Torsion angles	Atoms	Torsion angles
O(3)#1-Mg(1)-O(1)-C(1)	-128.8(2)	O(1)-C(1)-C(6)-C(8)	9.13(15)
O(2)-Mg(1)-O(1)-C(1)	5.2(2)	C(2)-C(1)-C(6)-C(8)	-169.00(9)
O(2)#1-Mg(1)-O(1)-C(1)	114.2(2)	C(3)-C(2)-C(7)-C(11)	5.61(14)
Mg(1)#1-Mg(1)-O(1)-C(1)	53.3(2)	C(1)-C(2)-C(7)-C(11)	-173.51(10)
O(1)-Mg(1)-O(2)-C(21)	-26.83(12)	C(3)-C(2)-C(7)-C(13)	124.39(11)
O(3)#1-Mg(1)-O(2)-C(21)	101.61(10)	C(1)-C(2)-C(7)-C(13)	-54.73(13)
O(2)#1-Mg(1)-O(2)-C(21)	-161.89(12)	C(3)-C(2)-C(7)-C(12)	-113.51(11)
Mg(1)#1-Mg(1)-O(2)-C(21)	-161.89(12)	C(1)-C(2)-C(7)-C(12)	67.37(12)
O(1)-Mg(1)-O(2)-Mg(1)#1	135.06(4)	C(5)-C(6)-C(8)-C(14)	-1.88(15)
O(3)#1-Mg(1)-O(2)-Mg(1)#1	-96.50(4)	C(1)-C(6)-C(8)-C(14)	175.27(10)
O(2)#1-Mg(1)-O(2)-Mg(1)#1	0.0	C(5)-C(6)-C(8)-C(15)	117.29(11)
Mg(1)-O(1)-C(1)-C(2)	-100.9(2)	C(1)-C(6)-C(8)-C(15)	-65.56(13)
Mg(1)-O(1)-C(1)-C(6)	81.0(2)	C(5)-C(6)-C(8)-C(16)	-120.45(11)
O(1)-C(1)-C(2)-C(3)	174.17(9)	C(1)-C(6)-C(8)-C(16)	56.69(13)
C(6)-C(1)-C(2)-C(3)	-7.70(14)	Mg(1)-O(2)-C(21)-C(22)	134.11(10)
O(1)-C(1)-C(2)-C(7)	-6.69(14)	Mg(1)#1-O(2)-C(21)-C(22)	-22.62(17)
C(6)-C(1)-C(2)-C(7)	171.44(9)	O(2)-C(21)-C(22)-C(23)	-64.94(15)
C(1)-C(2)-C(3)-C(4)	1.62(16)	C(21)-C(22)-C(23)-C(24)	90.06(13)
C(7)-C(2)-C(3)-C(4)	-177.52(10)	Mg(1)#1-O(3)-C(24)-N(1)	133.66(10)
C(2)-C(3)-C(4)-C(5)	3.87(17)	Mg(1)#1-O(3)-C(24)-C(23)	-47.57(16)
C(2)-C(3)-C(4)-C(9)	-178.11(11)	C(25)-N(1)-C(24)-O(3)	-0.92(17)
C(3)-C(4)-C(5)-C(6)	-3.30(17)	C(26)-N(1)-C(24)-O(3)	-177.99(11)
C(9)-C(4)-C(5)-C(6)	178.67(11)	C(25)-N(1)-C(24)-C(23)	-179.70(12)
C(4)-C(5)-C(6)-C(1)	-2.72(16)	C(26)-N(1)-C(24)-C(23)	3.23(17)
C(4)-C(5)-C(6)-C(8)	174.51(10)	C(22)-C(23)-C(24)-O(3)	-9.51(16)
O(1)-C(1)-C(6)-C(5)	-173.67(10)	C(22)-C(23)-C(24)-N(1)	169.25(10)
C(2)-C(1)-C(6)-C(5)	8.21(15)		

Symmetry transformations used to generate equivalent atoms: #1 -x, -y+1, -z+1

S2.8. Molecular structure of $\{(BHT)Mg[\mu\text{-}O(CH_2)_3CON(CH_3)_2]\}_2(THF)_3$ (7')

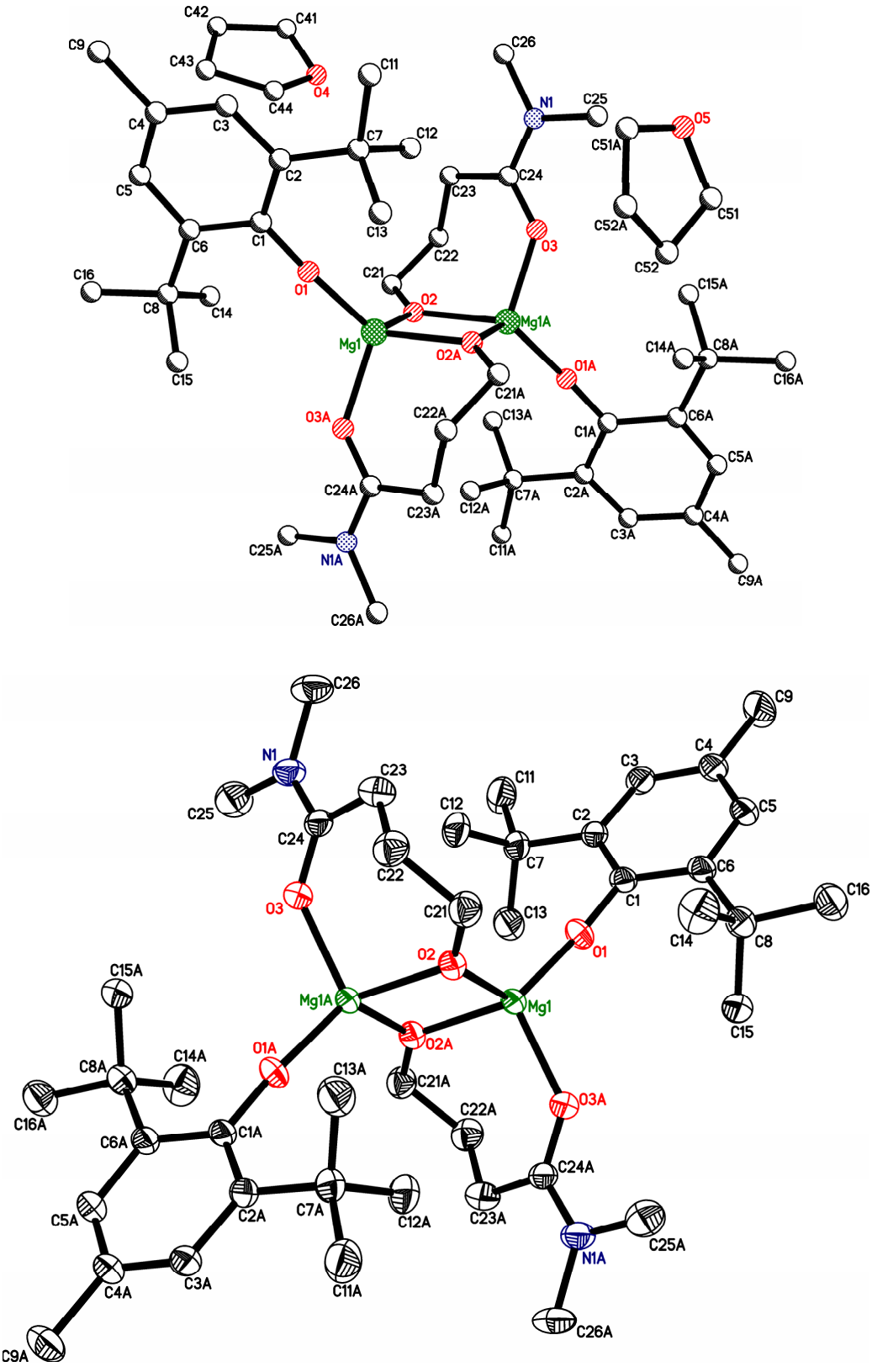

Fig. S19. Molecular structures of $\{(BHT)Mg[\mu\text{-}O(CH_2)_3CON(CH_3)_2]\}_2(THF)_3$: a ball-and-stick model of **7'** (top) and the moiety **7'** (bottom) with omitted hydrogen atoms and thermal ellipsoids of the 50% probability level.

{(BHT)Mg[μ-κ^{1}O:κ^{2}O,O'-O(CH$_2$)$_3$CON(CH$_3$)$_2$]}$_2$(THF)$_3$ **7'**, synthesized in the presence of THF, does not contain coordinated solvent molecules (Fig. S19). One of non-coordination THF molecules (O5-C51-C52-C52A-C51A) is located at a 2-fold screw axis. The dimeric molecule {(BHT)Mg[μ-O(CH$_2$)$_3$CON(CH$_3$)$_2$]}$_2$ lies on an inversion center. The hydroxylamide ligand displays the μ-κ^1:κ^2 semibridging coordination mode.

Table S31. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for {(BHT)Mg[μ-O(CH$_2$)$_3$CON(CH$_3$)$_2$]}$_2$(THF)$_3$ (**7'**). U(eq) is defined as one third of the trace of the orthogonalized U$_{ij}$ tensor.

Atom	x	y	z	U(eq)
Mg(1)	2213(1)	2016(1)	5492(1)	23(1)
N(1)	2950(1)	5283(1)	5723(1)	31(1)
O(1)	1988(1)	2192(1)	6453(1)	31(1)
O(2)	1966(1)	2821(1)	4521(1)	26(1)
O(3)	2925(1)	4157(1)	4897(1)	30(1)
C(1)	1785(1)	2404(1)	7081(1)	25(1)
C(2)	2154(1)	2900(1)	7820(1)	26(1)
C(3)	1916(1)	3121(1)	8460(1)	31(1)
C(4)	1343(1)	2876(1)	8413(1)	34(1)
C(5)	992(1)	2382(1)	7697(1)	30(1)
C(6)	1197(1)	2129(1)	7033(1)	26(1)
C(7)	2801(1)	3177(1)	7924(1)	30(1)
C(8)	792(1)	1566(1)	6268(1)	30(1)
C(9)	1105(1)	3134(2)	9121(2)	50(1)
C(11)	3124(1)	3686(2)	8782(1)	43(1)
C(12)	2774(1)	3751(1)	7146(1)	38(1)
C(13)	3205(1)	2410(1)	7975(2)	38(1)
C(14)	620(1)	2038(2)	5379(1)	45(1)
C(15)	1123(1)	740(1)	6255(2)	36(1)
C(16)	187(1)	1326(1)	6357(1)	39(1)
C(21)	1452(1)	3328(1)	4094(1)	32(1)
C(22)	1620(1)	4220(1)	3947(1)	33(1)
C(23)	1950(1)	4718(1)	4804(1)	35(1)
C(24)	2640(1)	4698(1)	5150(1)	26(1)
C(25)	3616(1)	5306(2)	6031(2)	43(1)
C(26)	2669(1)	5911(1)	6105(2)	41(1)
O(4)	987(2)	5227(2)	5893(3)	113(1)
C(41)	592(2)	5777(3)	6003(4)	111(1)
C(42)	199(2)	5382(4)	6400(3)	119(2)
C(43)	487(2)	4528(3)	6712(3)	91(1)
C(44)	1024(2)	4548(3)	6474(3)	90(1)
O(5)	5000	4507(2)	7500	81(1)
C(51)	5127(2)	3997(2)	6883(2)	88(1)
C(52)	5012(2)	3118(2)	7054(2)	92(1)

Table S32. Anisotropic displacement parameters ($Å^2 x10^3$) for {(BHT)Mg[μ-$O(CH_2)_3CON(CH_3)_2$]}$_2$(THF)$_3$ (**7'**). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U_{11}$ + ... + 2 h k a* b* U_{12}].

Atoms	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	31(1)	21(1)	25(1)	-2(1)	19(1)	-1(1)
N(1)	40(1)	25(1)	30(1)	-4(1)	18(1)	1(1)
O(1)	41(1)	33(1)	30(1)	-4(1)	26(1)	-2(1)
O(2)	30(1)	24(1)	29(1)	2(1)	17(1)	1(1)
O(3)	37(1)	24(1)	38(1)	-5(1)	24(1)	-2(1)
C(1)	36(1)	21(1)	26(1)	3(1)	20(1)	3(1)
C(2)	37(1)	21(1)	28(1)	3(1)	20(1)	1(1)
C(3)	47(1)	25(1)	29(1)	-4(1)	24(1)	-4(1)
C(4)	48(1)	30(1)	36(1)	-5(1)	30(1)	-3(1)
C(5)	37(1)	28(1)	35(1)	-1(1)	24(1)	1(1)
C(6)	33(1)	22(1)	27(1)	3(1)	18(1)	4(1)
C(7)	37(1)	28(1)	31(1)	1(1)	19(1)	-4(1)
C(8)	35(1)	31(1)	28(1)	-2(1)	17(1)	-1(1)
C(9)	63(2)	53(1)	53(1)	-23(1)	43(1)	-16(1)
C(11)	49(1)	45(1)	40(1)	-8(1)	22(1)	-16(1)
C(12)	50(1)	33(1)	40(1)	5(1)	26(1)	-6(1)
C(13)	37(1)	39(1)	44(1)	4(1)	20(1)	3(1)
C(14)	53(1)	52(1)	28(1)	4(1)	12(1)	-5(1)
C(15)	45(1)	29(1)	45(1)	-9(1)	29(1)	-6(1)
C(16)	34(1)	46(1)	39(1)	-6(1)	18(1)	-3(1)
C(21)	28(1)	32(1)	37(1)	3(1)	12(1)	0(1)
C(22)	35(1)	30(1)	33(1)	6(1)	11(1)	4(1)
C(23)	37(1)	29(1)	43(1)	-4(1)	19(1)	5(1)
C(24)	39(1)	20(1)	26(1)	2(1)	19(1)	1(1)
C(25)	43(1)	42(1)	43(1)	-12(1)	15(1)	-7(1)
C(26)	56(1)	30(1)	39(1)	-11(1)	20(1)	5(1)
O(4)	113(2)	105(2)	147(3)	27(2)	79(2)	17(2)
C(41)	103(3)	80(3)	151(4)	-7(3)	49(3)	-4(2)
C(42)	105(3)	172(4)	85(2)	9(3)	43(2)	85(3)
C(43)	85(2)	113(3)	81(2)	11(2)	37(2)	11(2)
C(44)	100(3)	80(2)	106(3)	23(2)	57(2)	30(2)
O(5)	122(3)	63(2)	57(2)	0	32(2)	0
C(51)	138(3)	71(2)	72(2)	-13(2)	58(2)	-29(2)
C(52)	150(4)	76(2)	64(2)	-9(2)	58(2)	-16(2)

Table S33. Bond lengths for non-hydrogen atoms (Å) for {(BHT)Mg[μ-$O(CH_2)_3CON(CH_3)_2$]}$_2$(THF)$_3$ (**7'**).

Atoms	Bond lengths	Atoms	Bond lengths	Atoms	Bond lengths
Mg(1)-O(1)	1.8494(13)	C(1)-C(2)	1.428(3)	C(8)-C(14)	1.541(3)
Mg(1)-O(2)	1.9448(13)	C(2)-C(3)	1.400(2)	C(21)-C(22)	1.520(3)
Mg(1)-O(2)#1	1.9617(13)	C(2)-C(7)	1.535(3)	C(22)-C(23)	1.536(3)
Mg(1)-O(3)#1	1.9630(14)	C(3)-C(4)	1.381(3)	C(23)-C(24)	1.507(3)
Mg(1)-Mg(1)#1	2.8993(11)	C(4)-C(5)	1.389(3)	O(4)-C(41)	1.340(5)
N(1)-C(24)	1.326(2)	C(4)-C(9)	1.514(3)	O(4)-C(44)	1.419(5)
N(1)-C(25)	1.457(3)	C(5)-C(6)	1.399(2)	C(41)-C(42)	1.454(7)
N(1)-C(26)	1.463(2)	C(6)-C(8)	1.538(3)	C(42)-C(43)	1.521(6)

O(1)-C(1)	1.324(2)	C(7)-C(13)	1.535(3)	C(43)-C(44)	1.457(5)
O(2)-C(21)	1.404(2)	C(7)-C(12)	1.541(3)	O(5)-C(51)#2	1.408(4)
O(2)-Mg(1)#1	1.9618(13)	C(7)-C(11)	1.543(3)	O(5)-C(51)	1.408(4)
O(3)-C(24)	1.256(2)	C(8)-C(16)	1.534(3)	C(51)-C(52)	1.475(5)
O(3)-Mg(1)#1	1.9630(14)	C(8)-C(15)	1.537(3)	C(52)-C(52)#2	1.470(6)
C(1)-C(6)	1.427(2)				

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, -y+1/2, -z+1; #2 -x+1, y, -z+3/2.

Table S34. Bond angles for non-hydrogen atoms (°) for {(BHT)Mg[μ-$O(CH_2)_3CON(CH_3)_2$]}$_2$$(THF)_3$ (**7'**).

Atoms	Bond angles	Atoms	Bond angles
O(1)-Mg(1)-O(2)	119.44(6)	C(5)-C(6)-C(1)	118.62(17)
O(1)-Mg(1)-O(2)#1	126.00(6)	C(5)-C(6)-C(8)	120.15(16)
O(2)-Mg(1)-O(2)#1	84.17(6)	C(1)-C(6)-C(8)	121.23(15)
O(1)-Mg(1)-O(3)#1	110.49(6)	C(2)-C(7)-C(13)	110.26(15)
O(2)-Mg(1)-O(3)#1	113.93(6)	C(2)-C(7)-C(12)	110.47(16)
O(2)#1-Mg(1)-O(3)#1	99.63(6)	C(13)-C(7)-C(12)	110.52(16)
O(1)-Mg(1)-Mg(1)#1	136.67(6)	C(2)-C(7)-C(11)	112.45(16)
O(2)-Mg(1)-Mg(1)#1	42.31(4)	C(13)-C(7)-C(11)	106.64(18)
O(2)#1-Mg(1)-Mg(1)#1	41.86(4)	C(12)-C(7)-C(11)	106.39(16)
O(3)#1-Mg(1)-Mg(1)#1	112.66(5)	C(16)-C(8)-C(15)	106.37(16)
C(24)-N(1)-C(25)	119.71(16)	C(16)-C(8)-C(6)	112.65(15)
C(24)-N(1)-C(26)	124.16(18)	C(15)-C(8)-C(6)	110.33(16)
C(25)-N(1)-C(26)	116.10(17)	C(16)-C(8)-C(14)	106.59(17)
C(1)-O(1)-Mg(1)	172.38(13)	C(15)-C(8)-C(14)	111.21(17)
C(21)-O(2)-Mg(1)	136.04(11)	C(6)-C(8)-C(14)	109.62(16)
C(21)-O(2)-Mg(1)#1	126.14(11)	O(2)-C(21)-C(22)	112.89(15)
Mg(1)-O(2)-Mg(1)#1	95.83(6)	C(21)-C(22)-C(23)	114.54(17)
C(24)-O(3)-Mg(1)#1	135.86(12)	C(24)-C(23)-C(22)	115.69(16)
O(1)-C(1)-C(6)	120.28(16)	O(3)-C(24)-N(1)	119.56(17)
O(1)-C(1)-C(2)	120.49(16)	O(3)-C(24)-C(23)	121.83(16)
C(6)-C(1)-C(2)	119.22(15)	N(1)-C(24)-C(23)	118.60(16)
C(3)-C(2)-C(1)	118.45(17)	C(41)-O(4)-C(44)	106.4(3)
C(3)-C(2)-C(7)	120.39(17)	O(4)-C(41)-C(42)	111.5(4)
C(1)-C(2)-C(7)	121.15(15)	C(41)-C(42)-C(43)	104.9(3)
C(4)-C(3)-C(2)	123.08(18)	C(44)-C(43)-C(42)	102.4(4)
C(3)-C(4)-C(5)	117.85(17)	O(4)-C(44)-C(43)	110.6(3)
C(3)-C(4)-C(9)	121.05(19)	C(51)#2-O(5)-C(51)	109.4(4)
C(5)-C(4)-C(9)	121.10(19)	O(5)-C(51)-C(52)	108.2(3)
C(4)-C(5)-C(6)	122.74(18)	C(52)#2-C(52)-C(51)	105.3(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, -y+1/2, -z+1 #2 -x+1, y, -z+3/2.

Table S35. Torsion angles (°) for $\{(BHT)Mg[\mu\text{-}O(CH_2)_3CON(CH_3)_2]\}_2(THF)_3$ (**7'**)

Atoms	Torsion angles	Atoms	Torsion angles
O(1)-Mg(1)-O(2)-C(21)	-35.34(19)	C(3)-C(2)-C(7)-C(11)	0.8(2)
O(2)#1-Mg(1)-O(2)-C(21)	-163.71(19)	C(1)-C(2)-C(7)-C(11)	-178.40(17)
O(3)#1-Mg(1)-O(2)-C(21)	98.31(17)	C(5)-C(6)-C(8)-C(16)	-1.6(2)
Mg(1)#1-Mg(1)-O(2)-C(21)	-163.71(19)	C(1)-C(6)-C(8)-C(16)	178.53(17)
O(1)-Mg(1)-O(2)-Mg(1)#1	128.38(7)	C(5)-C(6)-C(8)-C(15)	-120.29(18)
O(2)#1-Mg(1)-O(2)-Mg(1)#1	0.0	C(1)-C(6)-C(8)-C(15)	59.8(2)
O(3)#1-Mg(1)-O(2)-Mg(1)#1	-97.97(7)	C(5)-C(6)-C(8)-C(14)	116.9(2)
O(1)-C(1)-C(2)-C(3)	178.92(16)	C(1)-C(6)-C(8)-C(14)	-63.0(2)
C(6)-C(1)-C(2)-C(3)	-2.0(2)	Mg(1)-O(2)-C(21)-C(22)	134.56(15)
O(1)-C(1)-C(2)-C(7)	-1.9(3)	Mg(1)#1-O(2)-C(21)-C(22)	-25.2(2)
C(6)-C(1)-C(2)-C(7)	177.22(16)	O(2)-C(21)-C(22)-C(23)	-64.7(2)
C(1)-C(2)-C(3)-C(4)	0.5(3)	C(21)-C(22)-C(23)-C(24)	93.6(2)
C(7)-C(2)-C(3)-C(4)	-178.69(18)	Mg(1)#1-O(3)-C(24)-N(1)	149.78(14)
C(2)-C(3)-C(4)-C(5)	0.5(3)	Mg(1)#1-O(3)-C(24)-C(23)	-31.7(3)
C(2)-C(3)-C(4)-C(9)	-179.8(2)	C(25)-N(1)-C(24)-O(3)	1.9(3)
C(3)-C(4)-C(5)-C(6)	0.0(3)	C(26)-N(1)-C(24)-O(3)	-176.01(17)
C(9)-C(4)-C(5)-C(6)	-179.8(2)	C(25)-N(1)-C(24)-C(23)	-176.65(18)
C(4)-C(5)-C(6)-C(1)	-1.4(3)	C(26)-N(1)-C(24)-C(23)	5.5(3)
C(4)-C(5)-C(6)-C(8)	178.70(18)	C(22)-C(23)-C(24)-O(3)	-17.1(3)
O(1)-C(1)-C(6)-C(5)	-178.48(16)	C(22)-C(23)-C(24)-N(1)	161.37(17)
C(2)-C(1)-C(6)-C(5)	2.4(3)	C(44)-O(4)-C(41)-C(42)	-20.0(6)
O(1)-C(1)-C(6)-C(8)	1.4(3)	O(4)-C(41)-C(42)-C(43)	11.6(6)
C(2)-C(1)-C(6)-C(8)	-177.71(16)	C(41)-C(42)-C(43)-C(44)	1.4(5)
C(3)-C(2)-C(7)-C(13)	119.65(19)	C(41)-O(4)-C(44)-C(43)	21.0(5)
C(1)-C(2)-C(7)-C(13)	-59.5(2)	C(42)-C(43)-C(44)-O(4)	-13.3(5)
C(3)-C(2)-C(7)-C(12)	-117.90(19)	C(51)#2-O(5)-C(51)-C(52)	6.2(2)
C(1)-C(2)-C(7)-C(12)	62.9(2)	O(5)-C(51)-C(52)-C(52)#2	-16.0(6)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+1/2,-z+1; #2 -x+1,y,-z+3/2 .

S2.9. Molecular structure of $(BHT)_2Mg(DMSO)_2$ (8)

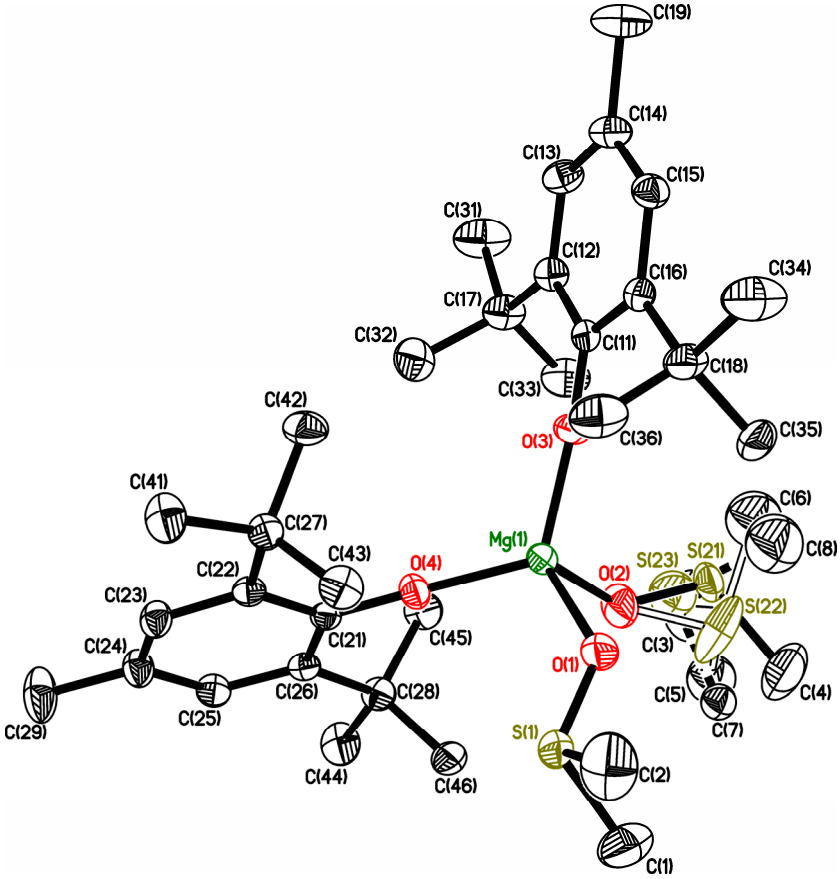

Fig. S20. Molecular structures of $(BHT)_2Mg(DMSO)_2$ (**8**). The disordered DMSO molecule is shown with open solid lines. H-atoms are omitted. Thermal ellipsoids are set to the 50% probability level.

Mg-atom (c.n.=4) is in distorted tetrahedral environment (Fig. S20). The O_{DMSO}-Mg-O_{DMSO} angle has the lowest value among O-Mg-O angles. Mg-O_{BHT} bond lengths are slightly shorter than Mg-O_{DMSO} (Table S38). One coordinated DMSO molecule in $(BHT)_2Mg(DMSO)_2$ is disordered over three positions.

Table S36. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2$ $x10^3$) for $(BHT)_2Mg(DMSO)_2$ (**8**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U(eq)
Mg(1)	3591(1)	3513(1)	6627(1)	22(1)
S(1)	2985(1)	1667(1)	6225(1)	32(1)
S(21)	3514(1)	4332(1)	4759(1)	34(1)
C(3)	2670(5)	5061(4)	4266(4)	80(2)
C(4)	3345(4)	3614(3)	3937(3)	69(1)
S(22)	3301(2)	3928(2)	4555(1)	61(1)
C(5)	2335(6)	4450(6)	3884(6)	57(2)
C(6)	4108(7)	4812(6)	4625(7)	73(3)
S(23)	3034(6)	4597(4)	4778(4)	52(2)
C(7)	2308(12)	4162(13)	3824(10)	29(4)
C(8)	4173(15)	4430(20)	4510(20)	75(9)

O(1)	3658(1)	2369(1)	6200(1)	35(1)
O(2)	3098(1)	3972(1)	5456(1)	40(1)
O(3)	4727(1)	4070(1)	7043(1)	25(1)
O(4)	2715(1)	3474(1)	7332(1)	24(1)
C(1)	2345(2)	1538(2)	5135(2)	56(1)
C(2)	3719(2)	790(1)	6303(2)	58(1)
C(11)	5538(1)	4416(1)	7423(1)	20(1)
C(12)	5566(1)	5239(1)	7724(1)	23(1)
C(13)	6435(1)	5560(1)	8163(1)	27(1)
C(14)	7286(1)	5132(1)	8298(1)	27(1)
C(15)	7256(1)	4350(1)	7967(1)	25(1)
C(16)	6415(1)	3978(1)	7534(1)	22(1)
C(17)	4657(1)	5767(1)	7579(1)	30(1)
C(18)	6435(1)	3099(1)	7206(1)	32(1)
C(19)	8212(1)	5502(1)	8787(2)	42(1)
C(21)	2052(1)	3480(1)	7796(1)	19(1)
C(22)	2249(1)	3159(1)	8659(1)	19(1)
C(23)	1529(1)	3177(1)	9124(1)	24(1)
C(24)	629(1)	3491(1)	8792(1)	26(1)
C(25)	444(1)	3795(1)	7950(1)	23(1)
C(26)	1124(1)	3798(1)	7441(1)	19(1)
C(27)	3228(1)	2794(1)	9084(1)	23(1)
C(28)	865(1)	4137(1)	6510(1)	24(1)
C(29)	-122(1)	3501(2)	9327(1)	44(1)
C(31)	4870(2)	6644(1)	7905(2)	47(1)
C(32)	3945(1)	5413(1)	8072(1)	39(1)
C(33)	4192(1)	5827(1)	6606(1)	39(1)
C(34)	7462(2)	2773(2)	7335(2)	58(1)
C(35)	6006(1)	3042(1)	6224(1)	42(1)
C(36)	5893(1)	2544(1)	7712(1)	39(1)
C(41)	3234(1)	2437(1)	9986(1)	35(1)
C(42)	4012(1)	3446(1)	9203(1)	32(1)
C(43)	3484(1)	2092(1)	8535(1)	30(1)
C(44)	-172(1)	4438(1)	6263(1)	37(1)
C(45)	1498(1)	4870(1)	6423(1)	32(1)
C(46)	961(1)	3467(1)	5853(1)	30(1)

Table S37. Anisotropic displacement parameters ($Å^2$ $x10^3$) for $(BHT)_2Mg(DMSO)_2$ (**8**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	20(1)	27(1)	20(1)	-1(1)	5(1)	-4(1)
S(1)	39(1)	32(1)	29(1)	-6(1)	15(1)	-11(1)
S(21)	29(1)	49(1)	26(1)	4(1)	13(1)	-5(1)
C(3)	107(4)	67(3)	68(3)	38(3)	24(3)	30(3)
C(4)	105(4)	64(3)	45(2)	-18(2)	31(2)	-12(3)
S(22)	110(2)	49(2)	23(1)	-1(1)	11(1)	36(1)
O(1)	36(1)	32(1)	40(1)	-12(1)	18(1)	-11(1)
O(2)	36(1)	59(1)	23(1)	10(1)	6(1)	-4(1)
O(3)	18(1)	24(1)	33(1)	-6(1)	5(1)	-2(1)
O(4)	21(1)	31(1)	21(1)	4(1)	6(1)	-1(1)
C(1)	61(2)	61(2)	40(1)	-15(1)	1(1)	-17(1)

C(2)	79(2)	37(1)	63(2)	12(1)	27(1)	9(1)
C(11)	21(1)	22(1)	19(1)	-1(1)	7(1)	-2(1)
C(12)	24(1)	20(1)	24(1)	2(1)	4(1)	0(1)
C(13)	33(1)	18(1)	28(1)	-1(1)	1(1)	-3(1)
C(14)	26(1)	26(1)	27(1)	3(1)	-2(1)	-6(1)
C(15)	20(1)	29(1)	25(1)	1(1)	2(1)	1(1)
C(16)	22(1)	24(1)	22(1)	-4(1)	7(1)	0(1)
C(17)	29(1)	20(1)	40(1)	-3(1)	3(1)	4(1)
C(18)	23(1)	31(1)	41(1)	-15(1)	3(1)	4(1)
C(19)	33(1)	29(1)	54(1)	0(1)	-12(1)	-7(1)
C(21)	19(1)	18(1)	19(1)	-1(1)	3(1)	-3(1)
C(22)	18(1)	19(1)	20(1)	1(1)	1(1)	1(1)
C(23)	24(1)	29(1)	18(1)	4(1)	4(1)	2(1)
C(24)	22(1)	33(1)	24(1)	3(1)	8(1)	3(1)
C(25)	18(1)	25(1)	25(1)	1(1)	2(1)	3(1)
C(26)	20(1)	17(1)	19(1)	1(1)	1(1)	-1(1)
C(27)	19(1)	26(1)	21(1)	4(1)	1(1)	2(1)
C(28)	24(1)	26(1)	20(1)	6(1)	0(1)	0(1)
C(29)	28(1)	76(2)	31(1)	14(1)	13(1)	14(1)
C(31)	42(1)	23(1)	69(2)	-9(1)	-4(1)	7(1)
C(32)	33(1)	35(1)	51(1)	-9(1)	16(1)	8(1)
C(33)	35(1)	32(1)	45(1)	6(1)	-4(1)	5(1)
C(34)	29(1)	49(1)	89(2)	-38(1)	0(1)	12(1)
C(35)	34(1)	53(1)	40(1)	-26(1)	11(1)	-1(1)
C(36)	41(1)	21(1)	50(1)	-4(1)	-1(1)	3(1)
C(41)	27(1)	50(1)	27(1)	14(1)	2(1)	10(1)
C(42)	23(1)	37(1)	33(1)	0(1)	-2(1)	-3(1)
C(43)	27(1)	28(1)	35(1)	3(1)	5(1)	7(1)
C(44)	30(1)	49(1)	28(1)	12(1)	-1(1)	10(1)
C(45)	39(1)	25(1)	29(1)	9(1)	5(1)	-2(1)
C(46)	30(1)	37(1)	20(1)	0(1)	1(1)	-6(1)

Table S38. Bond lengths for non-hydrogen atoms (Å) for $(BHT)_2Mg(DMSO)_2$ (**8**)

Atoms	Bond length	Atoms	Bond length	Atoms	Bond length
Mg(1)-O(4)	1.8565(12)	O(3)-C(11)	1.3192(18)	C(18)-C(34)	1.543(2)
Mg(1)-O(3)	1.8630(12)	O(4)-C(21)	1.3230(18)	C(21)-C(26)	1.429(2)
Mg(1)-O(2)	1.9777(14)	C(11)-C(16)	1.429(2)	C(21)-C(22)	1.430(2)
Mg(1)-O(1)	2.0091(14)	C(11)-C(12)	1.432(2)	C(22)-C(23)	1.394(2)
S(1)-O(1)	1.5124(13)	C(12)-C(13)	1.393(2)	C(22)-C(27)	1.542(2)
S(1)-C(2)	1.777(2)	C(12)-C(17)	1.544(2)	C(23)-C(24)	1.386(2)
S(1)-C(1)	1.777(2)	C(13)-C(14)	1.387(2)	C(24)-C(25)	1.390(2)
S(21)-O(2)	1.4853(15)	C(14)-C(15)	1.385(2)	C(24)-C(29)	1.510(2)
S(21)-C(4)	1.732(5)	C(14)-C(19)	1.514(2)	C(25)-C(26)	1.394(2)
S(21)-C(3)	1.762(5)	C(15)-C(16)	1.394(2)	C(26)-C(28)	1.540(2)
S(22)-O(2)	1.514(2)	C(16)-C(18)	1.539(2)	C(27)-C(43)	1.535(2)
S(22)-C(5)	1.773(8)	C(17)-C(32)	1.531(3)	C(27)-C(42)	1.537(2)
S(22)-C(6)	1.849(9)	C(17)-C(33)	1.537(3)	C(27)-C(41)	1.538(2)
S(23)-O(2)	1.472(6)	C(17)-C(31)	1.541(2)	C(28)-C(45)	1.534(2)
S(23)-C(7)	1.783(13)	C(18)-C(36)	1.534(3)	C(28)-C(44)	1.539(2)
S(23)-C(8)	1.801(15)	C(18)-C(35)	1.540(3)	C(28)-C(46)	1.540(2)

Table S39. Bond angles for non-hydrogen atoms (°) for $(BHT)_2Mg(DMSO)_2$ (**8**)

Atoms	Bond angles	Atoms	Bond angles
O(4)-Mg(1)-O(3)	117.60(6)	C(32)-C(17)-C(33)	109.75(15)
O(4)-Mg(1)-O(2)	114.95(6)	C(32)-C(17)-C(31)	107.02(17)
O(3)-Mg(1)-O(2)	104.40(6)	C(33)-C(17)-C(31)	106.52(16)
O(4)-Mg(1)-O(1)	104.96(6)	C(32)-C(17)-C(12)	110.46(14)
O(3)-Mg(1)-O(1)	118.43(6)	C(33)-C(17)-C(12)	110.70(15)
O(2)-Mg(1)-O(1)	94.51(6)	C(31)-C(17)-C(12)	112.24(15)
O(1)-S(1)-C(2)	104.34(11)	C(36)-C(18)-C(16)	109.52(14)
O(1)-S(1)-C(1)	105.36(10)	C(36)-C(18)-C(35)	110.56(15)
C(2)-S(1)-C(1)	98.23(13)	C(16)-C(18)-C(35)	111.30(16)
O(2)-S(21)-C(4)	105.7(2)	C(36)-C(18)-C(34)	107.81(18)
O(2)-S(21)-C(3)	104.3(2)	C(16)-C(18)-C(34)	111.70(15)
C(4)-S(21)-C(3)	99.4(3)	C(35)-C(18)-C(34)	105.86(16)
O(2)-S(22)-C(5)	104.5(3)	O(4)-C(21)-C(26)	120.74(13)
O(2)-S(22)-C(6)	98.9(4)	O(4)-C(21)-C(22)	120.45(13)
C(5)-S(22)-C(6)	93.1(5)	C(26)-C(21)-C(22)	118.80(13)
O(2)-S(23)-C(7)	105.4(8)	C(23)-C(22)-C(21)	118.55(13)
O(2)-S(23)-C(8)	98.6(12)	C(23)-C(22)-C(27)	119.44(13)
C(7)-S(23)-C(8)	97.7(13)	C(21)-C(22)-C(27)	122.01(13)
S(1)-O(1)-Mg(1)	128.88(8)	C(24)-C(23)-C(22)	123.29(14)
S(23)-O(2)-Mg(1)	153.9(3)	C(23)-C(24)-C(25)	117.58(14)
S(21)-O(2)-Mg(1)	136.35(9)	C(23)-C(24)-C(29)	121.07(15)
S(22)-O(2)-Mg(1)	139.05(12)	C(25)-C(24)-C(29)	121.34(15)
C(11)-O(3)-Mg(1)	173.25(11)	C(24)-C(25)-C(26)	122.68(14)
C(21)-O(4)-Mg(1)	176.00(11)	C(25)-C(26)-C(21)	119.09(13)
O(3)-C(11)-C(16)	120.45(14)	C(25)-C(26)-C(28)	119.87(13)
O(3)-C(11)-C(12)	121.09(14)	C(21)-C(26)-C(28)	121.04(13)
C(16)-C(11)-C(12)	118.46(14)	C(43)-C(27)-C(42)	109.47(14)
C(13)-C(12)-C(11)	118.66(14)	C(43)-C(27)-C(41)	106.39(14)
C(13)-C(12)-C(17)	119.90(14)	C(42)-C(27)-C(41)	107.28(14)
C(11)-C(12)-C(17)	121.44(14)	C(43)-C(27)-C(22)	110.89(13)
C(14)-C(13)-C(12)	123.31(15)	C(42)-C(27)-C(22)	110.87(13)
C(15)-C(14)-C(13)	117.39(15)	C(41)-C(27)-C(22)	111.79(13)
C(15)-C(14)-C(19)	121.09(16)	C(45)-C(28)-C(44)	106.61(14)
C(13)-C(14)-C(19)	121.52(16)	C(45)-C(28)-C(26)	110.22(13)
C(14)-C(15)-C(16)	122.99(15)	C(44)-C(28)-C(26)	112.07(13)
C(15)-C(16)-C(11)	119.06(14)	C(45)-C(28)-C(46)	111.14(14)
C(15)-C(16)-C(18)	120.00(14)	C(44)-C(28)-C(46)	106.53(14)
C(11)-C(16)-C(18)	120.92(14)	C(26)-C(28)-C(46)	110.18(13)

Table S40. Torsion angles (°) for $(BHT)_2Mg(DMSO)_2$ (**8**)

Atoms	Torsion angles	Atoms	Torsion angles
C(2)-S(1)-O(1)-Mg(1)	-150.20(13)	O(3)-C(11)-C(16)-C(15)	-177.72(14)
C(1)-S(1)-O(1)-Mg(1)	106.89(13)	C(12)-C(11)-C(16)-C(15)	3.0(2)
O(4)-Mg(1)-O(1)-S(1)	14.96(12)	O(3)-C(11)-C(16)-C(18)	0.7(2)
O(3)-Mg(1)-O(1)-S(1)	148.57(10)	C(12)-C(11)-C(16)-C(18)	-178.57(15)
O(2)-Mg(1)-O(1)-S(1)	-102.38(11)	C(13)-C(12)-C(17)-C(32)	-115.22(17)
C(7)-S(23)-O(2)-S(21)	91.7(8)	C(11)-C(12)-C(17)-C(32)	64.3(2)
C(8)-S(23)-O(2)-S(21)	-8.8(12)	C(13)-C(12)-C(17)-C(33)	123.01(17)
C(7)-S(23)-O(2)-S(22)	52.8(7)	C(11)-C(12)-C(17)-C(33)	-57.4(2)
C(8)-S(23)-O(2)-S(22)	-47.7(12)	C(13)-C(12)-C(17)-C(31)	4.1(2)
C(7)-S(23)-O(2)-Mg(1)	173.0(7)	C(11)-C(12)-C(17)-C(31)	-176.33(17)
C(8)-S(23)-O(2)-Mg(1)	72.5(14)	C(15)-C(16)-C(18)-C(36)	113.45(17)
C(4)-S(21)-O(2)-S(23)	-110.9(5)	C(11)-C(16)-C(18)-C(36)	-64.9(2)
C(3)-S(21)-O(2)-S(23)	-6.6(5)	C(15)-C(16)-C(18)-C(35)	-123.99(17)
C(4)-S(21)-O(2)-S(22)	-3.7(3)	C(11)-C(16)-C(18)-C(35)	57.6(2)
C(3)-S(21)-O(2)-S(22)	100.6(3)	C(15)-C(16)-C(18)-C(34)	-5.9(3)
C(4)-S(21)-O(2)-Mg(1)	108.1(3)	C(11)-C(16)-C(18)-C(34)	175.72(18)
C(3)-S(21)-O(2)-Mg(1)	-147.6(3)	O(4)-C(21)-C(22)-C(23)	-179.97(14)
C(5)-S(22)-O(2)-S(23)	-44.3(5)	C(26)-C(21)-C(22)-C(23)	-0.7(2)
C(6)-S(22)-O(2)-S(23)	51.3(5)	O(4)-C(21)-C(22)-C(27)	-0.1(2)
C(5)-S(22)-O(2)-S(21)	-86.7(4)	C(26)-C(21)-C(22)-C(27)	179.12(13)
C(6)-S(22)-O(2)-S(21)	8.9(4)	C(21)-C(22)-C(23)-C(24)	0.1(2)
C(5)-S(22)-O(2)-Mg(1)	171.2(4)	C(27)-C(22)-C(23)-C(24)	-179.77(15)
C(6)-S(22)-O(2)-Mg(1)	-93.2(4)	C(22)-C(23)-C(24)-C(25)	0.5(3)
O(4)-Mg(1)-O(2)-S(23)	110.3(8)	C(22)-C(23)-C(24)-C(29)	-179.51(18)
O(3)-Mg(1)-O(2)-S(23)	-20.0(8)	C(23)-C(24)-C(25)-C(26)	-0.4(3)
O(1)-Mg(1)-O(2)-S(23)	-140.9(8)	C(29)-C(24)-C(25)-C(26)	179.60(17)
O(4)-Mg(1)-O(2)-S(21)	160.25(16)	C(24)-C(25)-C(26)-C(21)	-0.2(2)
O(3)-Mg(1)-O(2)-S(21)	29.93(18)	C(24)-C(25)-C(26)-C(28)	179.41(15)
O(1)-Mg(1)-O(2)-S(21)	-90.95(17)	O(4)-C(21)-C(26)-C(25)	-179.94(14)
O(4)-Mg(1)-O(2)-S(22)	-155.0(3)	C(22)-C(21)-C(26)-C(25)	0.8(2)
O(3)-Mg(1)-O(2)-S(22)	74.6(3)	O(4)-C(21)-C(26)-C(28)	0.4(2)
O(1)-Mg(1)-O(2)-S(22)	-46.2(3)	C(22)-C(21)-C(26)-C(28)	-178.84(13)
O(3)-C(11)-C(12)-C(13)	176.66(14)	C(23)-C(22)-C(27)-C(43)	122.35(16)
C(16)-C(11)-C(12)-C(13)	-4.1(2)	C(21)-C(22)-C(27)-C(43)	-57.47(19)
O(3)-C(11)-C(12)-C(17)	-2.9(2)	C(23)-C(22)-C(27)-C(42)	-115.83(16)
C(16)-C(11)-C(12)-C(17)	176.35(14)	C(21)-C(22)-C(27)-C(42)	64.35(19)
C(11)-C(12)-C(13)-C(14)	2.2(2)	C(23)-C(22)-C(27)-C(41)	3.8(2)
C(17)-C(12)-C(13)-C(14)	-178.20(16)	C(21)-C(22)-C(27)-C(41)	-176.00(15)
C(12)-C(13)-C(14)-C(15)	0.8(3)	C(25)-C(26)-C(28)-C(45)	118.33(16)
C(12)-C(13)-C(14)-C(19)	-179.27(17)	C(21)-C(26)-C(28)-C(45)	-62.03(19)
C(13)-C(14)-C(15)-C(16)	-2.0(3)	C(25)-C(26)-C(28)-C(44)	-0.2(2)
C(19)-C(14)-C(15)-C(16)	178.11(17)	C(21)-C(26)-C(28)-C(44)	179.41(15)
C(14)-C(15)-C(16)-C(11)	0.0(2)	C(25)-C(26)-C(28)-C(46)	-118.65(16)
C(14)-C(15)-C(16)-C(18)	-178.39(16)	C(21)-C(26)-C(28)-C(46)	60.98(18)

S2.10. Molecular structure of $[Mg_6(BHT)_2(OCH_2COOEt)_{10}](THF)_3$

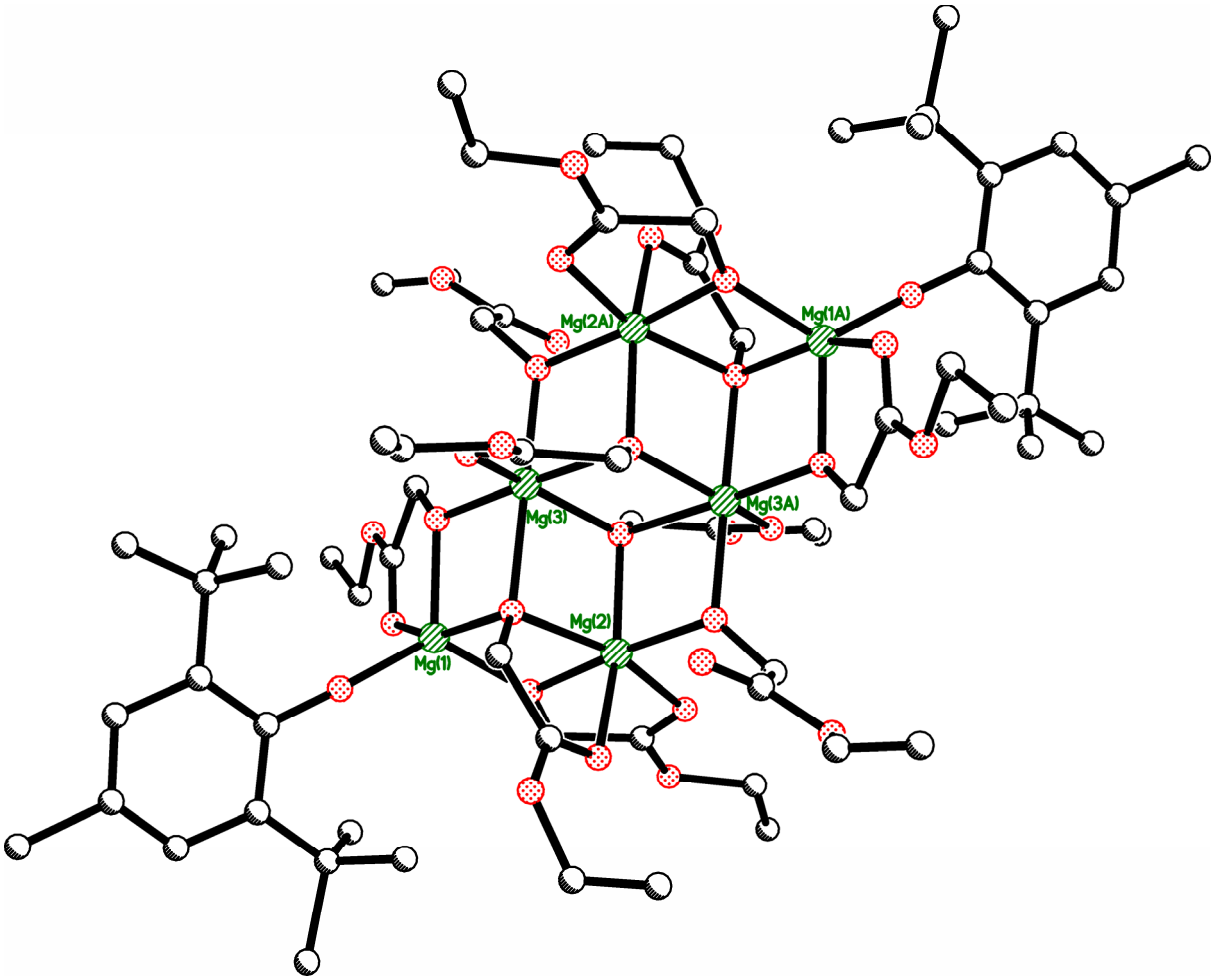

Fig. S21. The crystal structure of $[Mg_6(BHT)_2(OCH_2COOEt)_{10}](THF)_3$ (a ball-and-stick model). Non-coordinating THF molecules are omitted

Slow diffusion of $Mg(BHT)Bu(THF)_2$ and $HOCH_2COOEt$ solutions in THF into each other provided crystals of $[Mg_6(BHT)_2(OCH_2COOEt)_{10}](THF)_3$ (Fig. S21, Table S41). The crystal structure was not good enough to be published: hydrogen atoms were not located from the E-map, non-H atoms were refined with isotropic displacement parameters. The poor data were likely due to a small crystal size. Therefore, only the atom connectivity is avalibale for the structure. The structure is located at an inversion center. There are two terminal BHT ligands. Six OCH_2COOEt anions exhibit three folowing coordination modes: μ_3-κ^1O:κ^1O:κ^2O,O' (4 ligands), μ_2-κ^1O:κ^2O,O' (4 ligands), μ_2-κ^1O:κ^1O (2 ligands). Coordination numbers of Mg atoms are 5 (Mg1 and Mg1A) and 6 (the other 4 Mg atoms). The steric crowding and a relatively high Mg coordination number do not allow two OCH_2COOEt anions to use carbonyl groups for additional coordination with the nearest Mg atoms (Mg2, Mg3, Mg2A, Mg3A; c.n.=6). The polynuclear complex possesses an unprecedented Mg_6O_{10} core.[6,7] The core ressembles 4 joined cubes without 4 vertices (Fig. S22).

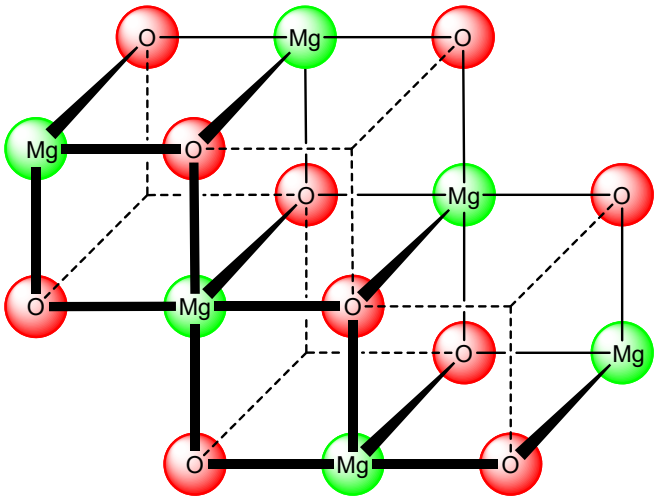

Fig. S22. An idelized Mg_6O_{10} tetracubic core of $[Mg_6(BHT)_2(OCH_2COOEt)_{10}]$

Table S41. Some crystal data for $[Mg_6(BHT)_2(OCH_2COOEt)_{10}](THF)_3$

Temperature (K)	150(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit Cell Dimensions	
a (Å)	12.8773(12)
b (Å)	21.347(2)
c (Å)	18.1672(17)
β (º)	106.286(2)
Volume ($Å^3$)	4793.55
Z	2

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S3. DOSY NMR experiments

S3.1. Mathematical formulae used in DOSY NMR

It is well-known that a size of a spherical molecule is related to diffusion coefficient (D) by the Stokes-Einstein equation (eq. 1), where k_B is the Boltzmann constant, T is the temperature, η is dynamic viscosity, R_S is the hydrodynamic radius of the solute (diffusing molecule). However for a regular molecule, the Stokes-Einstein equation has to be corrected for size[1] and shape (eq 2), where c is a size correlation factor (eq. 3)[2] between R_S and the van der Waals radius of the solvent (r_{solv}^{W}), f_s is a shape friction correction factor (eq. 4a-c).[3] Equations 2-4 can be found in the literature, for example [4-7]. Experimentally observed lg D values and R_S are related by eq.5.

$$D = \frac{k_B T}{6\pi\eta Rs} \quad (1)$$

$$D = \frac{k_B T}{cf_s \pi\eta Rs} \quad (2)$$

$$c = \frac{6}{1 + 0.695 \cdot \left(\frac{r_{solv}^{W}}{R_S}\right)^{2.234}} \quad (3)$$

For a prolate ellipsoid:

$$f_s = \frac{\sqrt{1-\left(\frac{b}{a}\right)^2}}{\left(\frac{b}{a}\right)^{\frac{2}{3}} \cdot \ln\left[\frac{1+\sqrt{1-\left(\frac{b}{a}\right)^2}}{\left(\frac{b}{a}\right)}\right]} \quad (4a)$$

For an oblate ellipsoid:

$$f_s = \frac{\sqrt{\left(\frac{b}{a}\right)^2 - 1}}{\left(\frac{b}{a}\right)^{\frac{2}{3}} \cdot \arctan\sqrt{\left(\frac{b}{a}\right)^2 - 1}} \quad (4b)$$

where a and b are semi-major and semi-minor axes of molecular spheroids

For a sphere: $f_s = 1$ (4c)

$$Rs = \frac{k_B T}{cf_s \pi\eta} \cdot 10^{-\lg D} \quad (5)$$

Measuring exact T and η values can be avoided if one of two molecules is used as an internal standard in the same DOSY NMR experiment. In this case, the ratio $R_{S(1)}/R_{S(2)}$ can be

described by eq. 6.[7] The latter may be rewritten as equation 7. The value of *const* (eq. 7) should be close to 1 for similar molecules, allowing to estimate $R_{S(2)}$ with a good presison, if $R_{S(1)}$ and $\Delta\lg D$ are known.

$$\frac{R_{S(1)}}{R_{S(2)}} = \frac{c_{(2)} f_{S(2)}}{c_{(1)} f_{S(1)}} \cdot \frac{D_{(2)}}{D_{(1)}} \quad (6)$$

$$\frac{R_{S(1)}}{R_{S(2)}} = \frac{c_{(2)} f_{S(2)}}{c_{(1)} f_{S(1)}} \cdot 10^{\lg D_{(2)} - \lg D_{(1)}} = const \cdot 10^{\Delta \lg D} \quad (7)$$

S3.2. Van der Waals and Connolly surfaces, their volumes and spherical equivalent radii

Van der Waals and solvent excluded (Connolly) surfaces and their volumes (V^W and V^{SES}) have been calculated by using Jmol software.[8] Connolly surfaces have been generated with THF probe radius of 2.60Å.[5] X-ray volumes ($V^{X\text{-}ray}$) for **1** and **3** have been calculated by dividing the unit cell volume by the number of molecules in it. Spherical equivalent radii ($R_{eq}{}^{W}$, $R_{eq}{}^{SES}$ and $R_{eq}{}^{X\text{-}ray}$) have been calculated from V^W, V^{SES} and $V^{X\text{-}ray}$ in usual manner, according to

$$R_{eq} = \sqrt[3]{\frac{3V}{4\pi}}$$

Table S42. $V^{X\text{-}ray}$, $R_{eq}{}^{X\text{-}ray}$ from the X-ray data.

	$V^{X\text{-}ray}$, Å^3	$R_{eq}{}^{X\text{-}ray}$, Å	$R_{eq}{}^{X\text{-}ray}{}_{(3)} / R_{eq}{}^{Xray}{}_{(1)}$
$[(BHT)_2Mg(thf)_2]$ (**1**)	915.295	6.023	1.114
1:1 mixture of cis- & trans- $[(BHT)Mg(OBn)(thf)]_2$ (**3**)	1264.65	6.709	

Table S43. V^w, V^{SES}, $R_{eq}{}^{W}$, $R_{eq}{}^{SES}$ from the X-ray data.

	V^W, Å^3	$R_{eq}{}^{W}$, Å	V^{SES}, Å^3	$R_{eq}{}^{ses}$, Å	$R_{eq}{}^{W}{}_{\mathbf{(dimer)}} / R_{eq}{}^{W}{}_{\mathbf{(1)}}$	$R_{eq}{}^{SES}{}_{\mathbf{(dimer)}} / R_{eq}{}^{SES}{}_{\mathbf{(1)}}$
$[(BHT)_2Mg(thf)_2]$ (**1**)	568.18	5.138	697.20	5.501	-	-
trans-$[(BHT)Mg(OBn)(thf)]_2$ (**3**)	769.79	5.686	979.11	6.160	1.107	1.120
cis-$[(BHT)Mg(OBn)(thf)]_2$ (**3**)	768.91	5.683	967.48	6.136	1.106	1.115
$[(BHT)Mg(OCH_2COOEt)(thf)]_2$ (**4**)	746.62	5.628	892.05	5.972	1.095	1.086

Table S44. V^w, V^{SES}, $R_{eq}{}^{W}$, $R_{eq}{}^{SES}$ from the DFT calculations.

	V^W, Å^3	$R_{eq}{}^{W}$, Å	V^{SES}, Å^3	$R_{eq}{}^{ses}$, Å	$R_{eq}{}^{W}{}_{\mathbf{(dimer)}} / R_{eq}{}^{W}{}_{\mathbf{(1)}}$	$R_{eq}{}^{SES}{}_{\mathbf{(dimer)}} / R_{eq}{}^{SES}{}_{\mathbf{(1)}}$
$[(BHT)_2Mg(thf)_2]$ (**1**)	595.85	5.220	740.72	5.613	-	-
$[(BHT)Mg(OBn)(thf)_2]$	474.20	4.838	590.96	5.206	0.927	0.927
trans-$[(BHT)Mg(OBn)(thf)]_2$ (**3**)	806.06	5.773	1039.82	6.285	1.106	1.120
$[(BHT)Mg(OCH_2COOEt)(thf)]$	392.61	4.542	481.08	4.861	0.870	0.866
$[(BHT)Mg(OCH_2COOEt)(thf)]_2$ (**4**)	781.51	5.714	937.21	6.071	1.095	1.082

Table S45. Van der Waals and Connolly surfaces generated from X-ray data

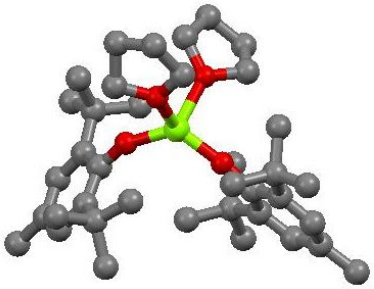
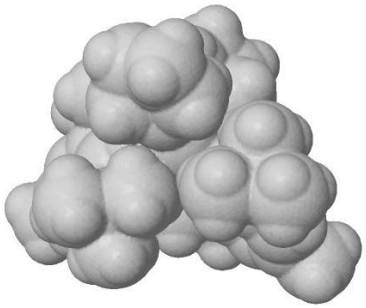
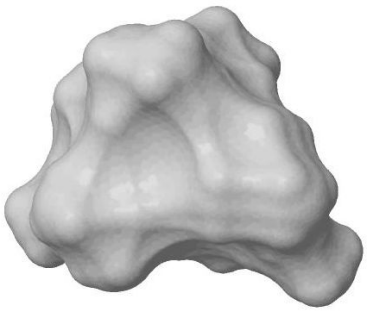
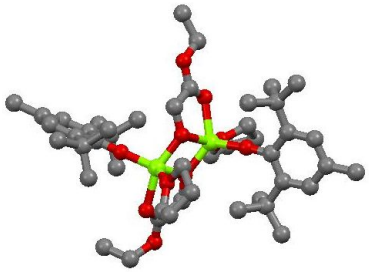
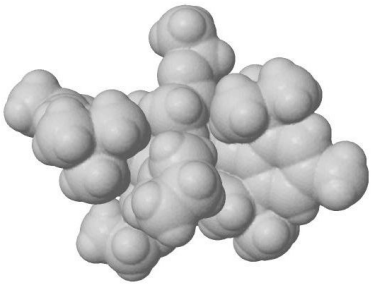
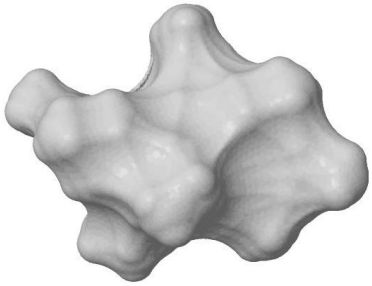
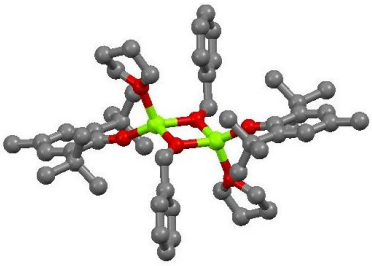
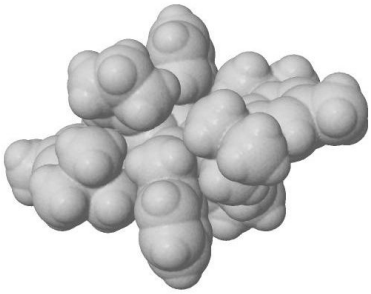
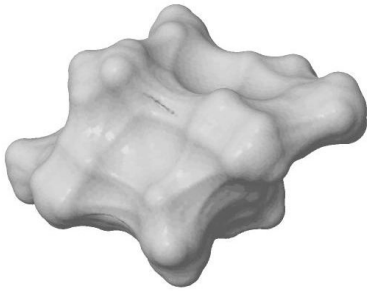
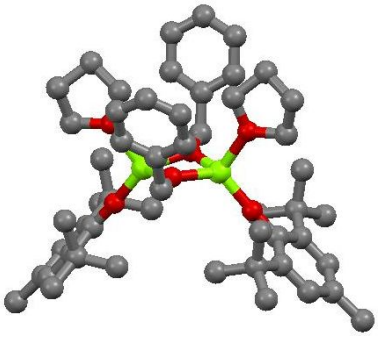
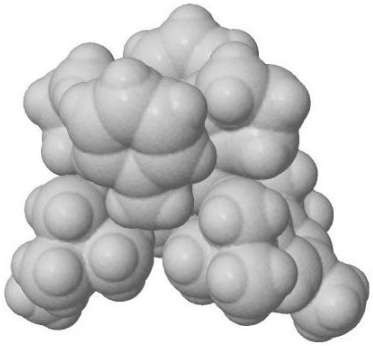
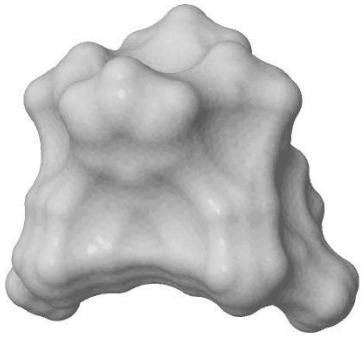
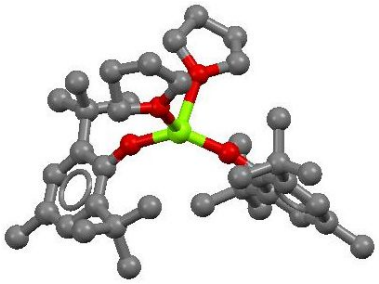
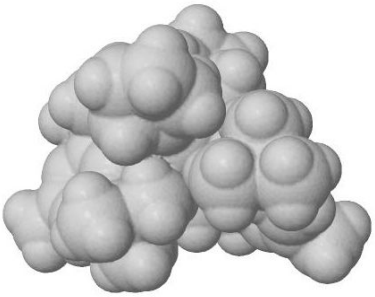
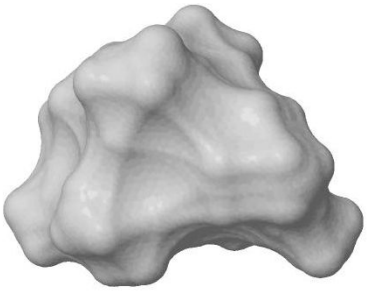
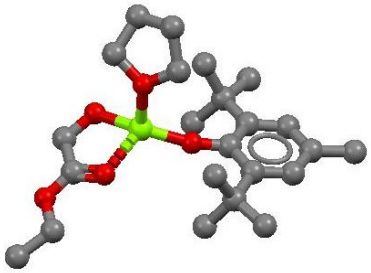
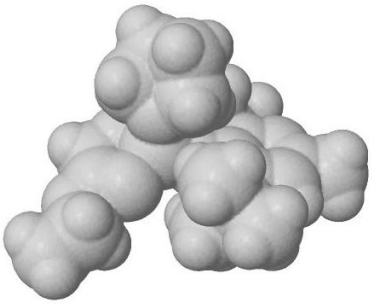
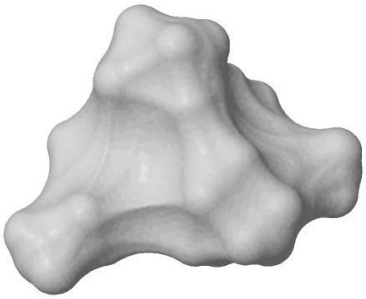
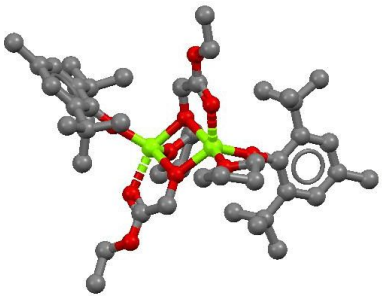
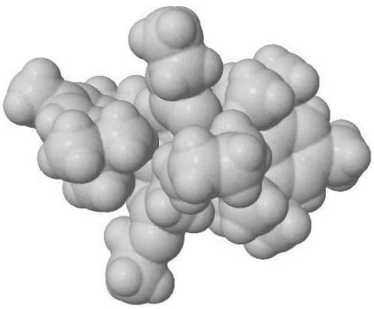
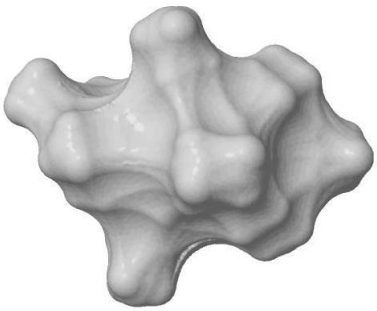
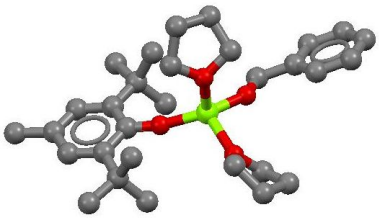
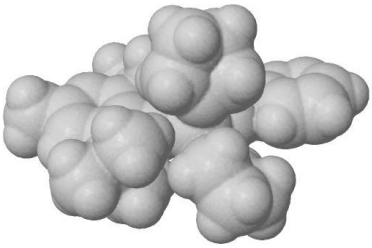
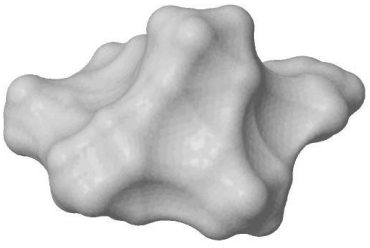
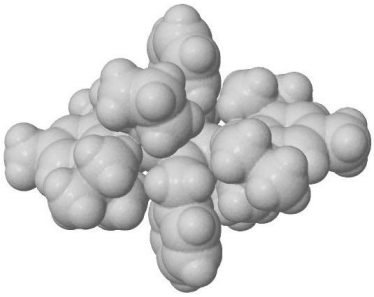
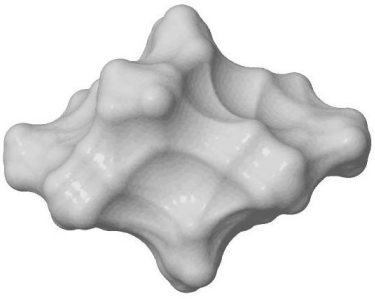
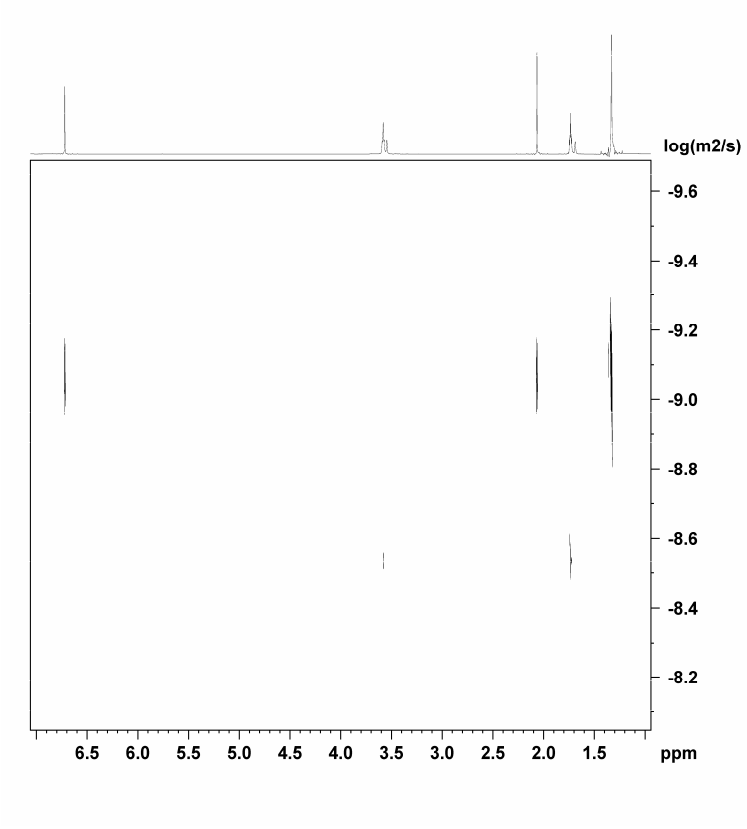
Complex	Van der Waals surface	Connolly surface
 $[(BHT)_2Mg(thf)_2]$		
 $[(BHT)Mg(OCH_2COOEt)(thf)]_2$		
 *trans*-$[(BHT)Mg(OBn)(thf)]_2$		
 *cis*-$[(BHT)Mg(OBn)(thf)]_2$		

Table S46. Van der Waals and Connolly surfaces generated from DFT calculation data

Complex	Van der Waals surface	Connolly surface
 $[(BHT)_2Mg(thf)_2]$		
 $[(BHT)Mg(OCH_2COOEt)(thf)]$		
 $[(BHT)Mg(OCH_2COOEt)(thf)]_2$		
 $[(BHT)Mg(OBn)(thf)_2]$		
 $[(BHT)Mg(OBn)(thf)]_2$		

S3.3. DOSY NMR spectra of BHT-Mg complexes

DOSY NMR spectra were acquired on a Bruker Avance III 600 spectrometer (600 MHz) at 303 K and referenced to solvent residual protons. DOSY experiments were performed with a standard dstegp3s pulse sequence, using a 2D sequence for diffusion measurement with double stimulated echo.[9,10]

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Current Data Parameters
NAME                  KBN040_4
EXPNO                      100
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20170531
Time                     15.46
INSTRUM                  spect
PROBHD   5 mm PABBO BB-
PULPROG               dstegp3s
TD                        9602
SOLVENT                    THF
NS                           8
DS                           0
SWH                   4801.537 Hz
FIDRES                0.500056 Hz
AQ                    0.9998882 sec
RG                         362
DW                     104.133 usec
DE                      11.20 usec
TE                       303.0 K
D1                  3.00000000 sec
D16                 0.00020000 sec
D20                 0.06000000 sec
D21                 0.00500000 sec

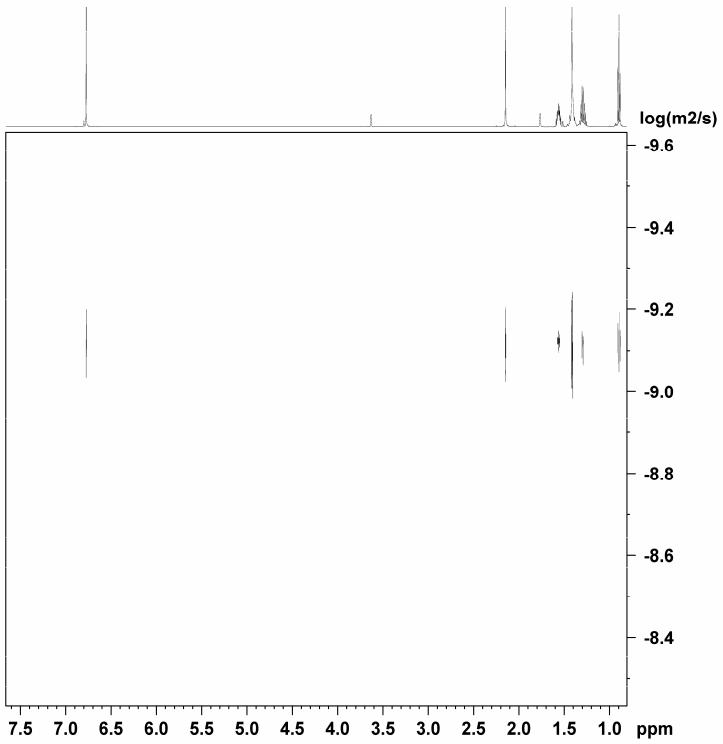
======== CHANNEL f1 ========
SFO1                600.1312003 MHz
NUC1                        1H
P1                       13.80 usec
PLW1                31.62299919 W

====== GRADIENT CHANNEL =====
GPNAM[6]            SMSQ10.100
GPNAM[7]            SMSQ10.100
GPNAM[8]            SMSQ10.100
GPNAM[9]            SMSQ10.100
GPZ6                     100.00 %
GPZ7                     -13.17 %
GPZ8                     -17.13 %
GPZ9                     -15.37 %
P19                      500.00 usec
P30                     2000.00 usec

F1 - Acquisition parameters
TD                           64
SFO1                600.1312 MHz
FIDRES              168.736496 Hz
SW                        8.997 ppm
FnMODE                       QF

F2 - Processing parameters
SI                       16384
SF                  600.1289282 MHz
```

Fig. S23. DOSY NMR spectrum of $(BHT)_2Mg(THF)_2$ (**1**) in THF_{d8} (600 Mhz, 303K)

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PROCNO                  1

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PULPROG          dstegp3s
TD                  9602
SOLVENT              THF
NS                     8
DS                     0
SWH              5405.405 Hz
FIDRES           0.562946 Hz
AQ              0.8881850 sec
RG                   101
DW                92.500 usec
DE                 8.71 usec
TE                303.0 K
D1           3.00000000 sec
D16          0.00020000 sec
D20          0.06000000 sec
D21          0.00500000 sec

======== CHANNEL f1 ========
SFO1         600.1324005 MHz
NUC1                1H
P1                 13.80 usec
PLW1        31.62299919 W

====== GRADIENT CHANNEL =====
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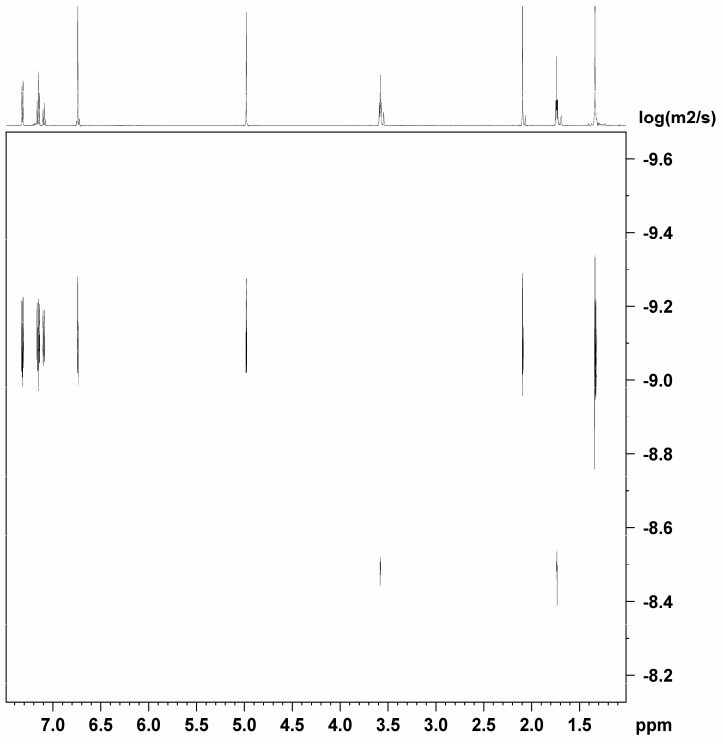
GPNAM[7]      SMSQ10.100
GPNAM[8]      SMSQ10.100
GPNAM[9]      SMSQ10.100
GPZ6              100.00 %
GPZ7              -13.17 %
GPZ8              -17.13 %
GPZ9              -15.37 %
P19               500.00 usec
P30              2000.00 usec

F1 - Acquisition parameters
TD                    64
SFO1            600.1324 MHz
FIDRES        168.736496 Hz
SW                8.997 ppm
FnMODE                QF

F2 - Processing parameters
SI                 16384
SF          600.1300000 MHz
```

Fig. S24. DOSY NMR spectrum of (BHT)Mg(n-Bu))THF)$_2$ (**2**) in THF$_{d8}$ (600 Mhz, 303K)

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Current Data Parameters
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EXPNO                 102
PROCNO                  1

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INSTRUM             spect
PROBHD   5 mm PAQNP 1H/
PULPROG          dstegp3s
TD                 16384
SOLVENT             DMSO
NS                     8
DS                     0
SWH              4801.537 Hz
FIDRES           0.293063 Hz
AQ              1.7061205 sec
RG                  71.8
DW                104.133 usec
DE                 11.26 usec
TE                303.0 K
D1           3.00000000 sec
D16          0.00020000 sec
D20          0.06000000 sec
D21          0.00500000 sec

======== CHANNEL f1 ========
SFO1         600.1330006 MHz
NUC1                1H
P1                 13.70 usec
PLW1        23.87800026 W

====== GRADIENT CHANNEL =====
GPNAM[6]      SMSQ10.100
GPNAM[7]      SMSQ10.100
GPNAM[8]      SMSQ10.100
GPNAM[9]      SMSQ10.100
GPZ6              100.00 %
GPZ7              -13.17 %
GPZ8              -17.13 %
GPZ9              -15.37 %
P19               500.00 usec
P30              2000.00 usec

F1 - Acquisition parameters
TD                    64
SFO1             600.133 MHz
FIDRES        150.096054 Hz
SW                8.003 ppm
FnMODE                QF

F2 - Processing parameters
SI                 16384
SF          600.1305012 MHz
```

Fig. S25. DOSY NMR spectrum of [(BHT)Mg(OBn)(THF)]$_2$ (**3**) in THF$_{d8}$ (600 Mhz, 303K)

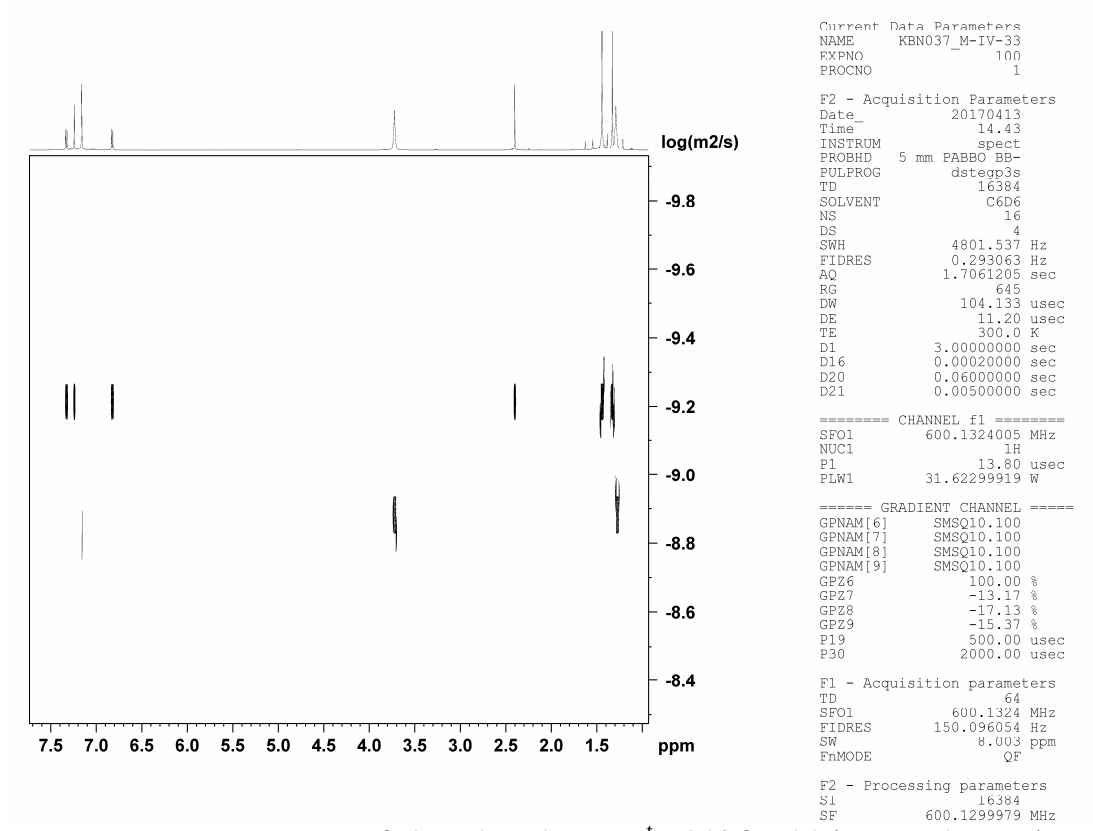

Fig. S26. DOSY NMR spectrum of $[(BHT)Mg(OC_6H_4\text{-}^tBu)(thf)]_2$ (**4**) in C_6D_6 (600 Mhz, 303K)

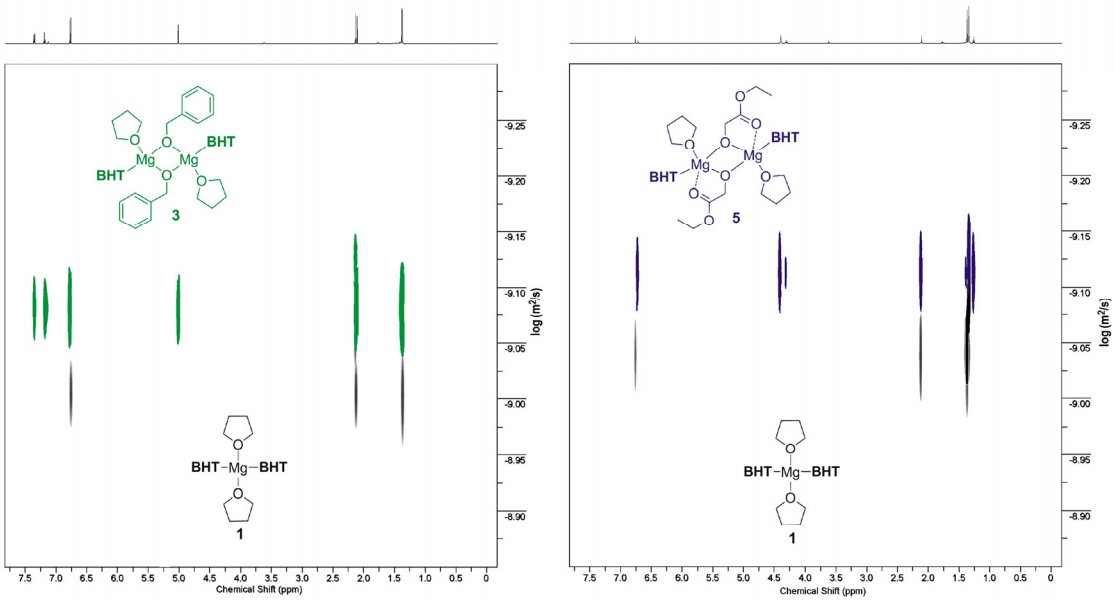

Fig. S27. DOSY NMR spectra (600 MHz, 303 K, THF-d_8) of $[(BHT)Mg(OBn)(THF)]_2$ (**3**, left) and $[(BHT)Mg(OCH_2COOEt)(THF)]_2$ (**4**, right) in the presence of $[(BHT)_2Mg(THF)_2]$ (**1**) as an internal standard

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S4. Polymerization experiments

S4.1. General experimental remarks

All of the synthetic and polymerization experiments were conducted under an argon atmosphere. Toluene was refluxed with Na/benzophenone/dibenzo-18-crown-6 and distilled prior to use. CH_2Cl_2 was refluxed over CaH_2, distilled and stored over molecular sieves 4Å. ε-Caprolactone (Sigma-Aldrich, 99 %) was purified prior to use by distillation under reduced pressure. (*DL*)-lactide, (3,6-dimethyl-1,4-dioxane-2,5-dione (DL), Sigma-Aldrich, 99 %) was purified by sublimation and subsequent recrystallizations from dry toluene followed by drying *in vacuo*.

$CDCl_3$ (Cambridge Isotope Laboratories, Inc., D 99.8 %) was used as purchased. The ^1H and ^{13}C NMR spectra were recorded on a Bruker AVANCE 400 spectrometer (400 MHz) at 20 °C. The chemical shifts are reported in ppm relative to the solvent residual peaks.

Size exclusion chromatography (SEC) was performed on an Agilent PL-GPC 220 chromatograph equipped with a PLgel column, and THF was used as the eluent (1 mL/min). The measurements were recorded with universal calibration according to a polystyrene standard at 40 °C. The molecular weights of PCL were corrected by a factor 0.56, PLAs were corrected by a factor of 0.58.[1]

S4.2. ε-CL and (*DL*)-LA polymerization, [monomer]/[cat] = 200

ε-CL polymerization was carried out at 20 °C in a 1 M solution. A preheated 20 ml glass ampoule was equipped with a magnetic stir bar and filled with dry argon. 1.54 ml (13.8 mmol) of ε-CL were transferred into the ampoule. Then, CH_2Cl_2 was added to achieve an overall volume of 13.5 ml. 0.4 ml of a 0.34 M (137 μmol) catalyst **3** solution in CH_2Cl_2 were injected into the stirred monomer solution at a temperature of 20 °C (ε-CL concentration 1M). After a certain time period, a 5-fold excess of acetic acid was injected into the ampoule to neutralize the catalyst and stop the process. The monomer conversion was determined using ^1H NMR spectroscopy by integration of the monomer $CH_2OC{=}O$ (δ = 4.20 ppm) and polymer $CH_2OC{=}O$ (δ = 4.05 ppm) resonance signals. The polymer was precipitated from the resulting solution with a 10-fold volume excess of diethyl ether. The polymer was filtered, washed with diethyl ether and dried under vacuum. Initiation fragments were determined using ^1H NMR spectroscopy.

The same experiment was performed using catalyst **2**, BnOH (138 μmol) was added to monomer solution before injection of the solution of **2**.

[1] M. Save, M. Schappacher and A. Soum, *Macromol. Chem. Phys.*, 2002, **203**, 889-899

(DL)-lactide polymerization was carried out at 20 °C in a 1 M solution. A preheated 20 ml glass ampoule was equipped with a magnetic stir bar and a septum and then filled with dry argon. 2.00 g (13.9 mmol) of (*DL*)-lactide was placed into the ampule. Then, CH_2Cl_2 was added to achieve an overall volume of 13.5 ml. 0.4 ml of a 0.35 M (140 μmol) solution of catalyst (**3**–**5** or **7**) in CH_2Cl_2 were injected into the stirred monomer solution at 20 °C (*rac*-LA concentration 1M). After a certain time period, a 5-fold excess of acetic acid was injected into the ampoule to neutralize the catalyst and stop the process. The monomer conversion was determined using ^{1}H NMR spectroscopy by integration of the monomer C*H*(CH_3)OC=O (δ = 5.04 ppm) and polymer C*H*(CH_3)OC=O (δ = 5.12 – 5.22 ppm) resonance signals. The resulting solution was poured into a 10-fold volume excess of diethyl ether. The precipitated polymer was filtered, washed with diethyl ether, and dried under vacuum.

The same experiment was performed using catalyst **2**, BnOH (69 μmol) was added to monomer solution before injection of the solution of **2**.

S4.3. (*DL*)-LA polymerization, [monomer]/[cat] = 75

(DL)-lactide polymerization was carried out at 20 °C in a 1 M solution. A preheated 10 ml glass ampoule was equipped with a magnetic stir bar and a septum and then filled with dry argon. 1.08 g (7.5 mmol) of (*DL*)-lactide was placed into the ampule. Then, CH_2Cl_2 was added to achieve an overall volume of 9.5 ml. 0.5 ml of a 0.2 M (100 μmol) solution of catalyst (**3**–**5** or **7**) in CH_2Cl_2 were injected into the stirred monomer solution at 20 °C. After a certain time period, a 5-fold excess of acetic acid was injected into the ampoule to neutralize the catalyst and stop the process. The monomer conversion was determined using ^{1}H NMR spectroscopy by integration of the monomer C*H*(CH_3)OC=O (δ = 5.04 ppm) and polymer C*H*(CH_3)OC=O (δ = 5.12 – 5.22 ppm) resonance signals. The resulting solution was poured into a 10-fold volume excess of diethyl ether. The precipitated polymer was filtered, washed with diethyl ether, and dried under vacuum. Initiation fragments were determined using ^{1}H NMR spectroscopy.

S4.3. ^{1}H NMR spectra of PCLs and PLAs

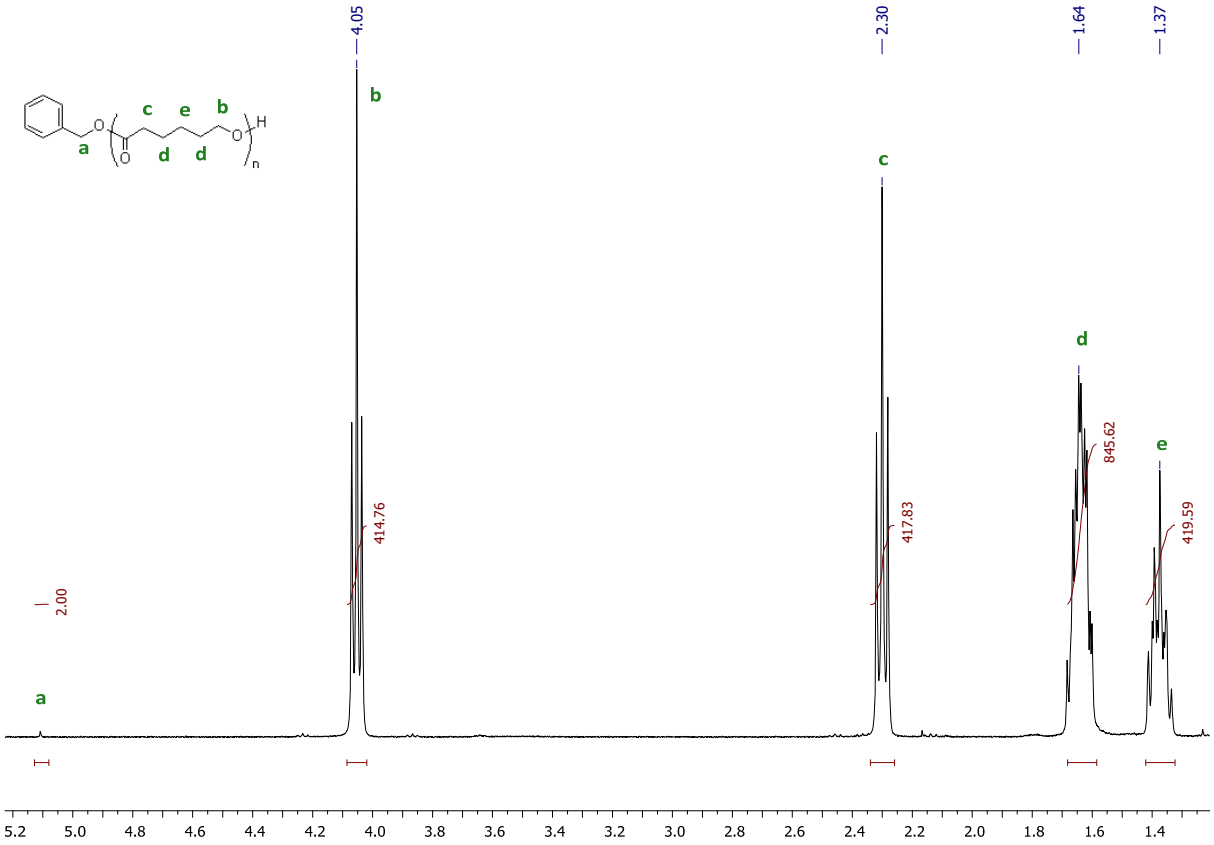

Fig. S28. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PCL obtained using complex **2** activated by BnOH; [εCL]/[**2**] = 200 (Table 1, run 1)

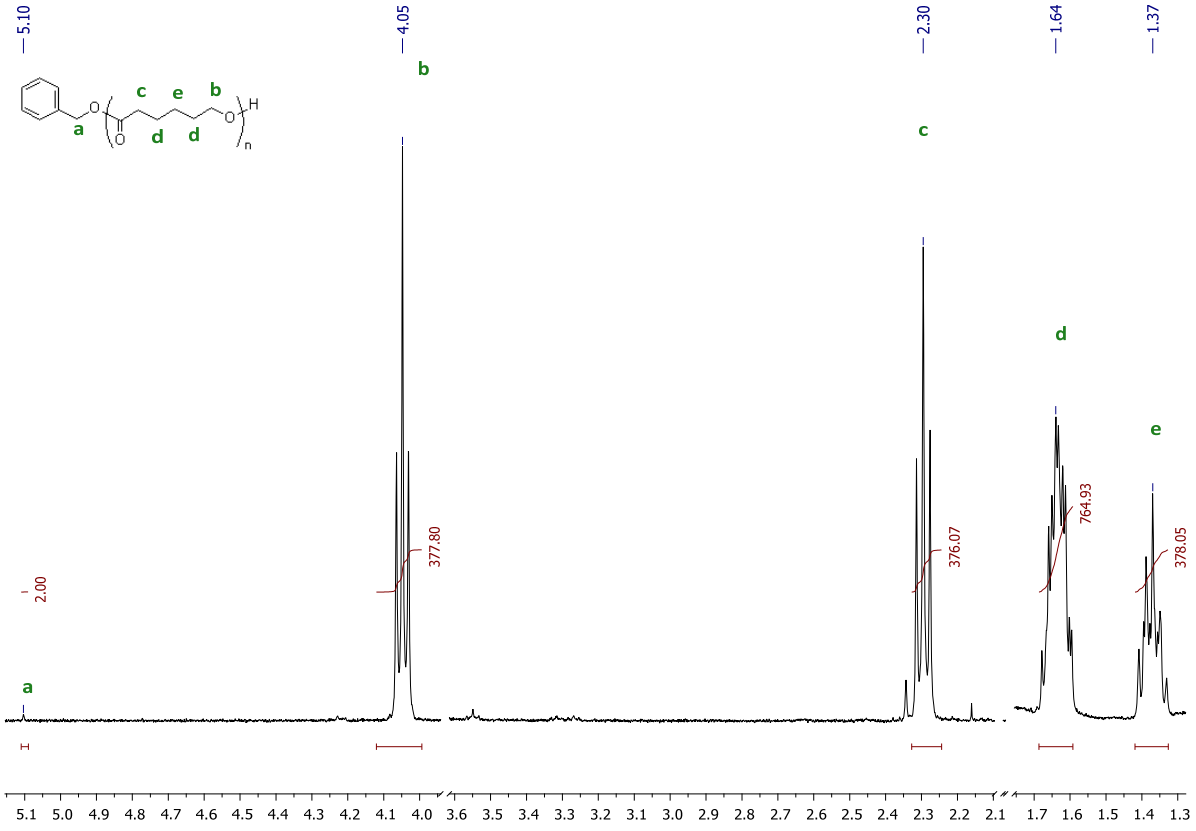

Fig. S29. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PCL obtained using complex **3**; [εCL]/[**3**] = 200 (Table 1, run 3)

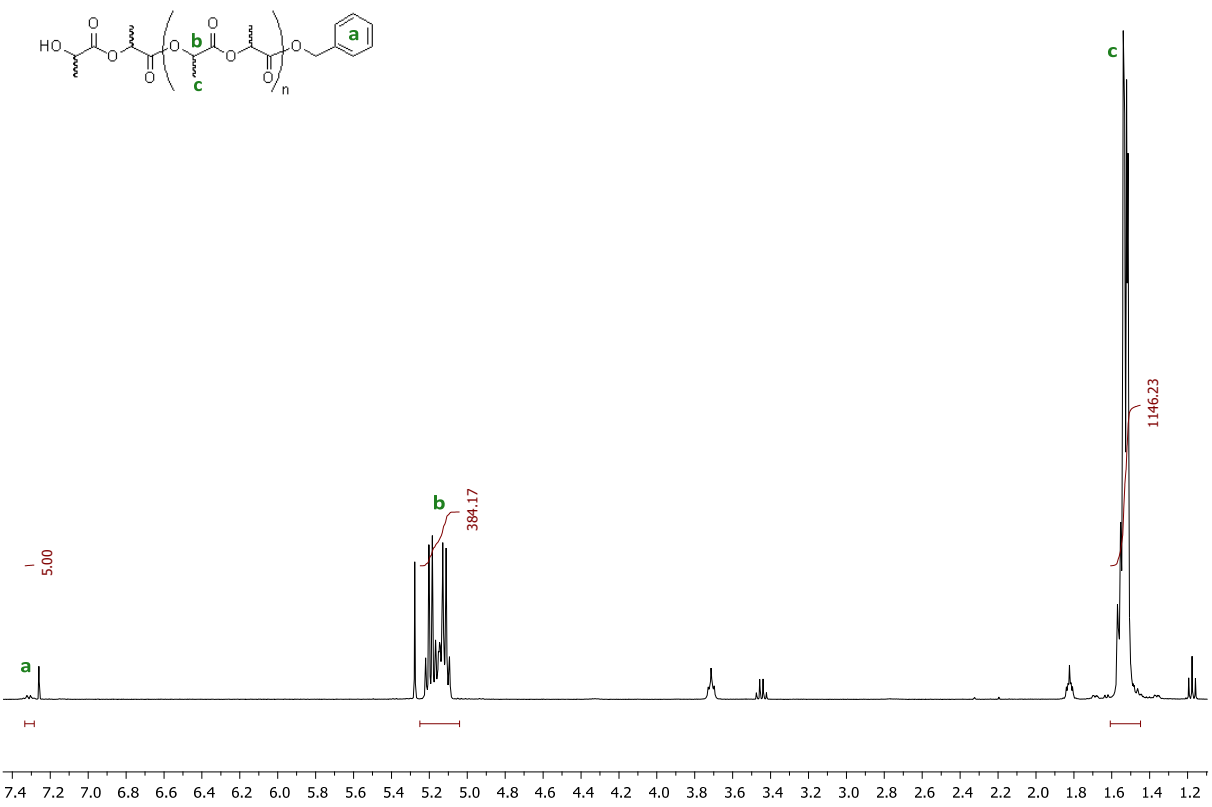

Fig. S30. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PLA obtained using complex **2** activated by BnOH; [LA]/[**2**] = 200 (Table 1, run 4)

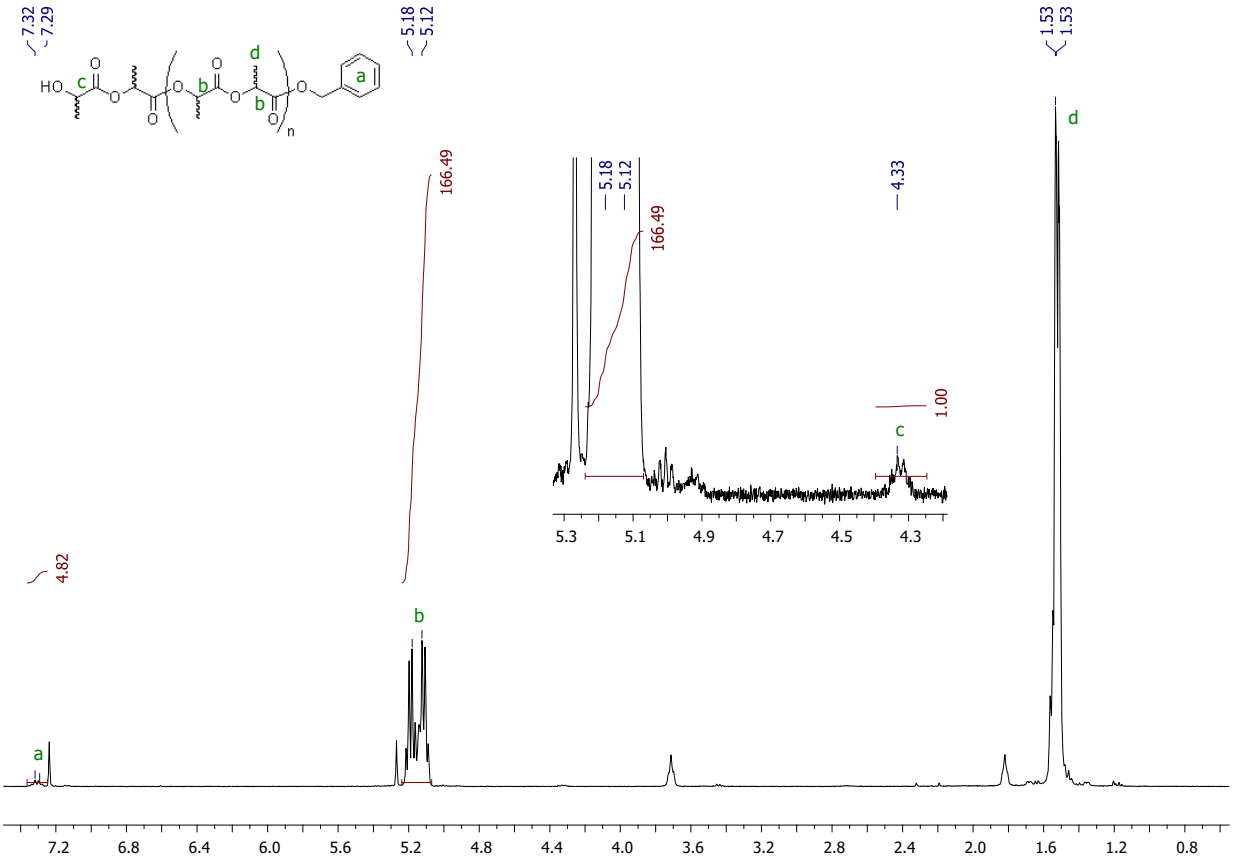

Fig. S31. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PLA obtained using complex **3** (Table 1, run 8)

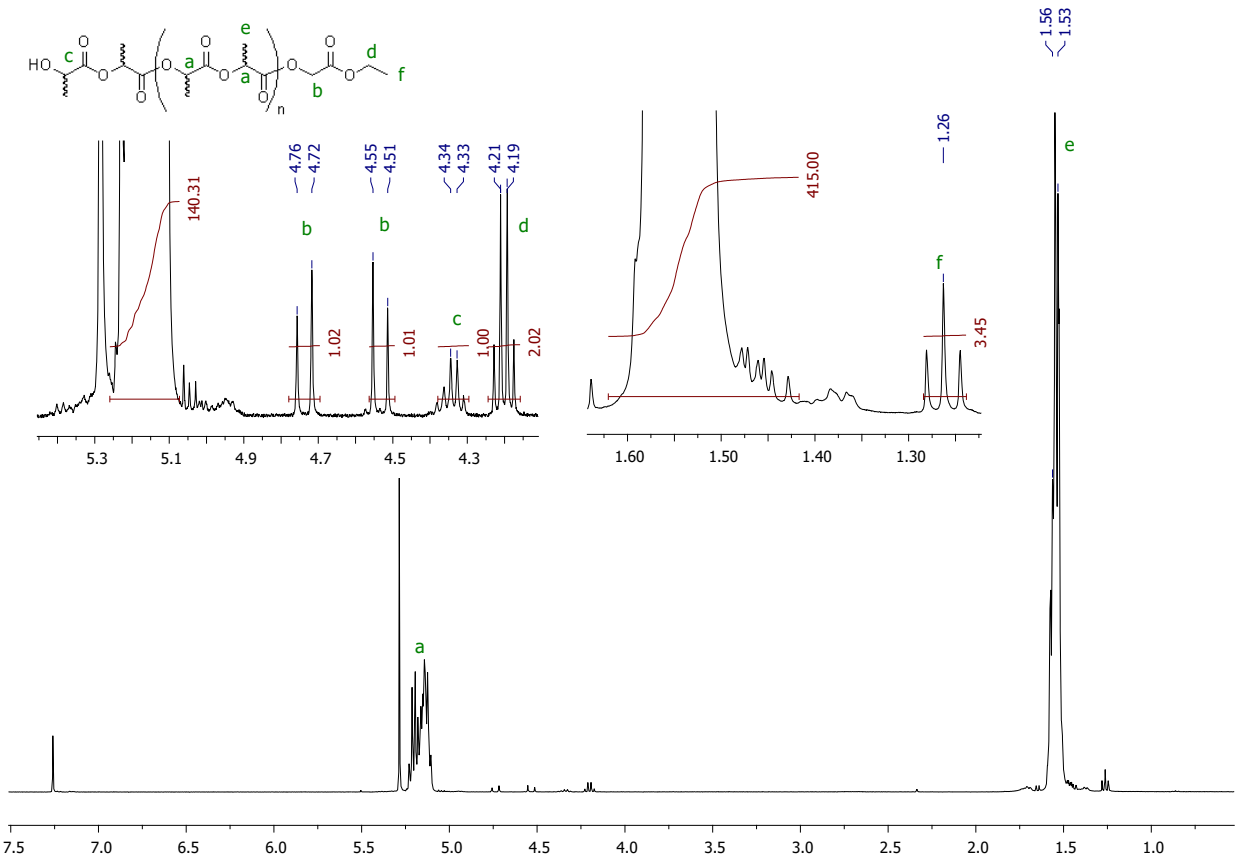

Fig. S32. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PLA obtained using complex **5** (Table 1, run 10)

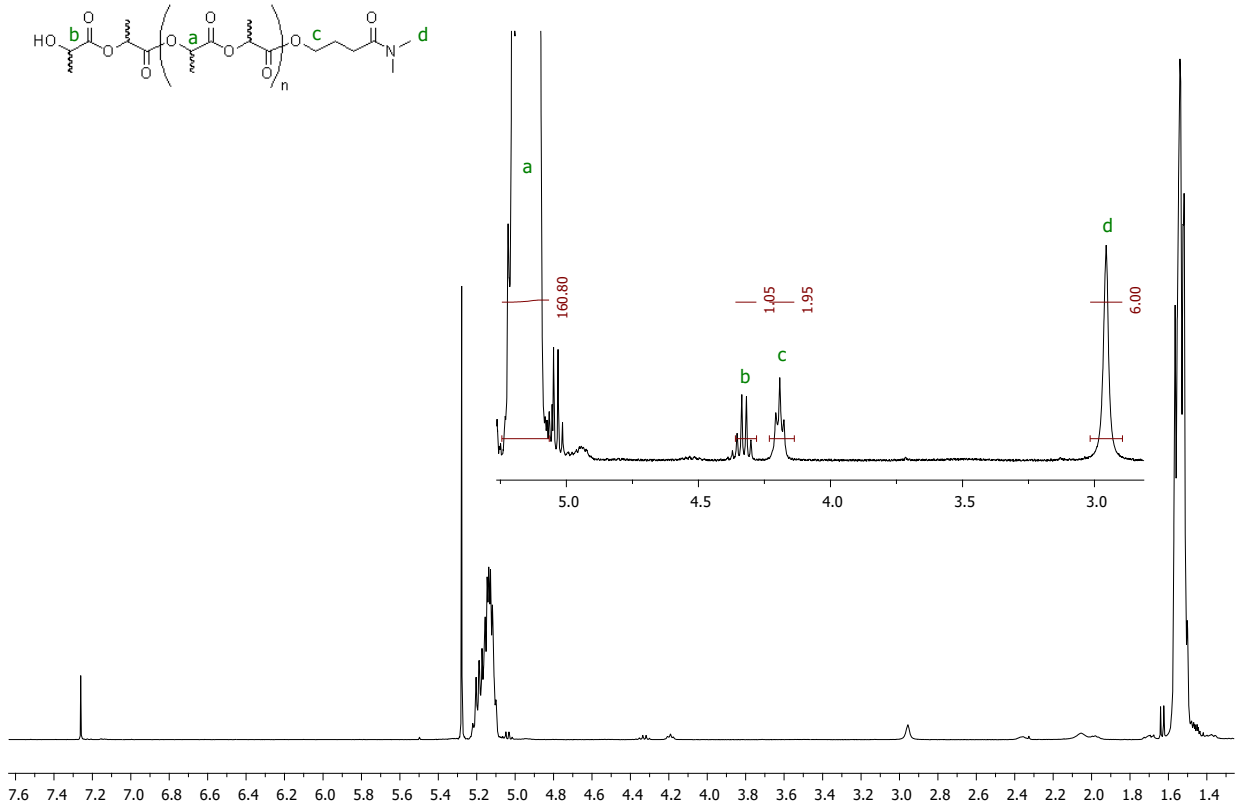

Fig. S33. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PLA obtained using complex **7** (Table , run 11)

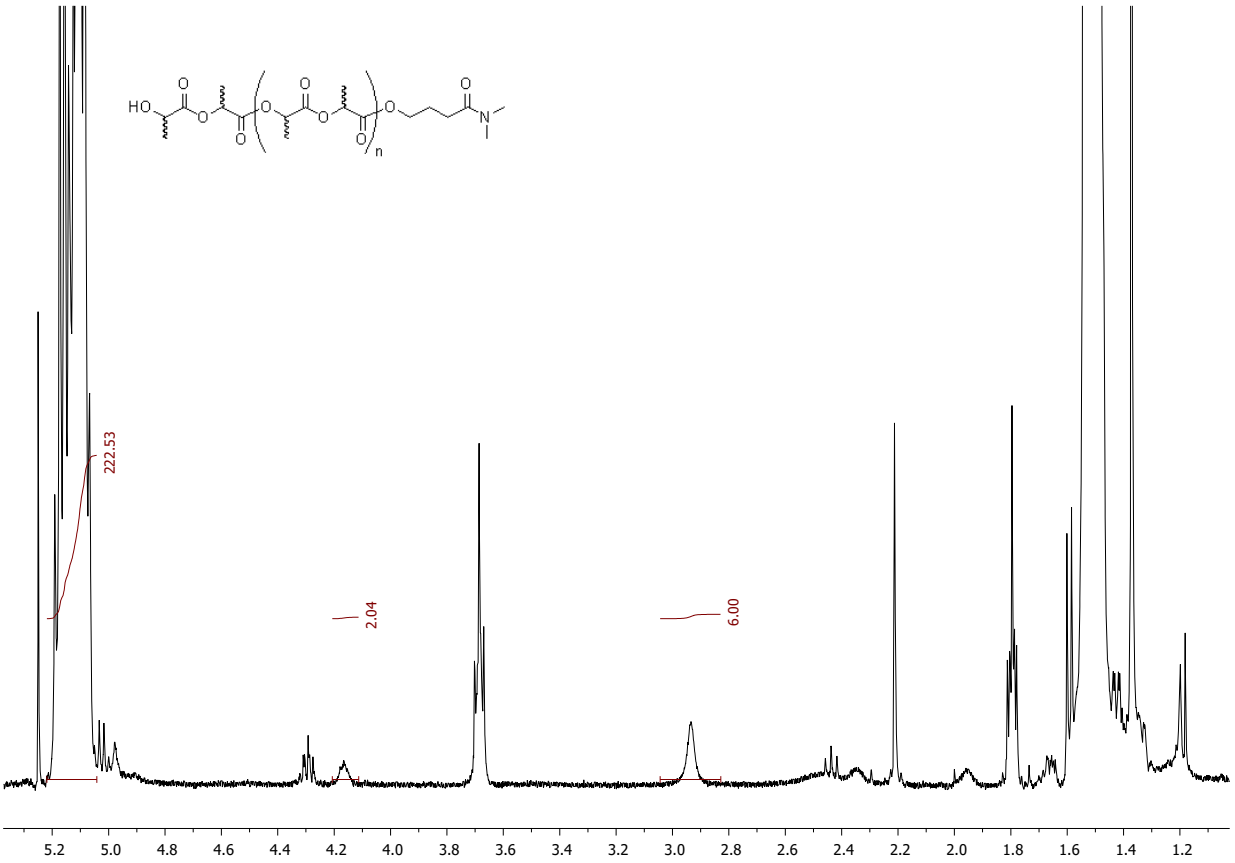

Fig. S34. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PLA obtained using complex **7** (Table 1, run 12)

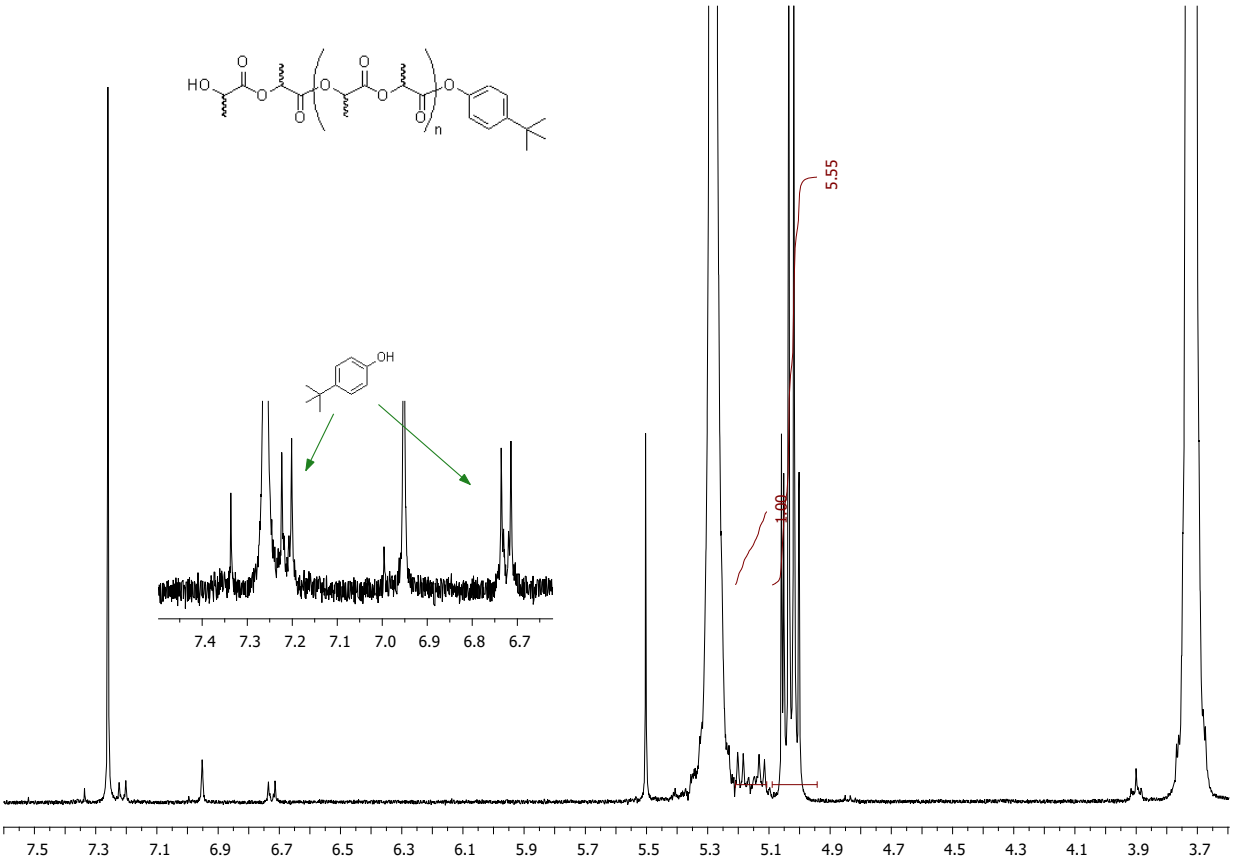

Fig. S35. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of hydrolized and dried reaction mixture of rac-LA polymerization using complex **4** (Table 1, run 13)

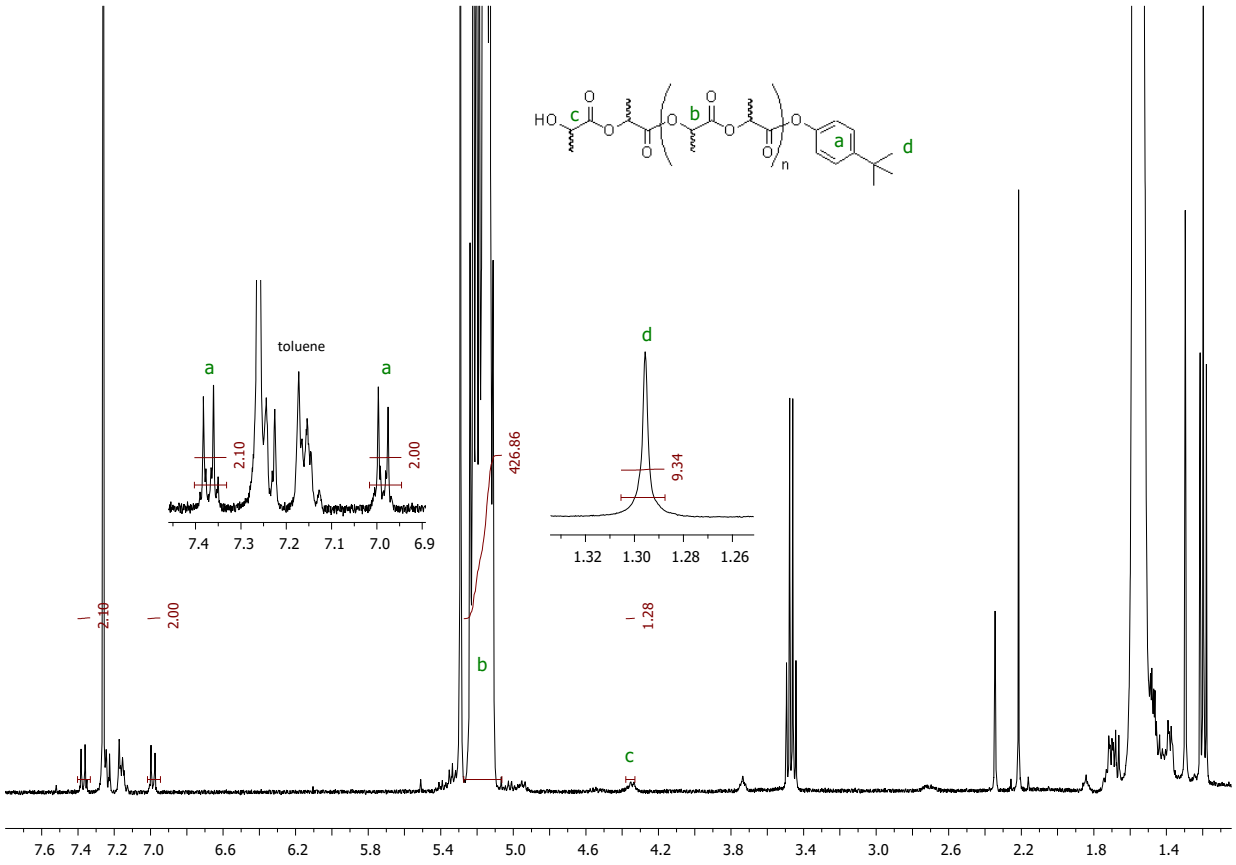

Fig. S36. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 20 °C) of PLA obtained using complex 4 (Table 1, run 14)

S5. DFT computational details

Structures of stationary points and transition states were optimized using density functional theory (DFT). The Gaussian 09 program was used for all single-point calculations. The B3PW91 hybrid functional and DGTZVP basis set[1,2] were used in the optimizations. The advantages of the B3PW91 functional as opposed to traditional B3LYP are examined elsewhere.[3,4] The B3PW91 functional has been used to successfully model ROP.[5–9] The ease and high efficiency of the DGTZVP basis set for systems not containing transition metals have also been demonstrated in a few publications.[10–12]

References

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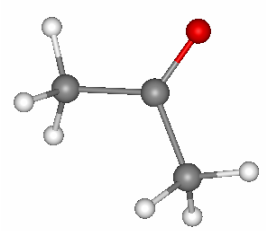
S5.1. Dimer-monomer equilibria

acetone

Zero-point vibrational energy	220907.2 (Joules/Mol)
	52.79808 (Kcal/Mol)
Zero-point correction =	0.084139 (Hartree/Particle)
Thermal correction to Energy =	0.089488
Thermal correction to Enthalpy =	0.090432
Thermal correction to Gibbs Free Energy =	0.056122
Sum of electronic and zero-point Energies =	-193.020725
Sum of electronic and thermal Energies =	-193.015376
Sum of electronic and thermal Enthalpies =	-193.014432
Sum of electronic and thermal Free Energies =	-193.048742



cartesian

6	0.00000000	0.18179999	0.00000000
8	0.00000000	1.40050006	0.00000000

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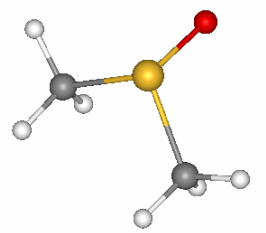
6	1.28840005	-0.61350000	-0.00270000
1	1.27429998	-1.38259995	-0.78189999
1	2.14059997	0.05080000	-0.14970000
1	1.40030003	-1.13450003	0.95510000
1	-1.27429998	-1.38259995	0.78200001
1	-2.14059997	0.05080000	0.14960000
1	-1.40030003	-1.13450003	-0.95510000

DMSO

Zero-point vibrational energy	209444.1 (Joules/Mol)
	50.05834 (Kcal/Mol)
Zero-point correction =	0.079773 (Hartree/Particle)
Thermal correction to Energy =	0.085437
Thermal correction to Enthalpy =	0.086381
Thermal correction to Gibbs Free Energy =	0.051413
Sum of electronic and zero-point Energies =	-552.992755
Sum of electronic and thermal Energies =	-552.987091
Sum of electronic and thermal Enthalpies =	-552.986147
Sum of electronic and thermal Free Energies =	-553.021115



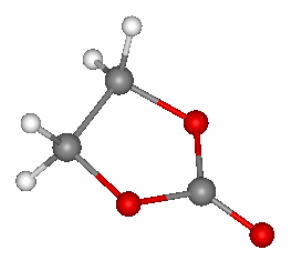
cartesian

16	0.00000000	0.23289999	-0.44769999
8	0.00000000	1.49189997	0.38970000

6	-1.35930002	-0.80820000	0.18460000
6	1.35930002	-0.80809999	0.18460000
1	-1.34590006	-1.78980005	-0.29629999
1	-1.26359999	-0.90060002	1.26929998
1	-2.28970003	-0.29150000	-0.05800000
1	1.34599996	-1.78970003	-0.29640001
1	2.28970003	-0.29130000	-0.05800000
1	1.26359999	-0.90060002	1.26929998

EC

Zero-point vibrational energy	198817.5 (Joules/Mol)
	47.51853 (Kcal/Mol)
Zero-point correction =	0.075726 (Hartree/Particle)
Thermal correction to Energy =	0.080569
Thermal correction to Enthalpy =	0.081513
Thermal correction to Gibbs Free Energy =	0.047263
Sum of electronic and zero-point Energies =	-342.245620
Sum of electronic and thermal Energies =	-342.240777
Sum of electronic and thermal Enthalpies =	-342.239833
Sum of electronic and thermal Free Energies =	-342.274082



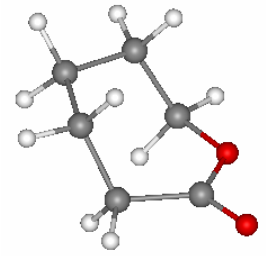
cartesian

6	0.84740001	0.00000000	-0.00010000
8	2.04349995	0.00000000	0.00000000

6	-1.29830003	-0.75580001	0.11230000
6	-1.29830003	0.75580001	-0.11230000
8	0.07100000	1.11220002	0.10100000
8	0.07100000	-1.11220002	-0.10100000
1	-1.91750002	1.30429995	0.59820002
1	-1.57749999	1.03170002	-1.13360000
1	-1.91750002	-1.30429995	-0.59820002
1	-1.57749999	-1.03170002	1.13360000

εCL

Zero-point vibrational energy	413924.6 (Joules/Mol)
	98.93035 (Kcal/Mol)
Zero-point correction =	0.157656 (Hartree/Particle)
Thermal correction to Energy =	0.164853
Thermal correction to Enthalpy =	0.165798
Thermal correction to Gibbs Free Energy =	0.126149
Sum of electronic and zero-point Energies =	-384.860246
Sum of electronic and thermal Energies =	-384.853048
Sum of electronic and thermal Enthalpies =	-384.852104
Sum of electronic and thermal Free Energies =	-384.891753



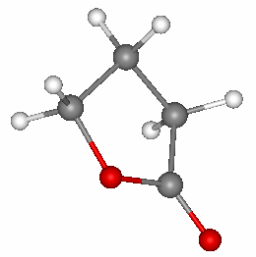
cartesian

8	-2.49640012	0.09650000	-0.41440001
6	-1.36909997	-0.02400000	0.01080000
8	-0.77679998	-1.24290001	-0.07160000
6	-0.58899999	1.13250005	0.60570002
6	0.55019999	-1.48150003	0.42449999
6	0.62889999	1.55929995	-0.23090000

6	1.64820004	-0.79979998	-0.38229999
1	0.65160000	-2.56620002	0.35339999
1	0.88940001	2.58470011	0.05370000
1	0.34410000	1.60000002	-1.28910005
1	-0.27320001	0.89160001	1.62860000
1	-1.30460000	1.95330000	0.67290002
6	1.86199999	0.67570001	-0.04630000
1	0.60909998	-1.21550000	1.48740005
1	1.42149997	-0.92960000	-1.44739997
1	2.58159995	-1.34459996	-0.19520000
1	2.20040011	0.75480002	0.99610001
1	2.67910004	1.06920004	-0.66170001

γBL

Zero-point vibrational energy	260676.4 (Joules/Mol)
	62.30315 (Kcal/Mol)
Zero-point correction =	0.099286 (Hartree/Particle)
Thermal correction to Energy =	0.104429
Thermal correction to Enthalpy =	0.105373
Thermal correction to Gibbs Free Energy =	0.070647
Sum of electronic and zero-point Energies =	-306.319710
Sum of electronic and thermal Energies =	-306.314568
Sum of electronic and thermal Enthalpies =	-306.313623
Sum of electronic and thermal Free Energies =	-306.348349

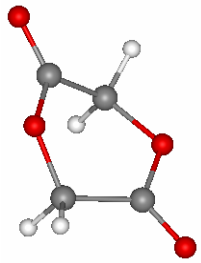


cartesian

6	0.88450003	-0.00260000	0.00300000
8	2.08690000	-0.02840000	-0.06870000
6	-1.26789999	-0.81800002	0.12690000
6	-1.40330005	0.66880000	-0.21420000
6	-0.02570000	1.20459998	0.16419999
8	0.12560000	-1.13399994	-0.04630000
1	-2.22779989	1.14240003	0.32319999
1	-1.57959998	0.79519999	-1.28639996
1	-1.83870006	-1.47800004	-0.52829999
1	-1.53989995	-1.02950001	1.16700006
1	0.33640000	2.03160000	-0.44740000
1	0.02450000	1.52020001	1.21229994

GL

Zero-point vibrational energy	223402.9 (Joules/Mol)
	53.39458 (Kcal/Mol)
Zero-point correction =	0.085090 (Hartree/Particle)
Thermal correction to Energy =	0.091684
Thermal correction to Enthalpy =	0.092628
Thermal correction to Gibbs Free Energy =	0.053775
Sum of electronic and zero-point Energies =	-455.526659
Sum of electronic and thermal Energies =	-455.520065
Sum of electronic and thermal Enthalpies =	-455.519121
Sum of electronic and thermal Free Energies =	-455.557974

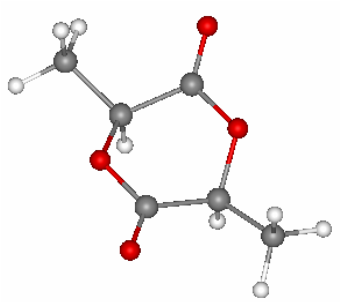


cartesian

8	-2.60920000	-0.01240000	-0.26240000
6	-1.42499995	-0.04330000	-0.04590000
6	-0.62419999	1.18149996	0.35299999
8	-0.72060001	-1.19299996	-0.14139999
8	0.72060001	1.19299996	-0.14139999
1	-1.11240005	2.06220007	-0.05880000
1	-0.61979997	1.26900005	1.44649994
6	0.62419999	-1.18149996	0.35299999
1	1.11240005	-2.06220007	-0.05880000
1	0.61979997	-1.26900005	1.44649994
6	1.42499995	0.04330000	-0.04590000
8	2.60920000	0.01240000	-0.26240000

LA

Zero-point vibrational energy	370616.7 (Joules/Mol)
	88.57951 (Kcal/Mol)
Zero-point correction =	0.141160 (Hartree/Particle)
Thermal correction to Energy =	0.150579
Thermal correction to Enthalpy =	0.151523
Thermal correction to Gibbs Free Energy =	0.106579
Sum of electronic and zero-point Energies =	-534.087278
Sum of electronic and thermal Energies =	-534.077859
Sum of electronic and thermal Enthalpies =	-534.076915
Sum of electronic and thermal Free Energies =	-534.121860

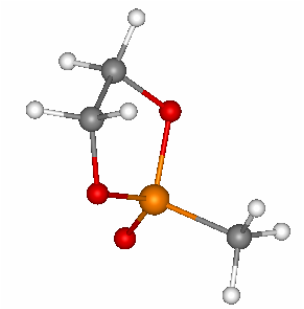


cartesian

8	-0.25319999	-1.35280001	-0.11950000
6	-1.25360000	-0.46730000	0.42940000
6	1.03890002	-0.96079999	-0.06110000
6	-1.03890002	0.96079999	-0.06120000
6	-2.61220002	-1.01740003	0.05490000
1	-1.14269996	-0.46180001	1.52359998
6	1.25360000	0.46730000	0.42940000
6	2.61220002	1.01740003	0.05500000
8	0.25319999	1.35270000	-0.11990000
1	-3.39499998	-0.39100000	0.48490000
1	-2.73480010	-1.02769995	-1.02980006
1	-2.71370006	-2.03559995	0.43599999
1	1.14250004	0.46200001	1.52349997
1	2.71329999	2.03600001	0.43540001
1	3.39499998	0.39160001	0.48590001
1	2.73539996	1.02680004	-1.02960002
8	1.92960000	-1.71019995	-0.37459999
8	-1.92960000	1.71029997	-0.37439999

Me-EP

Zero-point vibrational energy	287807.8 (Joules/Mol)
	68.78771 (Kcal/Mol)
Zero-point correction =	0.109620 (Hartree/Particle)
Thermal correction to Energy =	0.116957
Thermal correction to Enthalpy =	0.117901
Thermal correction to Gibbs Free Energy =	0.077871
Sum of electronic and zero-point Energies =	-685.352731
Sum of electronic and thermal Energies =	-685.345394
Sum of electronic and thermal Enthalpies =	-685.344450
Sum of electronic and thermal Free Energies =	-685.384481

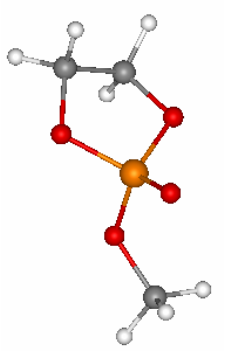


cartesian

8	1.41040003	-1.30190003	-0.64300001
15	0.64749998	-0.17100000	-0.08290000
8	-0.42829999	-0.48490000	1.11259997
8	-0.43070000	0.51480001	-1.10640001
6	-1.76520002	-0.44520000	0.58840001
6	-1.72940004	0.62010002	-0.50669998
1	-2.44099998	-0.19020000	1.40620005
1	-2.02710009	-1.43009996	0.18870001
1	-2.47790003	0.45269999	-1.28330004
1	-1.85220003	1.62720001	-0.09270000
6	1.66450000	1.16059995	0.58109999
1	1.05139995	1.99360001	0.92940003
1	2.25650001	0.77079999	1.41209996
1	2.34680009	1.50279999	-0.19949999

MeO-EP

Zero-point vibrational energy	303039.1 (Joules/Mol)
	72.42807 (Kcal/Mol)
Zero-point correction =	0.115421 (Hartree/Particle)
Thermal correction to Energy =	0.123826
Thermal correction to Enthalpy =	0.124770
Thermal correction to Gibbs Free Energy =	0.081434
Sum of electronic and zero-point Energies =	-760.559526
Sum of electronic and thermal Energies =	-760.551121
Sum of electronic and thermal Enthalpies =	-760.550177
Sum of electronic and thermal Free Energies =	-760.593513

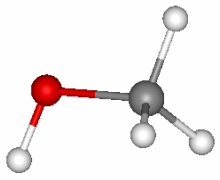


cartesian

8	0.93059999	1.58990002	0.62379998
15	0.25729999	0.39850000	0.08710000
8	-0.86940002	0.55760002	-1.06250000
8	-0.66130000	-0.41049999	1.15660000
6	-2.14350009	0.07260000	-0.60549998
6	-1.82290006	-0.93699998	0.49759999
1	-2.65860009	-0.37770000	-1.45519996
1	-2.72410011	0.91829997	-0.22520000
1	-2.62039995	-1.02370000	1.23679996
1	-1.58969998	-1.92509997	0.08710000
8	1.23060000	-0.67760003	-0.59359998
6	2.60759997	-0.75199997	-0.17450000
1	3.03449988	0.24820000	-0.08320000
1	2.68109989	-1.27820003	0.78079998
1	3.12719989	-1.31700003	-0.94819999

MEOH

Zero-point vibrational energy	135678.3 (Joules/Mol)
	32.42789 (Kcal/Mol)
Zero-point correction =	0.051677 (Hartree/Particle)
Thermal correction to Energy =	0.054980
Thermal correction to Enthalpy =	0.055924
Thermal correction to Gibbs Free Energy =	0.028947
Sum of electronic and zero-point Energies =	-115.642665
Sum of electronic and thermal Energies =	-115.639363
Sum of electronic and thermal Enthalpies =	-115.638418
Sum of electronic and thermal Free Energies =	-115.665396



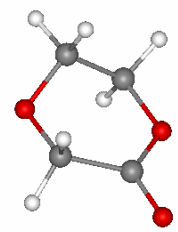
cartesian

8	-0.74860001	0.12270000	0.00000000
6	0.66500002	-0.02020000	0.00000000
1	-1.14289999	-0.75959998	0.00000000
1	1.02989995	-0.54460001	0.89349997
1	1.02989995	-0.54460001	-0.89349997
1	1.08179998	0.98820001	0.00000000

PDO

Zero-point vibrational energy	273656.0 (Joules/Mol)
	65.40535 (Kcal/Mol)
Zero-point correction =	0.104230 (Hartree/Particle)

Thermal correction to Energy =	0.110202
Thermal correction to Enthalpy =	0.111146
Thermal correction to Gibbs Free Energy =	0.074192
Sum of electronic and zero-point Energies =	-381.495816
Sum of electronic and thermal Energies =	-381.489845
Sum of electronic and thermal Enthalpies =	-381.488900
Sum of electronic and thermal Free Energies =	-381.525854

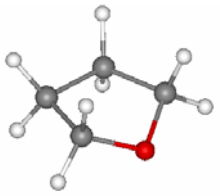


cartesian

8	2.29920006	-0.07070000	0.07390000
6	1.09300005	-0.05790000	0.00150000
6	0.32300001	1.25660002	-0.00070000
8	0.40160000	-1.21829998	-0.01190000
8	-1.05509996	1.17830002	-0.30860001
1	0.47880000	1.70570004	0.99220002
1	0.78960001	1.91209996	-0.73740000
6	-1.03040004	-1.20200002	-0.17749999
1	-1.40040004	-2.08119988	0.35519999
1	-1.24790001	-1.31420004	-1.24440002
6	-1.64510000	0.07230000	0.34999999
1	-1.51569998	0.15170000	1.44079995
1	-2.71409988	0.09690000	0.12580000

THF

Zero-point vibrational energy	309187.0 (Joules/Mol)
	73.89748 (Kcal/Mol)
Zero-point correction =	0.117763 (Hartree/Particle)
Thermal correction to Energy =	0.122713
Thermal correction to Enthalpy =	0.123657
Thermal correction to Gibbs Free Energy =	0.088546
Sum of electronic and zero-point Energies =	-232.274927
Sum of electronic and thermal Energies =	-232.269977
Sum of electronic and thermal Enthalpies =	-232.269033
Sum of electronic and thermal Free Energies =	-232.304144

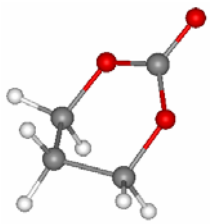


cartesian

6	1.12849998	-0.47139999	0.16010000
6	0.77840000	1.00950003	-0.05590000
8	-0.00350000	-1.20439994	-0.29100001
6	-1.13419998	-0.46360001	0.15109999
6	-0.76880002	1.01800001	-0.04390000
1	1.15939999	1.35979998	-1.01859999
1	1.21080005	1.64559996	0.72119999
1	-1.18030000	1.64250004	0.75379997
1	-1.16170001	1.39419997	-0.99180001
1	-1.33249998	-0.68030000	1.21270001
1	-1.99640000	-0.79040003	-0.43470001
1	1.30949998	-0.67860001	1.22689998
1	1.99570000	-0.81230003	-0.41010001

TMC

Zero-point vibrational energy	274569.8 (Joules/Mol)
	65.62376 (Kcal/Mol)
Zero-point correction =	0.104578 (Hartree/Particle)
Thermal correction to Energy =	0.110556
Thermal correction to Enthalpy =	0.111500
Thermal correction to Gibbs Free Energy =	0.074294
Sum of electronic and zero-point Energies =	-381.513681
Sum of electronic and thermal Energies =	-381.507703
Sum of electronic and thermal Enthalpies =	-381.506759
Sum of electronic and thermal Free Energies =	-381.543965

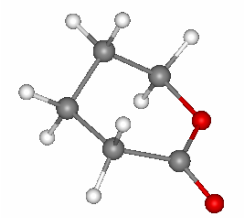


cartesian

8	2.29760003	0.00000000	-0.10490000
6	1.09909999	0.00000000	-0.01170000
8	0.41470000	-1.16600001	0.02670000
8	0.41470000	1.16600001	0.02670000
6	-1.01129997	-1.21710002	0.20530000
6	-1.01129997	1.21710002	0.20530000
1	-1.21870005	-1.29299998	1.27919996
1	-1.32550001	-2.14700007	-0.27169999
1	-1.32550001	2.14700007	-0.27169999
1	-1.21879995	1.29299998	1.27919996
6	-1.67850006	0.00000000	-0.39280000
1	-1.56910002	0.00000000	-1.48210001
1	-2.74729991	0.00000000	-0.15830000

δVL

Zero-point vibrational energy	337200.1 (Joules/Mol)
	80.59275 (Kcal/Mol)
Zero-point correction =	0.128433 (Hartree/Particle)
Thermal correction to Energy =	0.134656
Thermal correction to Enthalpy =	0.135600
Thermal correction to Gibbs Free Energy =	0.098132
Sum of electronic and zero-point Energies =	-345.589277
Sum of electronic and thermal Energies =	-345.583053
Sum of electronic and thermal Enthalpies =	-345.582109
Sum of electronic and thermal Free Energies =	-345.619577

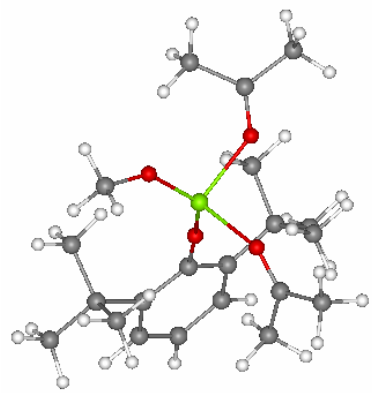


cartesian

8	-2.34209991	-0.03170000	0.00840000
6	-1.13230002	-0.01430000	-0.01190000
6	-0.34570000	1.28170002	-0.10550000
8	-0.46320000	-1.19430006	-0.03510000
6	1.12699997	1.19490004	0.28650001
1	-0.43520001	1.59150004	-1.15429997
1	-0.89349997	2.02539992	0.47729999
6	0.96149999	-1.27370000	0.17399999
1	1.22520006	1.15419996	1.37829995
1	1.65799999	2.09299994	-0.04460000
1	1.26779997	-2.18959999	-0.33570001
1	1.12679994	-1.41369998	1.24919999
6	1.72780001	-0.06450000	-0.32460001
1	1.68200004	-0.01560000	-1.41929996
1	2.78110003	-0.18300000	-0.04810000

I-1__DBP_Mg_OMe_acetone-2

Zero-point vibrational energy	1399836.6 (Joules/Mol)
	334.56898 (Kcal/Mol)
Zero-point correction =	0.533170 (Hartree/Particle)
Thermal correction to Energy =	0.568238
Thermal correction to Enthalpy =	0.569182
Thermal correction to Gibbs Free Energy =	0.464027
Sum of electronic and zero-point Energies =	-1322.113028
Sum of electronic and thermal Energies =	-1322.077960
Sum of electronic and thermal Enthalpies =	-1322.077015
Sum of electronic and thermal Free Energies =	-1322.182171



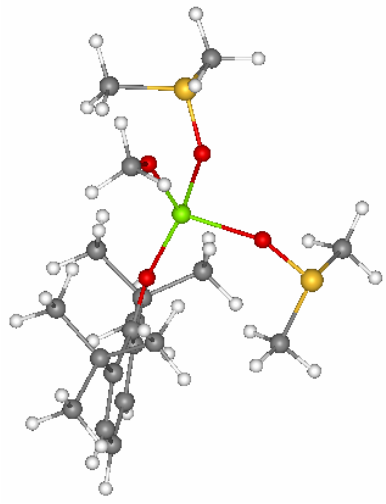
cartesian

12	-1.44615805	-0.75118232	0.05175648
8	-2.32105803	-2.20968223	0.79075646
8	0.26974201	-0.01658229	0.25075647
6	-2.33615804	-3.59368229	0.88325649
1	-2.64405799	-4.07858229	-0.06154353
1	-3.04835796	-3.93728232	1.65505648
6	1.55334198	0.31691772	0.27705649
6	1.93334198	1.69541776	0.17145647
6	3.29394197	2.01211786	0.11595647
1	3.60504198	3.04731774	0.02225647
6	4.28214216	1.03601778	0.18455647
6	3.90744209	-0.29308230	0.34805647
1	4.69274235	-1.03628230	0.43445647
6	2.56714201	-0.68758231	0.41195646
6	0.88324201	2.82361770	0.16165647
6	2.21984196	-2.16818213	0.66435647
6	0.04604200	2.76401782	1.45565653
1	-0.44125801	1.79461777	1.56615651
1	-0.72345799	3.54671764	1.45065653
1	0.68624198	2.92521763	2.32985640
6	-0.03445799	2.72291780	-1.07254350
1	-0.58175802	1.78071773	-1.08584356
1	0.55464196	2.79881763	-1.99404347

1	-0.76565802	3.54111767	-1.07354355
6	1.52524197	4.22141743	0.11435647
1	2.10724211	4.38131762	-0.79984355
1	2.17704201	4.40781736	0.97415650
1	0.73554200	4.98131752	0.13325648
6	3.47514200	-3.03668237	0.86655647
1	4.07344246	-2.70528221	1.72175646
1	4.12024212	-3.05548215	-0.01864353
1	3.16774201	-4.06958246	1.06495643
6	1.46894205	-2.77898216	-0.53494352
1	0.53824198	-2.25118232	-0.74964350
1	1.21854198	-3.82858229	-0.34084353
1	2.09254193	-2.74008226	-1.43554354
6	1.38444197	-2.30588222	1.95335650
1	1.94694197	-1.91898227	2.81005669
1	1.15394199	-3.35998225	2.14885664
1	0.44184202	-1.76048231	1.89675653
8	-2.83295798	0.74561769	0.48995647
1	-1.35335803	-4.01838255	1.15375650
1	5.33314228	1.31031775	0.13385648
6	-1.29385805	-0.55388230	-3.10834360
8	-1.83795798	-0.67098230	-2.00914335
6	-2.13625813	-0.52098233	-4.35184383
6	0.19224201	-0.44578227	-3.26134348
1	0.45214200	0.26621771	-4.04974365
1	0.67254198	-0.17518228	-2.32134342
1	0.57154197	-1.42488229	-3.58004332
1	-1.69075799	-1.13108230	-5.14274359
1	-3.15325809	-0.84928232	-4.13814354
1	-2.16265798	0.51001769	-4.72374344
6	-3.71215796	0.87191767	1.34795642
6	-3.83965802	-0.09078228	2.48585653
6	-4.67255783	2.02171779	1.25875652
1	-4.37365770	2.71981764	0.47705647
1	-5.67185783	1.62931776	1.03775644
1	-4.74345779	2.53321767	2.22375631
1	-3.48905802	-1.08038223	2.16165638
1	-3.17995811	0.25731772	3.29145670
1	-4.85775757	-0.11798228	2.88185644

I-1__DBP_Mg_OMe_DMSO-2

Zero-point vibrational energy	1378372.8 (Joules/Mol)
	329.43899 (Kcal/Mol)
Zero-point correction =	0.524994 (Hartree/Particle)
Thermal correction to Energy =	0.560463
Thermal correction to Enthalpy =	0.561407
Thermal correction to Gibbs Free Energy =	0.457008
Sum of electronic and zero-point Energies =	-2042.084316
Sum of electronic and thermal Energies =	-2042.048847
Sum of electronic and thermal Enthalpies =	-2042.047903
Sum of electronic and thermal Free Energies =	-2042.152302



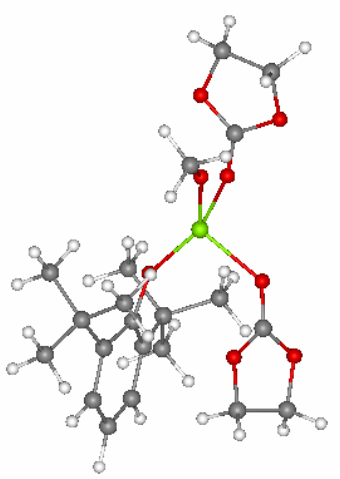
cartesian

12	-1.56345308	-0.59662908	-0.21364355
8	-2.62785292	-1.88022900	0.67675644
8	0.18904698	-0.02422909	0.23545645
6	-2.63405323	-3.26382923	0.84465647
1	-2.53245306	-3.81142926	-0.10904355
1	-3.57955313	-3.60652924	1.30335641
6	1.49064696	0.20937091	0.26015645
6	1.97634709	1.55897093	0.33155644
6	3.34944677	1.78487098	0.18945645
1	3.73354721	2.79937077	0.21015646
6	4.25754690	0.74297088	0.03375645
6	3.79264688	-0.56722909	0.09045644
1	4.52094698	-1.36972904	0.03585646
6	2.43464708	-0.87212908	0.22975646
6	1.03314698	2.74417090	0.62075645
6	1.99754703	-2.33982921	0.41115642
6	0.25924695	2.48097086	1.92895639
1	-0.31755301	1.55747092	1.86415637
1	-0.42635304	3.31177092	2.14005661
1	0.95404696	2.39307094	2.77125645
6	0.04044697	2.97547078	-0.53314352
1	-0.60855305	2.11017084	-0.66944355
1	0.57854700	3.18287086	-1.46674359
1	-0.60245299	3.83897090	-0.32144356
6	1.79854691	4.06537104	0.81605649
1	2.32684708	4.38167095	-0.09014355
1	2.52464676	4.00527096	1.63345647
1	1.08604693	4.85897112	1.06835639
6	3.20174694	-3.28972912	0.55515647
1	3.84134722	-3.01692915	1.40095639

1	3.82144690	-3.32582927	-0.34764355
1	2.83644676	-4.30722904	0.73465645
6	1.18884695	-2.85102916	-0.79544353
1	0.30084699	-2.24832916	-0.99014354
1	0.85824692	-3.88342929	-0.63024354
1	1.80734694	-2.84362912	-1.70144355
6	1.17684698	-2.48452926	1.70935643
1	1.77854693	-2.17642927	2.57165647
1	0.88484693	-3.53092909	1.85905635
1	0.27234697	-1.87552905	1.69605649
16	-4.15365314	1.10087097	0.78145641
8	-2.84695292	0.99697089	-0.03834355
1	-1.82185304	-3.61542916	1.50325644
1	5.31894732	0.94777089	-0.08454355
16	-0.96405303	-0.30902910	-3.54604340
8	-1.59235299	-0.83752912	-2.24844337
6	-5.20705271	-0.25022912	0.19725646
6	-3.76925325	0.43667090	2.42015648
6	-1.65905297	1.34767091	-3.77944350
6	0.74154699	0.16247091	-3.17054343
1	-6.09685278	-0.30092907	0.83095646
1	-5.49755287	-0.00772909	-0.82654357
1	-4.60435295	-1.16632903	0.24295644
1	-4.68965292	0.41597092	3.01055646
1	-3.34335279	-0.56472909	2.28045654
1	-3.05345297	1.12017095	2.88015652
1	0.77494693	0.84767091	-2.32314348
1	1.28194702	-0.75082910	-2.92164350
1	1.17454696	0.61457092	-4.06744337
1	-1.17815304	1.81477094	-4.64254379
1	-2.72445297	1.21907091	-3.97594333
1	-1.51035297	1.94167089	-2.87654352

I-1__DBP_Mg_OMe_EC-2

Zero-point vibrational energy	1355512.8 (Joules/Mol)
	323.97533 (Kcal/Mol)
Zero-point correction =	0.516288 (Hartree/Particle)
Thermal correction to Energy =	0.550738
Thermal correction to Enthalpy =	0.551682
Thermal correction to Gibbs Free Energy =	0.446670
Sum of electronic and zero-point Energies =	-1620.558358
Sum of electronic and thermal Energies =	-1620.523907
Sum of electronic and thermal Enthalpies =	-1620.522963
Sum of electronic and thermal Free Energies =	-1620.627976



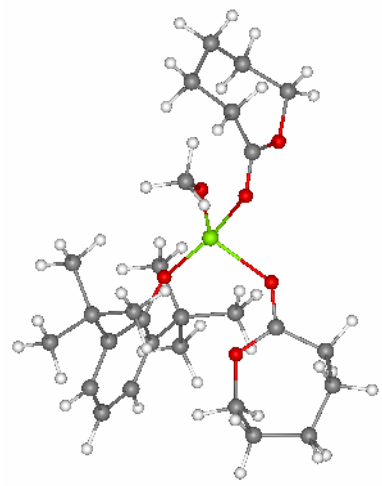
cartesian

12	1.60279357	0.05713393	-0.39049363
8	3.06319356	1.20323384	-0.62749362
8	0.02249354	0.06053393	0.64860636
6	3.43229365	2.48613405	-1.00409365
1	2.57319355	3.16093397	-1.16059363
1	4.00589371	2.49193406	-1.95039368
6	-1.29990649	0.02813393	0.68270636
6	-1.98800635	-1.21006608	0.92010635
6	-3.37960649	-1.23536611	0.76890635
1	-3.92020631	-2.16546607	0.91230637
6	-4.11350632	-0.09086607	0.46630633
6	-3.44960642	1.13213384	0.38980633
1	-4.04420662	2.02663398	0.23490635
6	-2.06130648	1.23483384	0.52250636
6	-1.24650645	-2.47096610	1.41280627
6	-1.39400649	2.62483406	0.55770636
6	-0.41210645	-2.12376595	2.66360641
1	0.32889354	-1.35346615	2.44850636
1	0.11029354	-3.01666594	3.02780652
1	-1.06130648	-1.76076615	3.46810651
6	-0.33520645	-3.07106590	0.32770634
1	0.45239353	-2.38256598	0.02510636
1	-0.91190648	-3.34756589	-0.56189364
1	0.15399353	-3.97906590	0.70070636
6	-2.22420645	-3.58556604	1.82970643
1	-2.80840635	-3.97126603	0.98640639
1	-2.92000651	-3.25556612	2.60820651
1	-1.65330648	-4.42846584	2.23500633
6	-2.43420649	3.76043391	0.58530635
1	-3.11990643	3.67183399	1.43450642
1	-3.02820635	3.80863404	-0.33429366
1	-1.91470647	4.72013378	0.68210638
6	-0.51340646	2.87953401	-0.67949367
1	0.33759353	2.19863391	-0.73239362
1	-0.10690647	3.89763403	-0.65069366
1	-1.08940649	2.77043390	-1.60349369
6	-0.55120647	2.76673388	1.84230638
1	-1.18800652	2.67403388	2.72890639
1	-0.07190648	3.75283408	1.87260652
1	0.22489354	2.00283408	1.90060639

6	4.11119366	-1.02066612	0.19080636
8	2.95239353	-1.40856612	0.24210635
1	4.06879330	2.97133398	-0.24079365
1	-5.19470692	-0.14016607	0.35880637
6	6.07169342	-0.36276609	-0.67739367
6	6.10659313	-0.19186607	0.84340638
8	4.76429367	-0.52066606	1.23860645
8	4.88999367	-1.15316606	-0.88299364
1	6.31409359	0.82983392	1.15960646
1	6.78609371	-0.88576609	1.34430647
1	6.92389393	-0.90936607	-1.08089364
1	5.93409348	0.58243394	-1.20469356
6	-0.28100646	-0.85046607	-2.59799361
8	0.85659355	-0.76936609	-2.16779375
6	-2.14550638	-1.72246611	-3.53169370
6	-2.44420648	-0.33236608	-2.96769357
8	-1.12420642	0.17323391	-2.67229366
8	-0.80620646	-1.98396611	-3.06349349
1	-3.00880647	-0.35086608	-2.03269362
1	-2.91090655	0.34283394	-3.68419361
1	-2.13240647	-1.75856614	-4.62369394
1	-2.79850650	-2.50026608	-3.13789368

I-1__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1784683.0 (Joules/Mol)
	426.54948 (Kcal/Mol)
Zero-point correction =	0.679750 (Hartree/Particle)
Thermal correction to Energy =	0.719103
Thermal correction to Enthalpy =	0.720047
Thermal correction to Gibbs Free Energy =	0.604580
Sum of electronic and zero-point Energies =	-1705.797246
Sum of electronic and thermal Energies =	-1705.757893
Sum of electronic and thermal Enthalpies =	-1705.756949
Sum of electronic and thermal Free Energies =	-1705.872416



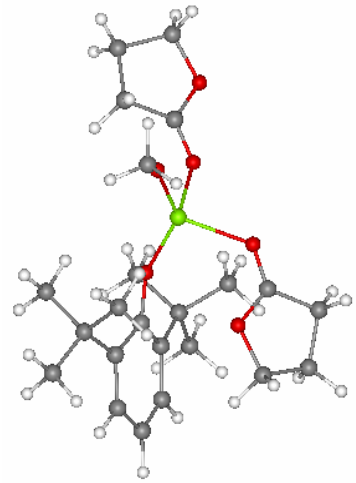
cartesian

8	-1.63320374	0.75279218	-2.54900122
6	-1.40160370	0.82269216	-3.91410136
1	-1.03700376	-0.13080782	-4.33640146
1	-0.65780371	1.59449220	-4.18610144
12	-0.80780369	0.56899220	-0.88910127
8	0.13459630	-0.89550781	-0.14480126
6	1.22249627	-1.51050782	0.28239873
6	2.20499635	-1.99840784	-0.64440125
6	3.39919639	-2.52220774	-0.13730127
1	4.16589642	-2.87290788	-0.82050127
6	3.64339638	-2.62950778	1.22909880
6	2.64119625	-2.25680780	2.12049866
1	2.82149625	-2.40140772	3.18099880
6	1.42389631	-1.72120786	1.68899870
6	1.96959639	-1.98390794	-2.16870117
6	0.32569629	-1.39340782	2.71959877
6	2.00169635	-0.54830784	-2.72600126
1	1.22779632	0.08459218	-2.29080129
1	1.84669626	-0.55240786	-3.81130123
1	2.97029638	-0.07790782	-2.52240133
6	0.62799633	-2.66250777	-2.51400137
1	-0.21590370	-2.15730786	-2.04460120
1	0.63289630	-3.70440793	-2.17460132
1	0.47189629	-2.66190791	-3.59970117
6	3.05809641	-2.76440787	-2.93000126
1	3.12749624	-3.80500793	-2.59570122
1	4.04889631	-2.30600786	-2.83710122
1	2.80979633	-2.77670789	-3.99730134
6	0.69249630	-1.87250781	4.13579845
1	1.56999624	-1.35650778	4.54119873
1	0.88229632	-2.95060778	4.16879845
1	-0.14370370	-1.66490781	4.81319857
6	-0.98840368	-2.10860777	2.34219885
1	-1.32730365	-1.81810784	1.34779871
1	-1.77440369	-1.86410785	3.06779885
1	-0.84570372	-3.19510794	2.35229874
6	0.09229630	0.12619218	2.81439877
1	1.01079631	0.63259214	3.13669872
1	-0.69010371	0.35279217	3.54929876
1	-0.22190370	0.54409218	1.85919869
8	0.18789630	2.31889224	-0.29470125
6	1.31929624	2.47839212	0.17269874
8	2.16109633	1.46659219	0.10809873
6	1.73529625	3.79649210	0.77209872
6	3.46119618	1.46709216	0.74919873
6	2.92789626	4.46169233	0.06189874
6	4.46029615	2.38929224	0.07159874
1	3.76279640	0.42199215	0.67419875
1	2.92339635	5.52069235	0.34079874

1	2.76799631	4.43219233	-1.02230132
1	1.96859622	3.64189219	1.83319879
1	0.85299629	4.43609238	0.72429872
6	4.29299641	3.86909223	0.41459873
1	3.33159637	1.70519221	1.81019878
1	4.40389633	2.22809219	-1.01120126
1	5.45969629	2.06109214	0.38019875
1	4.47169638	4.00689220	1.48959875
1	5.07019615	4.44599199	-0.09900127
8	-2.44980359	0.88429219	0.33769873
6	-3.67240381	0.92199218	0.20779873
6	-4.36730385	0.67469215	-1.10120130
8	-4.36890364	1.18019211	1.31499875
6	-5.16870356	-0.64060783	-1.11420131
1	-5.03230381	1.51969218	-1.32210124
1	-3.56980371	0.66189218	-1.85710120
6	-5.81350374	1.21099222	1.31009877
1	-4.55880356	-1.44370782	-0.68430126
1	-5.32900381	-0.91320783	-2.16200137
1	-6.16040373	1.96529222	0.59519875
1	-6.05050373	1.56709218	2.31359863
6	-6.52230358	-0.56210786	-0.40940127
1	-7.16130352	0.15109217	-0.94790125
1	-7.02310371	-1.53420782	-0.48150125
6	-6.45480347	-0.14640781	1.06049871
1	-5.91880369	-0.89490783	1.65619874
1	-7.47280359	-0.10070782	1.46559870
1	-2.32560372	1.07689226	-4.46610165
1	4.58229637	-3.04120779	1.59229875

I-1__DBP_Mg_OMe_gBL-2

Zero-point vibrational energy	1477576.0 (Joules/Mol)
	353.14913 (Kcal/Mol)
Zero-point correction =	0.562779 (Hartree/Particle)
Thermal correction to Energy =	0.598135
Thermal correction to Enthalpy =	0.599079
Thermal correction to Gibbs Free Energy =	0.491381
Sum of electronic and zero-point Energies =	-1548.710956
Sum of electronic and thermal Energies =	-1548.675600
Sum of electronic and thermal Enthalpies =	-1548.674656
Sum of electronic and thermal Free Energies =	-1548.782354



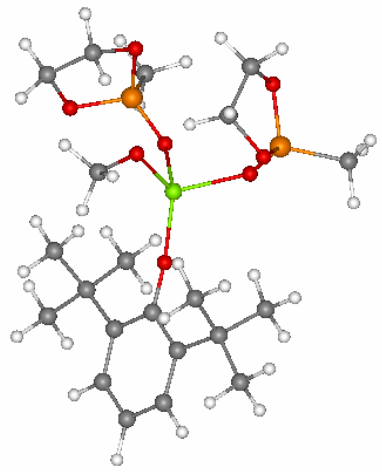
cartesian

12	1.33808494	0.45198941	-0.81619549
8	2.47228479	1.87438941	-1.21219540
8	0.00608483	0.16718940	0.50490451
6	2.51268482	3.12788939	-1.80429542
1	1.92668486	3.18588948	-2.74019551
1	3.54698467	3.41408944	-2.07149553
6	-1.26941514	0.02168941	0.82840455
6	-1.78401518	-1.27971065	1.14940464
6	-3.16631532	-1.43131065	1.30370462
1	-3.58221531	-2.41131067	1.51600456
6	-4.04191494	-0.35191059	1.22000456
6	-3.51561522	0.92758942	1.05920458
1	-4.20321512	1.76698935	1.07680464
6	-2.14551520	1.15628946	0.89600456
6	-0.85061520	-2.48551059	1.38180459
6	-1.61601520	2.60418940	0.83660460
6	0.22358483	-2.12091064	2.42780447
1	0.82298481	-1.27051055	2.10110450
1	0.88988483	-2.97551060	2.60060453
1	-0.24731517	-1.86181056	3.38250446
6	-0.17321518	-2.94461060	0.07790457
1	0.44988483	-2.16221070	-0.35259545
1	-0.92751521	-3.24261069	-0.66129541
1	0.46858484	-3.81511068	0.26150456
6	-1.60851526	-3.70461059	1.93840468
1	-2.34171534	-4.10561085	1.22950459
1	-2.12751532	-3.47351050	2.87450457
1	-0.89301521	-4.50791073	2.14780450
6	-2.71071529	3.63038945	1.18480456
1	-3.15781522	3.43918943	2.16610456
1	-3.51341534	3.65788937	0.43960455
1	-2.26711512	4.63178921	1.21460462
6	-1.10791516	2.97528934	-0.56899548
1	-0.23191518	2.39668941	-0.86489546
1	-0.81411517	4.03148937	-0.60009539
1	-1.88771534	2.81718946	-1.32089543
6	-0.48981518	2.79848933	1.87350452
1	-0.87091511	2.62818933	2.88670444
1	-0.10381517	3.82398939	1.82510459
1	0.33738482	2.10918951	1.70150459
6	4.00318480	-0.66211057	-0.03949543

8	2.86068487	-0.90791059	-0.40469542
1	2.12838483	3.92528939	-1.14279544
1	-5.11281490	-0.49791059	1.34160459
6	6.26178503	-0.97631061	0.13640457
6	5.92738485	0.16858940	1.09570456
6	4.51418495	0.56198943	0.66690457
8	4.98678493	-1.53371060	-0.27279544
1	6.64678478	0.98568940	1.01660454
1	5.93268490	-0.18771060	2.12940454
1	6.83538485	-1.78861058	0.58360457
1	6.76878500	-0.63451058	-0.77029538
6	-0.65011519	-0.70921057	-2.76569557
8	0.53018486	-0.51581061	-2.49149561
6	-2.69741511	-1.83021057	-3.18549562
6	-2.91891527	-0.38491058	-2.72779560
8	-1.60511518	0.10288940	-2.34439564
6	-1.22191525	-1.83501065	-3.58899546
1	-3.55251527	-0.28421059	-1.84679544
1	-3.28201532	0.26898941	-3.52569556
1	-3.37041521	-2.11061049	-3.99789548
1	-2.86431527	-2.51371050	-2.34999561
1	3.84488487	0.82898939	1.48640454
1	4.44528484	1.38028944	-0.06089544
1	-0.68531519	-2.76261067	-3.38969541
1	-1.07171512	-1.58091056	-4.64499569

I-1__DBP_Mg_OMe_Me-EP-2

Zero-point vibrational energy	1532763.9 (Joules/Mol)
	366.33937 (Kcal/Mol)
Zero-point correction =	0.583799 (Hartree/Particle)
Thermal correction to Energy =	0.623164
Thermal correction to Enthalpy =	0.624109
Thermal correction to Gibbs Free Energy =	0.508962
Sum of electronic and zero-point Energies =	-2306.798292
Sum of electronic and thermal Energies =	-2306.758926
Sum of electronic and thermal Enthalpies =	-2306.757982
Sum of electronic and thermal Free Energies =	-2306.873129



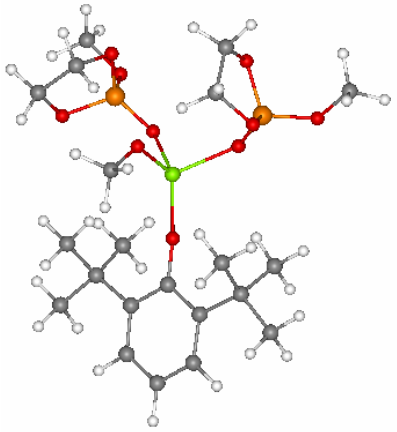
cartesian

12	0.76242131	-0.01046862	0.16538703
8	1.74462128	-0.01436862	-1.48361301
8	-1.10907876	-0.02916862	0.29968703
6	1.24842131	0.00823138	-2.79021311
1	0.17732130	0.26233137	-2.84911299
1	1.36402130	-0.96656859	-3.30051303
6	-2.42837858	-0.02806862	0.18138704
6	-3.14317870	-1.25976861	0.01308703
6	-4.53587866	-1.21826863	-0.10151297
1	-5.09357882	-2.14016867	-0.22951296
6	-5.24747849	-0.02436863	-0.05601297
6	-4.55077839	1.16773140	0.10908704
1	-5.11967850	2.09113145	0.14418703
6	-3.15857863	1.20493138	0.22918704
6	-2.41427851	-2.61526871	-0.03701296
6	-2.44337869	2.55663133	0.40698704
6	-1.66177881	-2.86176872	1.28618693
1	-0.94197869	-2.07116866	1.49688697
1	-1.12907875	-3.82226849	1.24468708
1	-2.36977863	-2.90816855	2.12138700
6	-1.44437873	-2.66236854	-1.23481297
1	-0.71927869	-1.84846866	-1.20801306
1	-1.99967873	-2.57806849	-2.17561293
1	-0.89467871	-3.61206865	-1.25071287
6	-3.38097858	-3.79926872	-0.21691296
1	-3.94577885	-3.73636866	-1.15321302
1	-4.09397840	-3.88296866	0.61038703
1	-2.80557871	-4.73196840	-0.24681297
6	-3.42507863	3.74223137	0.44358703
1	-4.12807846	3.67343140	1.28078699
1	-4.00117874	3.83413148	-0.48341298
1	-2.85937858	4.67303133	0.56868702
6	-1.49577868	2.81793141	-0.78071296
1	-0.77647877	2.00903130	-0.91561300
1	-0.93887877	3.75163150	-0.63611299
1	-2.07077861	2.90543151	-1.70951295
6	-1.67667878	2.58483148	1.74438715
1	-2.37547851	2.47893143	2.58178687
1	-1.15237868	3.54273129	1.86328697
1	-0.94647872	1.77913141	1.81178713
8	1.59952128	-1.52366865	1.25288701
15	2.57922149	-2.62246871	0.99878705
8	4.10692120	-2.10926867	0.85288703
8	2.47902131	-3.38676858	-0.41471297
6	4.63562155	-2.43236852	-0.45491296
6	3.42322135	-2.75916862	-1.32751298

1	5.31482124	-3.28286862	-0.34361297
1	5.18312120	-1.56176865	-0.81721294
1	2.95732141	-1.85106862	-1.72521305
1	3.64342141	-3.48406863	-2.11111307
6	2.50412130	-3.87376857	2.27668691
8	1.67072129	1.50173140	1.20268703
15	2.62472129	2.59623146	0.84848702
8	2.10882139	3.57193136	-0.32881296
8	4.02122116	2.16393137	0.16648704
6	2.99772143	3.52903128	-1.46961308
6	3.87092137	2.28783131	-1.27741289
1	3.57892132	4.45583153	-1.47611308
1	2.38282132	3.46593142	-2.36751294
1	3.37082148	1.38163137	-1.63821292
1	4.87122154	2.40553141	-1.69541287
6	3.03762150	3.58133149	2.28608704
1	-6.33127880	-0.02326863	-0.14621297
1	3.24182129	-4.65646839	2.09678698
1	2.69012141	-3.39886856	3.24188709
1	1.50002122	-4.30206871	2.28788686
1	3.71052146	4.39643145	2.01778698
1	2.11472130	3.98193145	2.70948696
1	3.51202130	2.93813133	3.02998686
1	1.78122127	0.74843138	-3.41911292

I-1__DBP_Mg_OMe_MeO-EP-2

Zero-point vibrational energy	1563934.1 (Joules/Mol)
	373.78921 (Kcal/Mol)
Zero-point correction =	0.595671 (Hartree/Particle)
Thermal correction to Energy =	0.636910
Thermal correction to Enthalpy =	0.637855
Thermal correction to Gibbs Free Energy =	0.518468
Sum of electronic and zero-point Energies =	-2457.201832
Sum of electronic and thermal Energies =	-2457.160592
Sum of electronic and thermal Enthalpies =	-2457.159648
Sum of electronic and thermal Free Energies =	-2457.279035



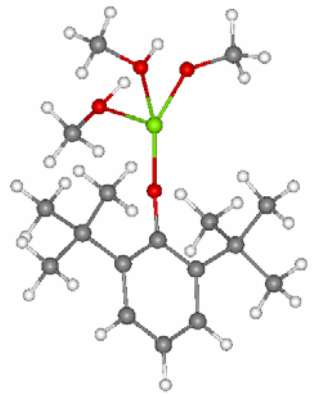
cartesian

12	0.56432343	-0.03587363	0.17754585
8	1.43602335	0.05532637	-1.53365421
8	-1.29017663	-0.05617363	0.40664583
6	0.82422340	0.04072637	-2.79235411
1	-0.26857662	0.17392637	-2.74955416
1	1.00082338	-0.90807366	-3.33295417
6	-2.61057663	-0.08647363	0.29654586
6	-3.30037642	-1.33767366	0.18254584
6	-4.69287682	-1.32647359	0.05984585
1	-5.23317671	-2.26297355	-0.03125416
6	-5.42627668	-0.14487363	0.05274585
6	-4.75337696	1.06582642	0.17724586
1	-5.33987665	1.97872639	0.17744584
6	-3.36257648	1.13352633	0.30164585
6	-2.54617643	-2.68027353	0.20554584
6	-2.67257643	2.50292635	0.43944585
6	-1.78877652	-2.84097362	1.53904581
1	-1.08527660	-2.02687359	1.70984578
1	-1.23287666	-3.78737354	1.55344582
1	-2.49717665	-2.85527372	2.37494588
6	-1.57907665	-2.77897358	-0.99125415
1	-0.86287665	-1.95677364	-1.01045418
1	-2.13617659	-2.75047374	-1.93445420
1	-1.01737666	-3.72097373	-0.95805413
6	-3.49337673	-3.88867354	0.09324585
1	-4.05777693	-3.89067364	-0.84575421
1	-4.20577669	-3.93447375	0.92374587
1	-2.90267658	-4.81187344	0.12014585
6	-3.67817688	3.66882634	0.45764583
1	-4.37497663	3.60192633	1.30014586
1	-4.26137686	3.73102641	-0.46755415
1	-3.13117647	4.61332655	0.56154585
6	-1.74237669	2.75412631	-0.76415414
1	-1.00177658	1.96122634	-0.87885410
1	-1.21107662	3.70702648	-0.64995414
1	-2.32547665	2.79732633	-1.69105411
6	-1.88987672	2.58192635	1.76554585
1	-2.57467651	2.47802639	2.61464572
1	-1.38707662	3.55362630	1.85594583
1	-1.13937664	1.79582632	1.84374595
8	1.52332342	-1.58047366	1.11614585
15	2.55212355	-2.58157372	0.74734586
8	4.04652357	-1.99777365	0.59414583
8	2.44522333	-3.27797365	-0.69435418
6	4.53622341	-2.18097353	-0.75495416
6	3.31192350	-2.54297352	-1.60155416
1	5.28452349	-2.97837353	-0.73335415
1	4.99672318	-1.24547362	-1.07375407
1	2.77232361	-1.64757359	-1.92875433

1	3.54812336	-3.20687366	-2.43305421
8	2.55992317	-3.73307371	1.82594585
8	1.55712342	1.44652641	1.19034576
15	2.44592333	2.55982637	0.77714586
8	1.80612338	3.61472631	-0.25175416
8	3.76242352	2.20012641	-0.07215416
6	2.52962351	3.63392639	-1.50395417
6	3.46002340	2.41432643	-1.47965407
1	3.07482338	4.58042669	-1.55625415
1	1.80002344	3.57752633	-2.31195426
1	2.95492315	1.51322639	-1.84495425
1	4.40692329	2.59752631	-1.98855424
8	2.92942333	3.32712626	2.07004595
1	-6.50937653	-0.16757363	-0.04285415
6	3.48752356	-4.83187342	1.74104595
6	3.75732327	4.50152683	1.97214580
1	1.21342337	0.84462637	-3.44725418
1	3.95522356	4.81082678	2.99724579
1	4.69702339	4.26402664	1.46804595
1	3.22492361	5.29562664	1.44334579
1	3.27602339	-5.46427345	2.60164571
1	3.32632351	-5.39377356	0.81854588
1	4.51512337	-4.46427345	1.79644585

I-1__DBP_Mg_OMe_MeOH-2

Zero-point vibrational energy	1233040.2 (Joules/Mol)
	294.70368 (Kcal/Mol)
Zero-point correction =	0.469640 (Hartree/Particle)
Thermal correction to Energy =	0.499790
Thermal correction to Enthalpy =	0.500734
Thermal correction to Gibbs Free Energy =	0.406273
Sum of electronic and zero-point Energies =	-1167.362607
Sum of electronic and thermal Energies =	-1167.332457
Sum of electronic and thermal Enthalpies =	-1167.331513
Sum of electronic and thermal Free Energies =	-1167.425974



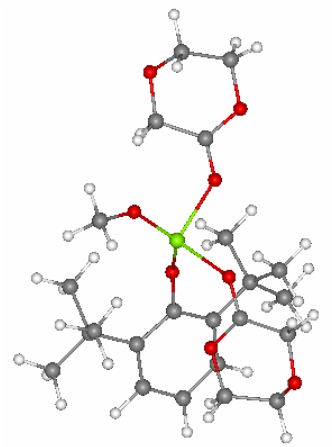
cartesian

12	-1.79139996	-0.05800000	-0.13779999
8	-3.46630001	0.86250001	-0.36950001
8	0.04580000	-0.06880000	-0.15320000
6	-4.01700020	2.05850005	-0.84780002
1	-3.70320010	2.92849994	-0.24940000
1	-5.11709976	2.02320004	-0.81639999
6	1.36020005	0.12040000	-0.07250000
6	1.90190005	1.44319999	-0.06630000
6	3.28760004	1.59280002	0.04800000
1	3.72420001	2.58579993	0.06050000
6	4.14139986	0.49959999	0.14440000
6	3.60599995	-0.78380001	0.11380000
1	4.28879976	-1.62440002	0.17670000
6	2.23119998	-1.01030004	0.00220000
6	1.00139999	2.68659997	-0.19300000
6	1.68729997	-2.45040011	-0.05280000
6	0.03750000	2.78279996	1.00740004
1	-0.57279998	1.88380003	1.11860001
1	-0.63419998	3.64299989	0.89980000
1	0.60140002	2.90639997	1.93830001
6	0.22319999	2.65310001	-1.52479994
1	-0.35850000	1.73670006	-1.64219999
1	0.91750002	2.70350003	-2.37010002
1	-0.45950001	3.50830007	-1.59619999
6	1.80710006	3.99830008	-0.19970000
1	2.51169991	4.04449987	-1.03639996
1	2.36560011	4.14860010	0.73009998
1	1.11880004	4.84439993	-0.30620000
6	2.80819988	-3.50270009	0.01440000
1	3.37439990	-3.44799995	0.95029998
1	3.51200008	-3.41260004	-0.81970000
1	2.36630011	-4.50419998	-0.03940000
6	0.94120002	-2.68740010	-1.38209999
1	0.11370000	-1.98870003	-1.51349998
1	0.54830003	-3.71169996	-1.42209995
1	1.62269998	-2.55920005	-2.23000002
6	0.75690001	-2.72799993	1.14540005
1	1.30530000	-2.62439990	2.08820009
1	0.36300001	-3.75119996	1.09720004
1	-0.08580000	-2.03489995	1.17130005
1	-3.72799993	2.26180005	-1.89090002
1	5.21500015	0.64609998	0.23330000
1	-3.61369991	-0.85460001	-1.22080004
8	-2.83719993	-1.46490002	-1.26359999
6	-3.21280003	-2.84220004	-1.15789998
1	-3.73370004	-3.03830004	-0.21540000
1	-2.29410005	-3.42630005	-1.19239998
6	-2.32859993	-0.19470000	3.09719992
8	-2.69289994	-0.40599999	1.72780001
1	-3.41759992	0.19870000	1.43239999

1	-3.14319992	-0.51190001	3.75460005
1	-1.44840002	-0.80640000	3.29139996
1	-2.08459997	0.85500002	3.28600001
1	-3.84829998	-3.12310004	-2.00230002

I-1__DBP_Mg_OMe_PDO-2

Zero-point vibrational energy	1503157.1 (Joules/Mol)
	359.26316 (Kcal/Mol)
Zero-point correction =	0.572522 (Hartree/Particle)
Thermal correction to Energy =	0.609351
Thermal correction to Enthalpy =	0.610295
Thermal correction to Gibbs Free Energy =	0.500546
Sum of electronic and zero-point Energies =	-1699.064634
Sum of electronic and thermal Energies =	-1699.027805
Sum of electronic and thermal Enthalpies =	-1699.026861
Sum of electronic and thermal Free Energies =	-1699.136611

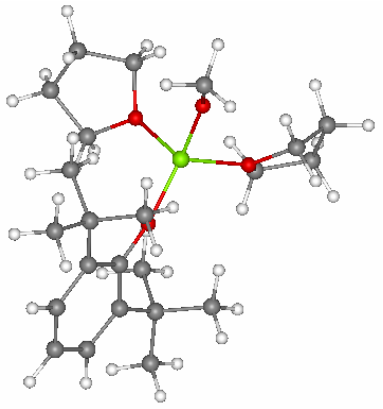


cartesian

8	0.06825855	0.41441467	-0.51451492
6	1.33145857	0.40661469	-0.90661502
6	1.84425843	-0.70908535	-1.65141499
6	3.21875858	-0.76918530	-1.90491498
1	3.63195872	-1.61698532	-2.44211483
6	4.08815861	0.24471468	-1.51061499
6	3.55985856	1.38661468	-0.91341496
1	4.23935843	2.19981456	-0.68041492
6	2.19695854	1.51691461	-0.62501490
6	0.91315854	-1.79958534	-2.21921492
6	1.66225851	2.84921455	-0.06061496
6	0.29515857	-2.66008544	-1.10191500
1	-0.31234145	-2.06498528	-0.42151496
1	-0.35004145	-3.43868542	-1.52701497
1	1.08215857	-3.16378546	-0.52611494
6	-0.20674144	-1.14768541	-3.05691481
1	-0.79534149	-0.45068532	-2.45971489
1	0.22165856	-0.59838533	-3.90241504
1	-0.87614143	-1.91778541	-3.45981479
6	1.65795851	-2.76598525	-3.15811491
1	2.13585854	-2.24178529	-3.99211478
1	2.42275858	-3.35438538	-2.63851476
1	0.94125855	-3.47718525	-3.58401489
6	2.73475862	3.95511460	-0.08021496
1	3.56925869	3.74741459	0.59888506
1	3.14015865	4.11791468	-1.08441496
1	2.28275871	4.89751482	0.24818504
6	0.49385855	3.36231470	-0.92821503
1	-0.32524145	2.64411473	-0.96931493
1	0.10785857	4.30571508	-0.52361500
1	0.83485854	3.54881454	-1.95261490
6	1.21235859	2.71181464	1.40588498
1	2.03265858	2.34781456	2.03368497
1	0.89245856	3.68421459	1.79858506
1	0.36925855	2.02991462	1.52488506
8	-2.36084127	1.42911458	1.73048496
6	-2.39714146	2.41331458	2.70908523
1	-3.43704128	2.68071461	2.97118521
1	-1.90374148	3.34901452	2.39228511
1	-1.91094148	2.10101461	3.65148520
8	-4.78484154	-1.72158539	-0.15481496
6	-3.94994140	-0.68988538	-0.16221496
8	-2.75804138	-0.91408539	0.02968504
6	-4.46244144	0.71651471	-0.34981498
12	-1.23054147	0.23521468	0.85468507
6	3.09065866	-0.96588528	2.12218499
8	1.67825854	-0.62288535	2.04518509
6	0.74605858	-1.49528539	2.34968519
6	1.11985850	-2.84438539	2.92438507
8	2.48595858	-2.99628544	3.22998524
6	3.28545856	-2.46078539	2.18238521
8	-0.43704143	-1.21728539	2.14918518
1	3.03295875	-2.92998528	1.22148502
1	4.32585859	-2.69148540	2.41928506
1	3.53705859	-0.51978534	1.23108506
1	3.47635865	-0.47898534	3.02098513
1	-4.16954136	1.25051463	0.57198501
1	0.54765856	-2.98378539	3.84428501
1	0.77715862	-3.59778547	2.19968510
1	5.15285826	0.17301467	-1.72031498
6	-6.20504141	-1.49698532	-0.34751496
1	-6.42094135	-1.65908539	-1.40671504
6	-6.60034180	-0.10218533	0.07348504
1	-6.69954157	-2.26818538	0.24618503
1	-7.65164137	0.07561466	-0.16401497
8	-5.83754158	0.83001471	-0.66631496
1	-6.45654154	0.03871466	1.15528500
1	-3.89814138	1.16911459	-1.16861498

I-1__DBP_Mg_OMe_THF-2

Zero-point vibrational energy	1577703.4 (Joules/Mol)
	377.08017 (Kcal/Mol)
Zero-point correction =	0.600915 (Hartree/Particle)
Thermal correction to Energy =	0.635197
Thermal correction to Enthalpy =	0.636142
Thermal correction to Gibbs Free Energy =	0.532661
Sum of electronic and zero-point Energies =	-1400.621994
Sum of electronic and thermal Energies =	-1400.587712
Sum of electronic and thermal Enthalpies =	-1400.586768
Sum of electronic and thermal Free Energies =	-1400.690248

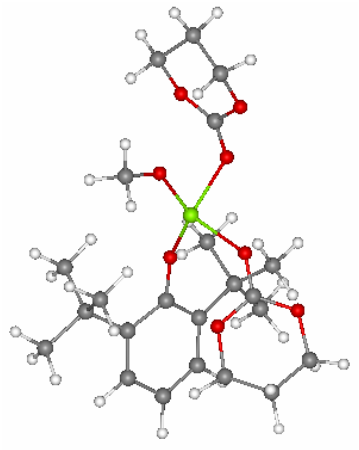


cartesian

12	1.10050440	-0.49806330	0.43258816
8	2.04230452	-1.82476330	1.33238828
8	-0.63809556	0.18693671	0.26318818
6	1.98680449	-2.92986321	2.16908813
1	1.22980440	-3.67096329	1.85638821
1	2.95500445	-3.46176314	2.19588828
6	-1.95119560	0.37763667	0.18468818
6	-2.87009549	-0.67856330	0.49208820
6	-4.23849535	-0.44526333	0.32178819
1	-4.95009518	-1.23536336	0.53628814
6	-4.73299551	0.77963674	-0.11111182
6	-3.84049559	1.81733668	-0.35521179
1	-4.24449539	2.77533674	-0.66501182
6	-2.45939565	1.65873671	-0.20831183
6	-2.39649558	-2.04036331	1.03488827
6	-1.52579558	2.86063671	-0.44691181
6	-1.52459562	-2.77606320	-0.00191182
1	-0.65719557	-2.18836331	-0.30611181
1	-1.16099560	-3.72836328	0.40198821
1	-2.10909557	-2.99006319	-0.90391183
6	-1.63519561	-1.84106338	2.36138821
1	-0.77619559	-1.17746329	2.25258827
1	-2.29949570	-1.39796340	3.11128831
1	-1.27509558	-2.80046320	2.75048828
6	-3.56679559	-2.98986316	1.35068822
1	-4.24319553	-2.57636333	2.10588813
1	-4.15449524	-3.23866320	0.46058816
1	-3.16769552	-3.92906332	1.74988818
6	-2.29809570	4.14523697	-0.79531181
1	-2.86899567	4.04823685	-1.72491181
1	-2.98649549	4.44353676	0.00228818
1	-1.58629560	4.96683693	-0.93591183
6	-0.71899557	3.16203666	0.83268815
1	-0.11719557	2.30433679	1.13678825
1	-0.05609557	4.02333689	0.67458814
1	-1.39489555	3.41083670	1.65818822
6	-0.57529557	2.58443666	-1.62741172
1	-1.14589560	2.40193677	-2.54521179
1	0.07900443	3.44783688	-1.80791175
1	0.04480443	1.70893669	-1.43351173
1	1.74710441	-2.66176319	3.21388817
1	-5.80239534	0.92963672	-0.23781182
6	3.30020452	0.94783670	2.01748824
6	4.60710478	1.60443664	1.60768819
8	2.44840431	1.05863667	0.84068817
6	2.95800447	2.08273673	-0.05131182
6	4.12530470	2.73003674	0.68818820
1	5.17370462	1.96813667	2.46838832
1	5.23440456	0.89463669	1.05848825
1	4.89550447	3.08813667	0.00058818
1	3.77690434	3.58193684	1.28038824
1	3.27710438	1.59183669	-0.97661185
1	2.14520431	2.77513671	-0.27601182
1	3.36020446	-0.11596330	2.25378823
1	2.81510448	1.48913670	2.83808827
6	0.76900440	-0.80916327	-2.70701170
6	1.04720438	-2.05126333	-3.56471181
8	1.66200447	-0.89886332	-1.55891180
6	2.63090444	-1.95356333	-1.79431176
6	1.87560439	-2.95806313	-2.64541173
1	0.12250443	-2.52546334	-3.90061188
1	1.62490439	-1.78086340	-4.45371199
1	2.54390430	-3.62446332	-3.19691181
1	1.22820437	-3.56816316	-2.00921178
1	3.48770452	-1.52636337	-2.33191180
1	2.93860435	-2.31246328	-0.81011182
1	0.98420441	0.12313670	-3.23641181
1	-0.24889557	-0.76406330	-2.31661177

I-1__DBP_Mg_OMe_TMC-2

Zero-point vibrational energy	1506208.4 (Joules/Mol)
	359.99244 (Kcal/Mol)
Zero-point correction =	0.573684 (Hartree/Particle)
Thermal correction to Energy =	0.610446
Thermal correction to Enthalpy =	0.611390
Thermal correction to Gibbs Free Energy =	0.500767
Sum of electronic and zero-point Energies =	-1699.102844
Sum of electronic and thermal Energies =	-1699.066082
Sum of electronic and thermal Enthalpies =	-1699.065138
Sum of electronic and thermal Free Energies =	-1699.175762

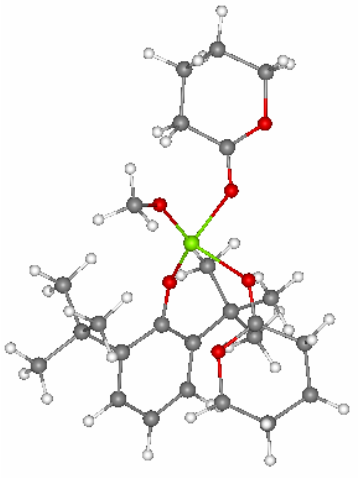


cartesian

12	-1.41703081	-0.18661475	0.27689257
8	-2.89753079	0.69378531	1.06189263
8	0.10966921	0.40128526	-0.67860746
6	-3.11683083	1.67018521	2.02719259
1	-2.50113082	1.53028524	2.93379259
1	-4.16843081	1.67138517	2.37299252
6	1.41856933	0.53268528	-0.80040741
6	2.16986918	-0.40611476	-1.58680737
6	3.56756926	-0.33851475	-1.54820740
1	4.15756941	-1.05641472	-2.10920739
6	4.24266911	0.64668524	-0.83110744
6	3.50166917	1.64108527	-0.19660743
1	4.04146910	2.44828534	0.28839257
6	2.10326934	1.63468528	-0.18370743
6	1.47616911	-1.41851473	-2.52260756
6	1.33686924	2.82168531	0.43499255
6	0.50926924	-0.67061472	-3.46470761
1	-0.25743079	-0.13301474	-2.90620756
1	0.01356922	-1.37971473	-4.13920736
1	1.05846930	0.05158526	-4.07900763
6	0.70866925	-2.50111461	-1.74390733
1	-0.10623078	-2.08451462	-1.15430737
1	1.38036919	-3.05001473	-1.07290733
1	0.26786920	-3.22931457	-2.43530750
6	2.48576927	-2.15731478	-3.42000747
1	3.16866922	-2.79631472	-2.84810758
1	3.08456922	-1.46731472	-4.02340746
1	1.94016933	-2.80941463	-4.11130762
6	2.27866936	3.97818518	0.81949258
1	2.86146927	4.33668518	-0.03550743
1	2.97466922	3.70458531	1.62039256
1	1.68166924	4.82008553	1.18779266
6	0.59936923	2.41758537	1.72429264
1	-0.14423078	1.64038527	1.54859257
1	0.07556921	3.28118539	2.15119243
1	1.30236912	2.04378533	2.47659254
6	0.33586919	3.39258528	-0.59120744
1	0.86736923	3.76088524	-1.47560740
1	-0.21523078	4.23408556	-0.15370743
1	-0.38163078	2.63888526	-0.91620743
8	-4.57063055	-1.61291480	0.22589257
6	-3.89403081	-0.90281475	-0.66850746
8	-4.49343061	0.04378526	-1.37860739
6	-5.67623091	0.69238520	-0.86530745
6	-6.58073092	-0.30431473	-0.17410742
6	-5.74893093	-1.05381477	0.84269255
8	-2.73793077	-1.22571480	-0.94610745
1	-5.40023088	-0.39921474	1.64549267
1	-6.27413082	-1.90811479	1.27099264
1	-7.01603079	-0.99781477	-0.90060747
1	-7.39953089	0.22108525	0.32669255
1	-6.14313078	1.15448523	-1.73560739
1	-5.33093071	1.47068524	-0.17990743
6	2.75176930	-1.07761478	2.26369262
8	1.32456923	-0.89281476	2.08679247
6	0.52346921	-1.90651476	1.81509256
8	0.93406922	-3.16271472	1.93729258
6	2.32406926	-3.48421454	2.18919253
6	3.01346922	-2.38851476	2.96939254
8	-0.63973081	-1.69331479	1.48559260
1	2.79576921	-3.64031458	1.21479261
1	2.29576921	-4.43411446	2.72379255
1	2.63886929	-2.35231471	3.99729252
1	4.08886909	-2.58471465	3.00709248
1	3.07046938	-0.21121475	2.84149241
1	3.21046925	-1.02391469	1.27229261
1	-2.90993071	2.69058537	1.65819263
1	5.32986927	0.67628527	-0.82160741

I-1__DBP_Mg_OMe_VL-2

Zero-point vibrational energy	1630983.4 (Joules/Mol)
	389.81438 (Kcal/Mol)
Zero-point correction =	0.621209 (Hartree/Particle)
Thermal correction to Energy =	0.658525
Thermal correction to Enthalpy =	0.659469
Thermal correction to Gibbs Free Energy =	0.548782
Sum of electronic and zero-point Energies =	-1627.256236
Sum of electronic and thermal Energies =	-1627.218920
Sum of electronic and thermal Enthalpies =	-1627.217975
Sum of electronic and thermal Free Energies =	-1627.328663

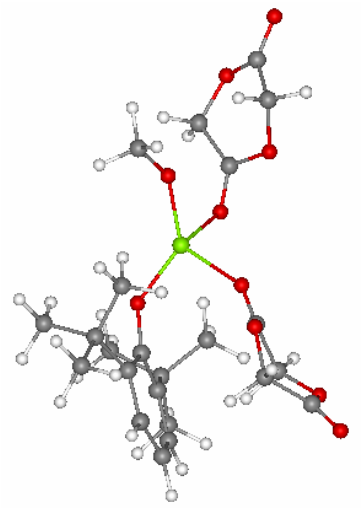


cartesian

8	4.63328218	-1.62660706	0.15950271
6	3.84818172	-0.56600696	-0.01249728
6	4.39018202	0.83269304	0.06790273
6	5.90878201	0.94079298	-0.02189727
6	6.54158211	-0.16980699	0.80710268
6	6.07418203	-1.51140702	0.28320274
8	2.65308166	-0.79390699	-0.19829726
1	6.48458195	-1.70700705	-0.71299732
1	6.35688210	-2.33680701	0.93870270
1	6.26658201	-0.06110699	1.86300278
1	7.63528204	-0.14630699	0.75260270
1	6.23008204	1.92749298	0.32300273
1	6.23038197	0.85239303	-1.06649733
6	-3.26091814	-0.81830698	-1.90749729
8	-1.84701824	-0.48800698	-2.03559732
6	-0.92781824	-1.38800704	-2.32179713
6	-1.31311822	-2.73140693	-2.88719726
6	-2.75041819	-3.15260696	-2.58869720
6	-3.68221831	-1.96520710	-2.80139732
8	0.25748181	-1.08000708	-2.17449713
1	-2.82841825	-3.49960709	-1.55249727
1	-3.02881813	-3.99540710	-3.22819734
1	-3.66741824	-1.65190709	-3.85239720
1	-4.71701813	-2.22430706	-2.55549717
1	-3.77371836	0.11269300	-2.14809728
1	-3.42211819	-1.03320706	-0.84749722
1	4.03518200	1.21679294	1.03360271
1	3.84328175	1.40509295	-0.69819725
1	-0.57491815	-3.45250702	-2.53109717
1	-1.15771818	-2.64050698	-3.97029734
8	2.08778191	1.65259290	-1.79789722
6	2.03638172	2.63459301	-2.77569723
1	1.50008178	3.54139304	-2.44299722
1	1.53928173	2.29509306	-3.70339727
12	1.08158183	0.36129302	-0.90459728
8	-0.13171819	0.47259301	0.55340278
6	-1.35841823	0.42299300	1.04300272
6	-2.25921822	1.53109300	0.88800275
6	-3.59171820	1.36489296	1.27970278
1	-4.29871798	2.17669296	1.14290273
6	-4.05541801	0.18819302	1.86220276
6	-3.14451814	-0.82880700	2.13440275
1	-3.50271821	-1.70810699	2.66030264
6	-1.79591823	-0.73480695	1.77310276
6	-1.79061818	2.89669299	0.34470272
6	-0.80951816	-1.83620703	2.21210265
6	-1.46451819	2.83169293	-1.15889728
1	-0.63001817	2.16519284	-1.37809730
1	-1.18881822	3.82509303	-1.53289723
1	-2.33251834	2.48569298	-1.73069727
6	-0.55911815	3.38969302	1.13250279
1	0.27158180	2.68739295	1.06220281
1	-0.81091815	3.51689291	2.19140267
1	-0.22581819	4.36029339	0.74510276
6	-2.87211823	3.98209310	0.50580275
1	-3.19021821	4.09539318	1.54760277
1	-3.75971818	3.78739285	-0.10639727
1	-2.46371818	4.94519329	0.17990273
6	-1.46571827	-2.85850716	3.15870285
1	-2.26071835	-3.43410707	2.67100286
1	-1.88391829	-2.38410711	4.05270243
1	-0.70801818	-3.57690716	3.49170280
6	0.36518183	-1.20650709	2.98890281
1	0.89318180	-0.47190699	2.38030267
1	1.07558179	-1.98400700	3.29680276
1	-0.00151819	-0.70620698	3.89200282
6	-0.27261817	-2.63440704	1.01020277
1	-1.09941828	-3.10580707	0.46360275
1	0.39898181	-3.43340707	1.34790277
1	0.28948182	-2.00510693	0.32270274
1	3.05038166	2.96209288	-3.07109714
1	-5.09891796	0.08869302	2.15180278

I-1__DBP_Mg_OMe_GL-2

Zero-point vibrational energy	1405019.0 (Joules/Mol)
	335.80761 (Kcal/Mol)
Zero-point correction =	0.535143 (Hartree/Particle)
Thermal correction to Energy =	0.572809
Thermal correction to Enthalpy =	0.573753
Thermal correction to Gibbs Free Energy =	0.461343
Sum of electronic and zero-point Energies =	-1847.121529
Sum of electronic and thermal Energies =	-1847.083863
Sum of electronic and thermal Enthalpies =	-1847.082919
Sum of electronic and thermal Free Energies =	-1847.195329



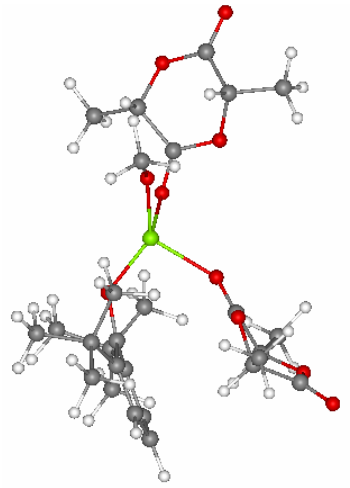
cartesian

8	0.00096560	1.10860598	-0.39149079
6	-1.29493439	0.97150588	-0.14529079
6	-2.13923454	0.28480595	-1.08419085
6	-3.44713449	-0.02809408	-0.69189084
1	-4.10053444	-0.56959409	-1.36899078
6	-3.96853447	0.37990594	0.53480923
6	-3.19623423	1.20250595	1.35350919
1	-3.64933443	1.58990598	2.26000929
6	-1.87633431	1.54160595	1.03620923
6	-1.68903434	0.03540593	-2.54029059
6	-1.10443437	2.54080582	1.92080915
6	-0.47153443	-0.89949405	-2.67209077
1	0.45286560	-0.40679407	-2.36549067
1	-0.32713443	-1.17959404	-3.72209072
1	-0.59373438	-1.82489407	-2.10149074
6	-1.34203446	1.39940596	-3.17559075
1	-0.54163438	1.89810598	-2.62499070
1	-2.21753454	2.05700588	-3.18179083
1	-1.01473439	1.26200593	-4.21339083
6	-2.81333447	-0.58769405	-3.38729072
1	-3.71513414	0.03210592	-3.40199065
1	-3.08983421	-1.59199405	-3.04479074
1	-2.47103453	-0.68479407	-4.42289114
6	-2.02153444	3.21120596	2.95940924
1	-2.40933418	2.50330591	3.70020938
1	-2.87063456	3.72010565	2.49130940
1	-1.44883442	3.96580601	3.50920939
6	-0.51893443	3.67040586	1.04790914
1	0.16616559	3.28080606	0.29420921
1	0.02226558	4.38750601	1.67680919
1	-1.32023442	4.21320581	0.53480923
6	0.02506560	1.84760582	2.70370936
1	-0.37343442	1.05600595	3.34900928
1	0.53796560	2.56950569	3.35070920
1	0.77556562	1.41320598	2.04480934
6	-2.41293430	-3.58599424	0.26690921
8	-1.05403435	-3.13719416	0.07380921
6	-0.61683440	-2.19269419	0.89580917
6	-1.48153436	-1.88609409	2.08880925
8	-2.13993454	-3.04869413	2.60960937
6	-2.74653435	-3.86349392	1.71910918
8	0.45556560	-1.64459407	0.68370920
1	-3.09253454	-2.82619429	-0.13419080
1	-2.51083422	-4.50499439	-0.30549082
1	-0.85933435	-1.49469411	2.89050937
1	-2.21583462	-1.11819410	1.80620921
8	-3.48793459	-4.74529409	2.06680918
1	-4.98853445	0.12640592	0.81310916
12	1.48006558	-0.07579407	-0.20579079
8	2.99976540	-0.44279408	-1.26909077
6	3.30756569	-0.70959407	-2.60419083
1	3.12906551	-1.76389408	-2.87619066
1	4.37136555	-0.50009406	-2.81729078
8	4.26036549	-1.39119411	1.20360923
6	3.99166536	-0.11019406	1.00290918
6	5.11806583	0.77030587	0.52500916
8	6.42646551	0.26040596	0.80250919
6	6.63776588	-1.06449413	0.63500917
6	5.39076567	-1.91019404	0.48040920
8	2.88976574	0.34820592	1.30380917
1	5.10936594	-1.98939407	-0.57439077
1	5.58516550	-2.90049410	0.88500917
1	2.72696543	-0.09259406	-3.30939078
1	5.04576588	1.73070586	1.03400922
1	4.97786570	0.92140591	-0.54889083
8	7.74896574	-1.52799404	0.62680924

I-1__ DBP_Mg_OMe_ssLA-2

Zero-point vibrational energy	1697611.7 (Joules/Mol)

	405.73893 (Kcal/Mol)
Zero-point correction =	0.646586 (Hartree/Particle)
Thermal correction to Energy =	0.690352
Thermal correction to Enthalpy =	0.691296
Thermal correction to Gibbs Free Energy =	0.565143
Sum of electronic and zero-point Energies =	-2004.241213
Sum of electronic and thermal Energies =	-2004.197446
Sum of electronic and thermal Enthalpies =	-2004.196502
Sum of electronic and thermal Free Energies =	-2004.322655

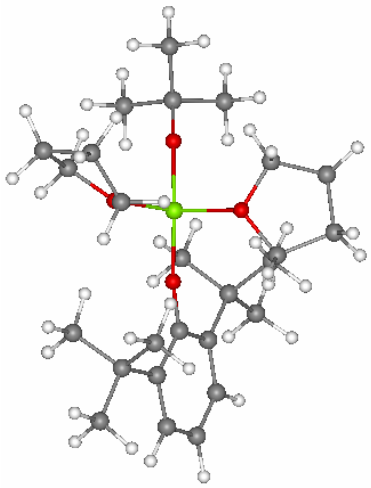


cartesian

8	-0.24022797	1.45164871	-0.55365765
6	-1.51572788	1.38534880	-0.19355768
6	-2.47382784	0.73924875	-1.04545772
6	-3.74682784	0.47194874	-0.52585769
1	-4.48542833	-0.03815125	-1.13715768
6	-4.12492800	0.88894874	0.75004232
6	-3.25082803	1.69494867	1.47904229
1	-3.60082793	2.11034870	2.41854239
6	-1.96382785	1.99984860	1.02284241
6	-2.17592788	0.49934876	-2.54135776
6	-1.10532796	3.05054879	1.75754237
6	-0.97862792	-0.43425125	-2.80585766
1	-0.03012797	0.07094875	-2.61445761
1	-0.95952797	-0.73155129	-3.86105752
1	-1.02502787	-1.35105133	-2.20985770
6	-1.88162804	1.86934876	-3.19075775
1	-1.02242792	2.34914875	-2.71635771
1	-2.74492788	2.53654861	-3.09785771
1	-1.66152787	1.74534869	-4.25835800
6	-3.38542795	-0.10465126	-3.27585769
1	-4.27602816	0.52684873	-3.20005774
1	-3.64232802	-1.10535121	-2.90805769
1	-3.14882803	-0.20355125	-4.34045792
6	-1.90702796	3.77884865	2.85144234
1	-2.20112801	3.11484861	3.67194223
1	-2.80892801	4.25604868	2.45384240
1	-1.28332794	4.56694889	3.28724241
6	-0.64922798	4.12454891	0.74694234
1	-0.04142797	3.68984866	-0.04795767
1	-0.05692795	4.89294863	1.25794232
1	-1.51472795	4.61614847	0.28964233
6	0.12777205	2.43554878	2.44134235
1	-0.16962796	1.71924877	3.21484232
1	0.71537209	3.21944880	2.93454242
1	0.78307199	1.93274879	1.73214233
6	-2.73892784	-3.11435127	0.00394233
8	-1.36952794	-2.61945128	-0.07455768
6	-0.93822789	-1.83375120	0.89974231
6	-1.79292798	-1.75795126	2.14704227
8	-2.43672800	-3.02375126	2.40824223
6	-3.01762795	-3.68625140	1.38674235
8	0.11627205	-1.22315121	0.77594233
1	-3.39432788	-2.24705124	-0.14865768
6	-2.92132783	-4.12975121	-1.10055768
6	-1.00432789	-1.39505124	3.38734221
1	-2.56392789	-0.99655128	1.94734228
8	-3.70012784	-4.65985107	1.58264232
1	-5.11892796	0.66744876	1.13124228
12	1.13267207	0.12614876	-0.43605769
8	2.47167206	-0.56555128	-1.57425773
6	2.60967207	-1.25485134	-2.77655768
1	2.33267212	-2.32015133	-2.69045758
1	3.65517211	-1.22645128	-3.13555765
1	1.99757206	-0.82995123	-3.58925772
8	3.99667215	-1.11175132	0.94974232
6	3.77197218	0.11144873	0.49594232
6	4.89317179	0.75394875	-0.30045769
8	6.18137169	0.31474876	0.18644233
6	6.36267185	-1.00765133	0.39534232
6	5.08887196	-1.84175134	0.33084232
8	2.73217201	0.69584876	0.79984230
1	4.81367207	-1.98445129	-0.72165769
6	5.21487188	-3.17285132	1.03484225
6	4.87177181	2.26644874	-0.24835768
1	4.75727177	0.40584874	-1.33065772
8	7.45617199	-1.46045136	0.62324232
1	5.69957161	2.65804863	-0.84275770
1	3.93227196	2.63634872	-0.66015768
1	4.97127199	2.62354875	0.77874231
1	6.01087189	-3.75535131	0.56894231
1	5.46377182	-3.03225136	2.08854246
1	4.27427197	-3.72125125	0.95484233
1	-1.68642795	-1.32375121	4.23654270
1	-0.24952796	-2.15525126	3.60004234
1	-0.51072800	-0.43525124	3.24374223
1	-3.95142770	-4.48835135	-1.09285772
1	-2.70852804	-3.66965127	-2.06725764
1	-2.25852799	-4.98495150	-0.95365763

I-1__DBP_Mg_OtBu_THF-2

Zero-point vibrational energy	1798856.5 (Joules/Mol)
	429.93702 (Kcal/Mol)
Zero-point correction =	0.685148 (Hartree/Particle)
Thermal correction to Energy =	0.723318
Thermal correction to Enthalpy =	0.724262
Thermal correction to Gibbs Free Energy =	0.612046
Sum of electronic and zero-point Energies =	-1518.453519
Sum of electronic and thermal Energies =	-1518.415350
Sum of electronic and thermal Enthalpies =	-1518.414405
Sum of electronic and thermal Free Energies =	-1518.526622



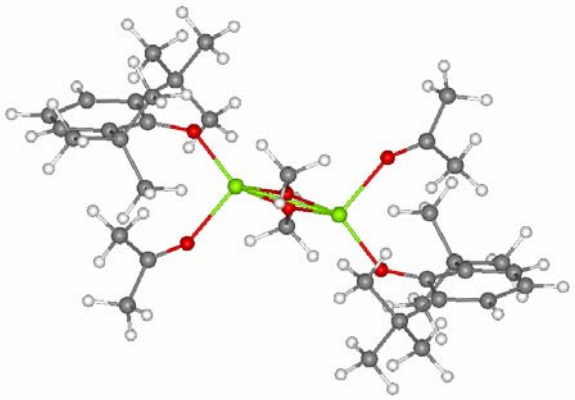
cartesian

12	0.82381451	0.10707406	0.05442853
8	2.32601452	-0.82532597	0.60992855
8	-1.04138553	0.11927406	0.26302853
8	1.03831446	0.10647406	-2.04107141
6	-0.06138552	0.03337406	-2.99417138
1	-0.21358553	1.03107405	-3.41617131
1	-0.95058548	-0.24912593	-2.42997146
6	0.36011446	-0.99302602	-4.05807161
1	0.56051451	-0.49402592	-5.01057148
1	-0.41928554	-1.73792601	-4.23127174
6	1.64681447	-1.61552596	-3.49497128
1	1.42051446	-2.47712588	-2.86107135
1	2.33941436	-1.93632591	-4.27737141
6	2.21131444	-0.49122593	-2.64567137
1	2.85891438	-0.80342597	-1.82477152
1	2.71611452	0.26757404	-3.25887132
6	-2.36338568	-0.01662594	0.29582852
6	-2.96248555	-1.31462598	0.40272853
6	-4.35648537	-1.41522598	0.35582852
1	-4.82898521	-2.38932586	0.42012852
6	-5.17628527	-0.29922593	0.23642854
6	-4.59248543	0.96147406	0.19142854
1	-5.24688530	1.82407403	0.12832855
6	-3.20668554	1.14127398	0.23012854
6	-2.11918545	-2.58792591	0.60342854
6	-2.62898564	2.56907392	0.21822855
6	-1.21118557	-2.85032606	-0.61337149
1	-0.50418550	-2.03632593	-0.78037149
1	-1.81518555	-2.96512604	-1.52087152
1	-0.63328552	-3.77162600	-0.47357148
6	-1.28608561	-2.46242595	1.89422858
1	-1.94828558	-2.35712600	2.76052856
1	-0.62838548	-1.59252596	1.87202847
1	-0.67138553	-3.35772586	2.04692864
6	-2.98668551	-3.84952593	0.76722854
1	-3.65928555	-3.78082585	1.62832856
1	-2.33408546	-4.71432590	0.93252856
1	-3.58718562	-4.06242609	-0.12377147
6	-3.72398567	3.65067410	0.22142854
1	-3.25098562	4.63927412	0.24032854
1	-4.37068510	3.58307409	1.10242856
1	-4.35458517	3.61147404	-0.67327148
6	-1.77568555	2.80737400	1.48022854
1	-1.35008562	3.81937408	1.46912849
1	-0.95968550	2.08817410	1.55312848
1	-2.39408565	2.71367407	2.37972856
6	-1.79148555	2.80177402	-1.05317152
1	-1.39528561	3.82547402	-1.07197142
1	-2.40948558	2.66597414	-1.94787145
1	-0.95478553	2.10507393	-1.10997152
6	3.06621432	-1.80802596	1.26572847
6	2.77801442	-1.77482593	2.77702856
6	4.56481457	-1.54122591	1.03232849
6	2.71171451	-3.19972587	0.71382850
8	1.56991446	2.05337405	0.41462854
6	1.90201449	3.06697392	-0.56117147
1	1.87411439	2.60047412	-1.54747152
1	1.14391446	3.85667396	-0.51717144
6	3.27191448	3.57587409	-0.14297146
1	4.05461454	2.89997411	-0.50117147
1	3.47611451	4.57827425	-0.52727145
6	3.17071438	3.52487397	1.38402855
1	2.64231443	4.40707397	1.75912857
1	4.14461470	3.47907400	1.87692857
6	2.35241437	2.25967407	1.62762856
1	1.65591443	2.35037398	2.46502876
1	2.96681452	1.36577404	1.75632858
1	-6.25738525	-0.40922594	0.19932854
1	5.20141459	-2.27992606	1.53342855
1	4.79111481	-1.56712592	-0.03967146
1	4.83341455	-0.54742599	1.40792859

1	3.34661436	-2.53612590	3.32432866
1	3.04071450	-0.79462594	3.19062853
1	1.71261442	-1.94562602	2.96122861
1	3.28911448	-3.99752617	1.19622850
1	1.64781439	-3.40372586	0.86862850
1	2.91071439	-3.23912597	-0.36327147

DI-1__DBP-2_Mg-2_OMe-2_acetone-2

Zero-point vibrational energy	2358063.5 (Joules/Mol)
	563.59071 (Kcal/Mol)
Zero-point correction =	0.898139 (Hartree/Particle)
Thermal correction to Energy =	0.955240
Thermal correction to Enthalpy =	0.956184
Thermal correction to Gibbs Free Energy =	0.802662
Sum of electronic and zero-point Energies =	-2258.218866
Sum of electronic and thermal Energies =	-2258.161765
Sum of electronic and thermal Enthalpies =	-2258.160821
Sum of electronic and thermal Free Energies =	-2258.314342



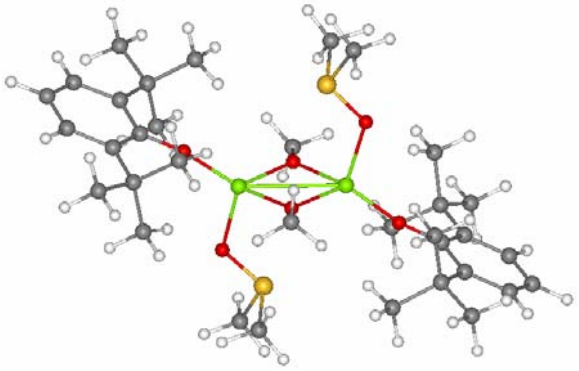
cartesian

12	1.45819998	-0.11210000	0.13600001
8	0.00610000	-0.98589998	-0.86320001
8	3.08290005	0.19589999	-0.80839998
6	0.06860000	-1.80820000	-2.00729990
1	1.03380001	-1.70510006	-2.51909995
1	-0.06320000	-2.86649990	-1.74419999
6	4.36859989	0.25180000	-0.47569999
6	5.18200016	-0.92949998	-0.52010000
6	6.45609999	-0.87629998	0.05600000
1	7.07660007	-1.76639998	0.07830000
6	6.97730017	0.30050001	0.58920002
6	6.24919987	1.48020005	0.45370001
1	6.70809984	2.40529990	0.78740001
6	4.96700001	1.50059998	-0.10420000
6	4.72170019	-2.20449996	-1.25820005
6	4.25979996	2.84619999	-0.36489999
6	3.55660009	-2.91770005	-0.54909998
1	2.65269995	-2.30839992	-0.52859998
1	3.30640006	-3.84870005	-1.07229996
1	3.82209992	-3.17840004	0.48130000
6	4.30259991	-1.83089995	-2.69560003
1	3.50370002	-1.08759999	-2.69400001
1	5.15420008	-1.41550004	-3.24530005
1	3.95530009	-2.72119999	-3.23469996
6	5.85620022	-3.23860002	-1.37940001
1	6.73750019	-2.82529998	-1.88030005
1	6.16769981	-3.63739991	-0.40740001
1	5.50579977	-4.08720016	-1.97739995
6	5.19019985	4.04339981	-0.09860000
1	5.46490002	4.13549995	0.95810002
1	6.11019993	3.98979998	-0.68970001
1	4.67409992	4.96859980	-0.37770000
6	3.83750010	2.92659998	-1.84689999
1	3.16580009	2.10890007	-2.11339998
1	3.32739997	3.87770009	-2.04460001
1	4.71649981	2.87470007	-2.49860001
6	3.02559996	3.04310012	0.53380001
1	3.29029989	2.95609999	1.59379995
1	2.60010004	4.04309988	0.38360000
1	2.23429990	2.32660007	0.30910000
12	-1.45829999	0.11250000	-0.13620000
8	-0.00620000	0.98640001	0.86290002
8	-3.08290005	-0.19589999	0.80820000
6	-0.06860000	1.80879998	2.00699997
1	-1.03380001	1.70580006	2.51880002
1	0.06320000	2.86710000	1.74370003
6	-4.36850023	-0.25189999	0.47580001
6	-5.18209982	0.92930001	0.52039999
6	-6.45629978	0.87599999	-0.05550000
1	-7.07679987	1.76600003	-0.07760000
6	-6.97749996	-0.30080000	-0.58859998
6	-6.24930000	-1.48049998	-0.45330000
1	-6.70819998	-2.40560007	-0.78689998
6	-4.96689987	-1.50070000	0.10430000
6	-4.72179985	2.20429993	1.25849998
6	-4.25960016	-2.84629989	0.36469999
6	-3.55699992	2.91770005	0.54930001
1	-2.65289998	2.30850005	0.52859998
1	-3.30679989	3.84870005	1.07239997
1	-3.82259989	3.17840004	-0.48120001
6	-4.30240011	1.83060002	2.69569993
1	-3.50340009	1.08749998	2.69400001
1	-5.15380001	1.41520000	3.24559999
1	-3.95510006	2.72090006	3.23480010
6	-5.85640001	3.23830009	1.37989998
1	-6.73750019	2.82489991	1.88100004
1	-6.16809988	3.63709998	0.40810001
1	-5.50600004	4.08690023	1.97790003

6	-5.19000006	-4.04360008	0.09880000
1	-5.46519995	-4.13560009	-0.95779997
1	-6.10979986	-3.99000001	0.69029999
1	-4.67379999	-4.96880007	0.37750000
6	-3.83669996	-2.92680001	1.84660006
1	-3.16490006	-2.10910010	2.11279988
1	-3.32649994	-3.87779999	2.04410005
1	-4.71540022	-2.87490010	2.49869990
6	-3.02570009	-3.04320002	-0.53439999
1	-3.29089999	-2.95619988	-1.59430003
1	-2.60010004	-4.04309988	-0.38440001
1	-2.23440003	-2.32649994	-0.31020001
6	2.96149993	-2.47670007	3.55380011
6	2.95630002	-1.20480001	2.75659990
6	4.00040007	-0.17829999	3.06030011
8	2.10940003	-1.03620005	1.87740004
6	-4.00059986	0.17839999	-3.05979991
6	-2.95639992	1.20500004	-2.75679994
6	-2.96149993	2.47639990	-3.55480003
8	-2.10940003	1.03690004	-1.87750006
1	0.71660000	1.54589999	2.73079991
1	-0.71649998	-1.54519999	-2.73119998
1	-7.96689987	-0.31140000	-1.03950000
1	7.96659994	0.31099999	1.04020000
1	2.30520010	-3.22070003	3.10299993
1	2.61120009	-2.25399995	4.56869984
1	-2.30509996	3.22059989	-3.10450006
1	-2.61120009	2.25300002	-4.56949997
1	3.67729998	0.81500000	2.75090003
1	4.89839983	-0.42420000	2.47639990
1	4.27850008	-0.18860000	4.11770010
1	3.97959995	-2.86520004	3.64949989
1	-3.97959995	2.86490011	-3.65079999
1	-3.67750001	-0.81480002	-2.74979997
1	-4.27880001	0.18810000	-4.11709976
1	-4.89849997	0.42469999	-2.47589993

DI-1__DBP-2_Mg-2_OMe-2_DMSO-2

Zero-point vibrational energy	2336549.0 (Joules/Mol)
	558.44860 (Kcal/Mol)
Zero-point correction =	0.889945 (Hartree/Particle)
Thermal correction to Energy =	0.947976
Thermal correction to Enthalpy =	0.948920
Thermal correction to Gibbs Free Energy =	0.793981
Sum of electronic and zero-point Energies =	-2978.191113
Sum of electronic and thermal Energies =	-2978.133081
Sum of electronic and thermal Enthalpies =	-2978.132137
Sum of electronic and thermal Free Energies =	-2978.287076



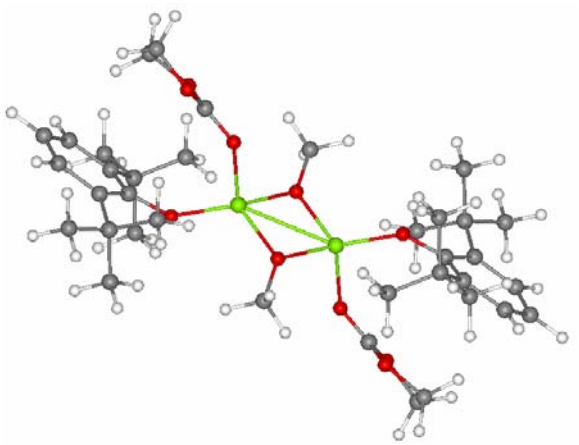
cartesian

16	-0.29980001	1.23119998	-3.02440000
8	1.12440002	0.89940000	-2.51830006
6	-0.41970000	3.03010011	-2.91980004
6	-0.14250000	1.06770003	-4.81680012
1	-1.34959996	3.35590005	-3.39140010
1	0.45280001	3.47830009	-3.40000010
1	-0.44279999	3.27410007	-1.85800004
1	-1.06690001	1.40670002	-5.28999996
1	0.01320000	0.00890000	-5.02710009
1	0.71619999	1.64900005	-5.15799999
12	1.36339998	0.21310000	-0.61440003
8	-0.04540000	1.27419996	0.30960000
8	3.16840005	0.05360000	-0.13900000
6	0.00050000	2.51049995	0.98699999
1	0.83279997	3.13070011	0.63040000
1	-0.92970002	3.07540011	0.84310001
6	4.49179983	0.02740000	-0.03320000
6	5.19910002	1.15789998	0.49120000
6	6.59310007	1.09870005	0.57760000
1	7.14540005	1.94719994	0.96759999
6	7.31160021	-0.02310000	0.17950000
6	6.62020016	-1.12549996	-0.31000000
1	7.19399977	-1.99710000	-0.60619998
6	5.22700024	-1.13829994	-0.42510000
6	4.45989990	2.42129993	0.96600002
6	4.51819992	-2.39870000	-0.95289999
6	3.72059989	3.08270001	-0.21450000
1	3.02810001	2.39450002	-0.70160002
1	3.16149998	3.96440005	0.12420000
1	4.43900013	3.41210008	-0.97320002
6	3.48289990	2.06299996	2.10459995
1	2.76309991	1.30439997	1.79349995
1	4.03959990	1.66859996	2.96269989
1	2.93549991	2.95300007	2.43950009
6	5.41319990	3.48839998	1.53209996
1	5.97580004	3.12280011	2.39770007
1	6.12709999	3.84820008	0.78380001
1	4.82770014	4.35309982	1.86510003
6	5.49980021	-3.54169989	-1.26849997

1	6.21400023	-3.26999998	-2.05270004
1	6.06320000	-3.86170006	-0.38540000
1	4.93730021	-4.41050005	-1.62960005
6	3.54809999	-2.94020009	0.11650000
1	2.79730010	-2.19479990	0.38409999
1	3.04130006	-3.84450006	-0.24450000
1	4.10279989	-3.20659995	1.02380002
6	3.77629995	-2.08949995	-2.26859999
1	4.49259996	-1.80250001	-3.04620004
1	3.23149991	-2.97320008	-2.62400007
1	3.06929994	-1.26590002	-2.16129994
12	-1.37650001	-0.19090000	0.52029997
8	0.01460000	-1.24090004	-0.44589999
8	-3.20169997	-0.06610000	0.12200000
6	-0.06620000	-2.46269989	-1.14649999
1	-0.40459999	-2.31680012	-2.18280005
1	-0.78060001	-3.14849997	-0.67100000
6	-4.52969980	-0.04670000	0.09980000
6	-5.26809978	-1.23950005	-0.19110000
6	-6.66489983	-1.18069994	-0.19630000
1	-7.24079990	-2.07520008	-0.40799999
6	-7.35710001	-0.00270000	0.06050000
6	-6.63660002	1.15629995	0.32499999
1	-7.19000006	2.06970000	0.51609999
6	-5.23899984	1.17240000	0.35100001
6	-4.56129980	-2.56830001	-0.51239997
6	-4.49919987	2.48769999	0.65240002
6	-3.72650003	-3.04349995	0.69360000
1	-3.00230002	-2.29469991	1.01709998
1	-3.18869996	-3.96900010	0.44960001
1	-4.38019991	-3.25079989	1.54809999
6	-3.68039989	-2.40269995	-1.76709998
1	-2.94190001	-1.60990000	-1.64049995
1	-4.30359983	-2.14660001	-2.63140011
1	-3.15560007	-3.33850002	-1.99670005
6	-5.55159998	-3.70449996	-0.82590002
1	-6.17740011	-3.48079991	-1.69630003
1	-6.20800018	-3.93129992	0.02110000
1	-4.99030018	-4.61780024	-1.05470002
6	-5.45660019	3.67899990	0.83370000
1	-6.13689995	3.54130006	1.68050003
1	-6.05649996	3.86870003	-0.06280000
1	-4.87130022	4.58419991	1.03289998
6	-3.56769991	2.85610008	-0.52060002
1	-2.83220005	2.07200003	-0.70840001
1	-3.04250002	3.79730010	-0.31150001
1	-4.15549994	2.99600005	-1.43540001
6	-3.70810008	2.35940003	1.96940005
1	-4.39449978	2.18860006	2.80579996
1	-3.14529991	3.27789998	2.17820001
1	-3.00900006	1.52199996	1.94749999
1	0.90920001	-2.96379995	-1.18470001
1	0.13800000	2.37599993	2.06990004
1	-8.44429970	0.01270000	0.05040000
1	8.39610004	-0.04020000	0.25520000
16	0.41720000	-1.18190002	2.84209991
8	-1.03499997	-0.85490000	2.41820002
6	0.36710000	-1.00179994	4.63880014
6	0.53310001	-2.98180008	2.74699998
1	1.31819999	-1.33630002	5.05919981
1	-0.46980000	-1.57969999	5.03550005
1	0.22450000	0.05910000	4.84779978
1	1.48780000	-3.30229998	3.17050004
1	0.49939999	-3.23499990	1.68770003
1	-0.31140000	-3.42659998	3.27780008

DI-1__DBP-2_Mg-2_OMe-2_EC-2

Zero-point vibrational energy	2314488.3 (Joules/Mol)
	553.17597 (Kcal/Mol)
Zero-point correction =	0.881542 (Hartree/Particle)
Thermal correction to Energy =	0.938305
Thermal correction to Enthalpy =	0.939249
Thermal correction to Gibbs Free Energy =	0.784691
Sum of electronic and zero-point Energies =	-2556.669944
Sum of electronic and thermal Energies =	-2556.613181
Sum of electronic and thermal Enthalpies =	-2556.612237
Sum of electronic and thermal Free Energies =	-2556.766796



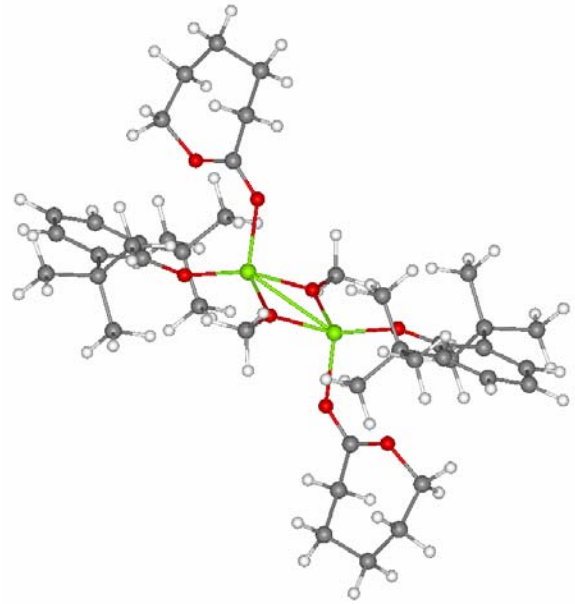
cartesian

12	-1.46370006	-0.10150000	-0.04210000
8	0.04450000	-1.02939999	0.80680001
8	-3.04010010	0.20100001	0.98600000
6	0.07060000	-1.92499995	1.89760005
1	-0.81519997	-1.80209994	2.53369999
1	0.09740000	-2.96749997	1.55309999
6	-4.35500002	0.28240001	0.83910000
6	-5.17479992	-0.89039999	0.96579999
6	-6.52720022	-0.79519999	0.61510003
1	-7.16020012	-1.67509997	0.66820002
6	-7.11009979	0.41029999	0.23150000
6	-6.34130001	1.57249999	0.27759999
1	-6.83059978	2.51749992	0.06540000
6	-4.98190022	1.55219996	0.60409999
6	-4.63630009	-2.19239998	1.59759998
6	-4.21239996	2.87639999	0.78410000
6	-3.56159997	-2.88779998	0.74269998
1	-2.65190005	-2.29290009	0.66320002
1	-3.27929997	-3.84430003	1.19920003
1	-3.92529988	-3.09780002	-0.26820001
6	-4.05499983	-1.86140001	2.98869991
1	-3.25539994	-1.12189996	2.91810012
1	-4.83489990	-1.45889997	3.64409995
1	-3.65339994	-2.76780009	3.45900011
6	-5.75360012	-3.22919989	1.81599998
1	-6.56570005	-2.83839989	2.43750000
1	-6.18149996	-3.58909988	0.87330002
1	-5.33710003	-4.10050011	2.33290005
6	-5.13430023	4.10129976	0.64789999
1	-5.54909992	4.20340014	-0.36140001
1	-5.96420002	4.07620001	1.36189997
1	-4.55579996	5.00909996	0.85130000
6	-3.60789990	2.92409992	2.20339990
1	-2.93720007	2.08109999	2.37750006
1	-3.04220009	3.85360003	2.34310007
1	-4.40030003	2.89479995	2.95930004
6	-3.09270000	3.05060005	-0.25830001
1	-3.47469997	2.93580008	-1.27789998
1	-2.65159988	4.05130005	-0.17460001
1	-2.28379989	2.33500004	-0.10930000
12	1.46360004	0.10150000	0.04220000
8	-0.04460000	1.02929997	-0.80680001
8	3.04010010	-0.19990000	-0.98619998
6	-0.07040000	1.92429996	-1.89800000
1	0.81500000	1.80050004	-2.53439999
1	-0.09640000	2.96709991	-1.55400002
6	4.35489988	-0.28169999	-0.83920002
6	5.17490005	0.89109999	-0.96499997
6	6.52729988	0.79540002	-0.61420000
1	7.16050005	1.67519999	-0.66659999
6	7.10979986	-0.41049999	-0.23130000
6	6.34089994	-1.57249999	-0.27829999
1	6.82999992	-2.51780009	-0.06680000
6	4.98150015	-1.55180001	-0.60509998
6	4.63670015	2.19350004	-1.59599996
6	4.21180010	-2.87570000	-0.78609997
6	3.56180000	2.88840008	-0.74089998
1	2.65190005	2.29349995	-0.66240001
1	3.27979994	3.84529996	-1.19679999
1	3.92499995	3.09739995	0.27030000
6	4.05579996	1.86350000	-2.98749995
1	3.25609994	1.12390006	-2.91759992
1	4.83589983	1.46140003	-3.64299989
1	3.65440011	2.77020001	-3.45729995
6	5.75409985	3.23040009	-1.81340003
1	6.56640005	2.84010005	-2.43490005
1	6.18179989	3.58960009	-0.87019998
1	5.33780003	4.10220003	-2.32969999
6	5.13350010	-4.10080004	-0.65069997
1	5.54820013	-4.20389986	0.35859999
1	5.96350002	-4.07530022	-1.36450005
1	4.55499983	-5.00839996	-0.85490000
6	3.60750008	-2.92230010	-2.20560002
1	2.93709993	-2.07909989	-2.37919998
1	3.04159999	-3.85159993	-2.34599996
1	4.40010023	-2.89269996	-2.96129990
6	3.09200001	-3.05049992	0.25600001
1	3.47379994	-2.93630004	1.27569997
1	2.65079999	-4.05109978	0.17160000
1	2.28309989	-2.33470011	0.10730000
1	-0.95599997	1.75820005	-2.52670002
1	0.95580000	-1.75849998	2.52679992
1	8.16520023	-0.45640001	0.02850000
1	-8.16539955	0.45580000	-0.02810000
6	-3.35949993	-0.84480000	-2.31590009
8	-2.28730011	-0.97890002	-1.75269997
6	-5.25470018	-1.36459994	-3.43359995
6	-5.27810001	0.11040000	-3.02579999
8	-3.92880011	0.33100000	-2.55960011
8	-4.07550001	-1.87000000	-2.77430010
1	-5.46269989	0.79299998	-3.85509992
1	-5.95340014	0.32020000	-2.19370008
1	-6.11269999	-1.92760003	-3.06839991
1	-5.12989998	-1.52049994	-4.50769997
6	3.35980010	0.84329998	2.31620002
8	2.28780007	0.97790003	1.75290000
6	5.27820015	-0.11250000	3.02600002
6	5.25489998	1.36230004	3.43460011
8	4.07579994	1.86819994	2.77550006
8	3.92910004	-0.33260000	2.55929995
1	5.13009977	1.51769996	4.50869989
1	6.11289978	1.92540002	3.06970000
1	5.95370007	-0.32200000	2.19409990

1 5.46229982 -0.79540002 3.85509992

DI-1__DBP-2_Mg-2_OMe-2_eCL-2

Zero-point vibrational energy	2741870.0 (Joules/Mol)
	655.32265 (Kcal/Mol)
Zero-point correction =	1.044323 (Hartree/Particle)
Thermal correction to Energy =	1.106188
Thermal correction to Enthalpy =	1.107132
Thermal correction to Gibbs Free Energy =	0.939188
Sum of electronic and zero-point Energies =	-2641.906101
Sum of electronic and thermal Energies =	-2641.844236
Sum of electronic and thermal Enthalpies =	-2641.843292
Sum of electronic and thermal Free Energies =	-2642.011236



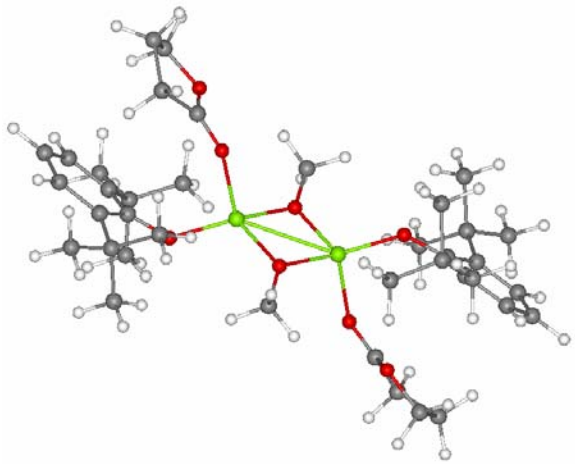
cartesian

12	1.47029996	-0.02270000	0.07830000
8	-0.05910000	0.31200001	1.27400005
8	2.96050000	1.13469994	-0.04140000
6	-0.12180000	0.70789999	2.62459993
1	0.86979997	0.97790003	3.00640011
1	-0.51789999	-0.09770000	3.25790000
6	4.23309994	1.48670006	-0.12700000
6	4.96700001	1.84780002	1.05320001
6	6.33650017	2.10750008	0.94150001
1	6.91069984	2.36190009	1.82640004
6	7.00099993	2.06699991	-0.28040001
6	6.26620007	1.81040001	-1.43390000
1	6.78660011	1.83519995	-2.38569999
6	4.89440012	1.53960001	-1.40009999
6	4.27829981	1.98409998	2.42440009
6	4.13320017	1.31930006	-2.72129989
6	3.79250002	0.61369997	2.93230009
1	3.09380007	0.14990000	2.23530006
1	3.29180002	0.71230000	3.90350008
1	4.64209986	-0.06710000	3.06279993
6	3.10100007	2.97620010	2.32760000
1	2.36780000	2.66350007	1.58369994
1	3.46849990	3.96840000	2.04270005
1	2.59960008	3.07100010	3.29909992
6	5.22499990	2.53620005	3.50589991
1	5.62830019	3.51810002	3.23709989
1	6.06519985	1.86420000	3.71329999
1	4.66909981	2.65549994	4.44280005
6	5.00400019	1.61580002	-3.95659995
1	5.85519981	0.93220001	-4.04659986
1	5.38570023	2.64219999	-3.95339990
1	4.39729977	1.49329996	-4.86100006
6	2.91930008	2.26710010	-2.81119990
1	2.22620010	2.12240005	-1.98259997
1	2.37989998	2.10450006	-3.75270009
1	3.25309992	3.31049991	-2.79189992
6	3.68670011	-0.14870000	-2.84669995
1	4.55919981	-0.81140000	-2.86689997
1	3.11999989	-0.30669999	-3.77200007
1	3.06060004	-0.45580000	-2.00819993
12	-1.46879995	-0.02090000	-0.06260000
8	0.06090000	-0.37070000	-1.25440001
8	-2.97620010	-1.15550005	0.05950000
6	0.12540001	-0.78200001	-2.60019994
1	-0.85650003	-1.10590005	-2.96460009
1	0.47389999	0.03260000	-3.25009990
6	-4.25719976	-1.47889996	0.13630000
6	-4.98740005	-1.83739996	-1.04690003
6	-6.36320019	-2.06570005	-0.94590002
1	-6.93429995	-2.31760001	-1.83360004
6	-7.03849983	-1.99650002	0.26879999
6	-6.30929995	-1.74310005	1.42659998
1	-6.83939981	-1.74559999	2.37339997
6	-4.93160009	-1.50290000	1.40330005
6	-4.28879976	-2.00419998	-2.40969992
6	-4.17859983	-1.28470004	2.72950006
6	-3.76970005	-0.65020001	-2.92880011
1	-3.06820011	-0.19220001	-2.23079991
1	-3.26180005	-0.77060002	-3.89369988
1	-4.60370016	0.04630000	-3.07550001
6	-3.13380003	-3.01979995	-2.28990006
1	-2.40129995	-2.71390009	-1.54240000
1	-3.52500010	-4.00040007	-1.99699998
1	-2.62549996	-3.13689995	-3.25530005
6	-5.23670006	-2.54909992	-3.49370003
1	-5.66319990	-3.51900005	-3.21729994

1	-6.06029987	-1.86210001	-3.71740007
1	-4.67449999	-2.69140005	-4.42369986
6	-5.06769991	-1.54809999	3.95919991
1	-5.90439987	-0.84490001	4.03340006
1	-5.47219992	-2.56579995	3.96350002
1	-4.46719980	-1.42910004	4.86829996
6	-2.98720002	-2.25830007	2.84170008
1	-2.28279996	-2.13800001	2.01850009
1	-2.45370007	-2.09809995	3.78690004
1	-3.34419990	-3.29410005	2.82979989
6	-3.70070004	0.17430000	2.84380007
1	-4.55849981	0.85640001	2.84649992
1	-3.14150000	0.33019999	3.77399993
1	-3.05800009	0.45829999	2.00970006
1	0.81419998	-1.62940001	-2.72790003
1	-0.76990002	1.58630002	2.75559998
1	-8.10949993	-2.17910004	0.31810001
1	8.06709957	2.27360010	-0.33790001
8	4.35760021	-1.67480004	0.21960001
6	3.34920001	-2.39420009	0.66990000
6	3.57170010	-3.76340008	1.25639999
1	4.20559978	-3.66880012	2.14720011
6	5.74660015	-2.06069994	0.36910000
1	6.27479982	-1.15859997	0.05980000
6	6.13590002	-3.25379992	-0.48710001
1	5.95499992	-2.22930002	1.43130004
1	5.74100018	-3.09960008	-1.49790001
6	5.70179987	-4.60970020	0.06950000
1	7.22830009	-3.23790002	-0.57810003
1	2.59150004	-4.10699987	1.58899999
6	4.19509983	-4.76980019	0.27280000
1	3.67100000	-4.71110010	-0.68849999
1	3.99830008	-5.77299976	0.66490000
1	6.20870018	-4.77939987	1.02909994
1	6.05259991	-5.40030003	-0.60310000
8	2.21350002	-1.91939998	0.57669997
8	-4.33190012	1.67340004	-0.24710000
6	-3.30609989	2.37800002	-0.68140000
6	-3.49880004	3.75139999	-1.26859999
1	-4.12260008	3.66840005	-2.16770005
6	-5.71229982	2.08229995	-0.41319999
1	-6.25909996	1.18859994	-0.11190000
6	-6.09289980	3.28020000	0.44049999
1	-5.90469980	2.25629997	-1.47749996
1	-5.71320009	3.11770010	1.45580006
6	-5.63009977	4.63000011	-0.10780000
1	-7.18650007	3.28169990	0.51789999
1	-2.50889993	4.07959986	-1.58790004
6	-4.11850023	4.76630020	-0.29139999
1	-3.60789990	4.69780016	0.67629999
1	-3.90070009	5.76669979	-0.67949998
1	-6.12179995	4.80940008	-1.07350004
1	-5.97690010	5.42479992	0.56180000
8	-2.17930007	1.88549995	-0.57279998

DI-1__DBP-2_Mg-2_OMe-2_gBL-2

Zero-point vibrational energy	2437311.3 (Joules/Mol)
	582.53137 (Kcal/Mol)
Zero-point correction =	0.928323 (Hartree/Particle)
Thermal correction to Energy =	0.985591
Thermal correction to Enthalpy =	0.986535
Thermal correction to Gibbs Free Energy =	0.831849
Sum of electronic and zero-point Energies =	-2484.819543
Sum of electronic and thermal Energies =	-2484.762275
Sum of electronic and thermal Enthalpies =	-2484.761331
Sum of electronic and thermal Free Energies =	-2484.916017



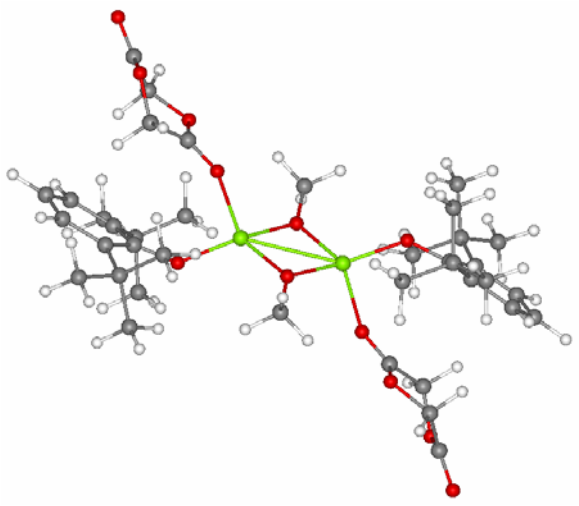
cartesian

12	-1.46809995	0.07160000	-0.04070000
8	0.07300000	1.28649998	-0.20050000
8	-3.00419998	0.44690001	-1.12699997
6	0.15970001	2.61919999	-0.65799999
1	-0.66759998	2.86209989	-1.33710003
1	0.12770000	3.32909989	0.17960000
6	-4.30989981	0.37300000	-0.90270001
6	-5.03859997	1.51950002	-0.43740001
6	-6.36660004	1.34399998	-0.03200000
1	-6.93009996	2.18849993	0.35170001
6	-7.01060009	0.11170000	-0.12020000
6	-6.34429979	-0.95230001	-0.72469997
1	-6.89190006	-1.87730002	-0.87629998
6	-5.02059984	-0.84579998	-1.16610003
6	-4.41650009	2.93009996	-0.44080001
6	-4.39169979	-1.97609997	-2.00710011
6	-3.30800009	3.07259989	0.61799997
1	-2.47390008	2.39669991	0.43200001

1	-2.90750003	4.09359980	0.61629999
1	-3.69370008	2.86780000	1.62269998
6	-3.85080004	3.23729992	-1.84280002
1	-3.10489988	2.49920011	-2.14070010
1	-4.65439987	3.23049998	-2.58759999
1	-3.38860011	4.23229980	-1.85609996
6	-5.45779991	4.02150011	-0.13370000
1	-6.30039978	3.99510002	-0.83260000
1	-5.85309982	3.95180011	0.88590002
1	-4.98420000	5.00500011	-0.22679999
6	-5.39510012	-3.11030006	-2.28200006
1	-5.69439983	-3.63499999	-1.36699998
1	-6.29899979	-2.75149989	-2.78469992
1	-4.92880011	-3.85139990	-2.94039989
6	-3.97040009	-1.40030003	-3.37560010
1	-3.25690007	-0.58300000	-3.25399995
1	-3.50340009	-2.18160009	-3.98830009
1	-4.84170008	-1.01970005	-3.91969991
6	-3.16790009	-2.62269998	-1.33169997
1	-3.37820005	-2.90159988	-0.29449999
1	-2.87840009	-3.53349996	-1.86969995
1	-2.29970002	-1.96239996	-1.34790003
12	1.46980000	-0.10020000	-0.10650000
8	-0.06820000	-1.31180000	0.04670000
8	2.98679996	-0.44940001	1.00220001
6	-0.12400000	-2.64949989	0.49579999
1	0.75629997	-2.90120006	1.10119998
1	-0.16190000	-3.34949994	-0.35020000
6	4.30100012	-0.30370000	0.88709998
6	5.10869980	-1.37030005	0.36649999
6	6.44840002	-1.09959996	0.06340000
1	7.07189989	-1.87810004	-0.36489999
6	7.03039980	0.13820000	0.32640001
6	6.28240013	1.10200000	1.00059998
1	6.77860022	2.02230000	1.29250002
6	4.93809986	0.90270001	1.33010006
6	4.56930017	-2.81209993	0.25130001
6	4.20160007	1.92069995	2.22460008
6	3.48860002	-2.96639991	-0.83310002
1	2.60060000	-2.37409997	-0.61580002
1	3.17129993	-4.01380014	-0.90600002
1	3.86750007	-2.66700006	-1.81620002
6	3.99329996	-3.24020004	1.61769998
1	3.19309998	-2.57080007	1.93750000
1	4.77640009	-3.22690010	2.38369989
1	3.59529996	-4.26100016	1.55980003
6	5.68270016	-3.81649995	-0.09740000
1	6.50129986	-3.79270005	0.62910002
1	6.10330009	-3.64800000	-1.09549999
1	5.26739979	-4.83029985	-0.09120000
6	5.14739990	3.02449989	2.73230004
1	5.52069998	3.66260004	1.92309999
1	6.00699997	2.61549997	3.27349997
1	4.60220003	3.67249990	3.42720008
6	3.65079999	1.19379997	3.46970010
1	2.96650004	0.39160001	3.18779993
1	3.11229992	1.90059996	4.11339998
1	4.46880007	0.75989997	4.05520010
6	3.04660010	2.63129997	1.49539995
1	3.38010001	3.07060003	0.55019999
1	2.64870000	3.44050002	2.12010002
1	2.21609998	1.95480001	1.28929996
1	-1.01349998	-2.82419991	1.11510003
1	1.09829998	2.79119992	-1.20239997
1	8.07429981	0.32089999	0.08110000
1	-8.04100037	0.00200000	0.21010000
6	-3.45210004	-0.67360002	2.27200007
8	-2.47720003	-0.13420001	1.76540005
6	-5.26779985	-1.18649995	3.71799994
6	-4.91279984	-2.35179996	2.79489994
8	-3.63360000	-1.99179995	2.20479989
6	-4.57520008	-0.01380000	3.02579999
1	-4.77050018	-3.30760002	3.29929996
1	-5.62179995	-2.46550012	1.97119999
1	-6.34709978	-1.05649996	3.81130004
1	-4.85179996	-1.34920001	4.71649981
6	3.39000010	0.58139998	-2.40630007
8	2.38840008	0.01960000	-1.97959995
6	5.03669977	2.16709995	-2.55739999
6	5.55999994	0.93129998	-3.29110003
6	4.28389978	0.12520000	-3.53060007
8	3.80960011	1.73710001	-1.90649998
1	6.08960009	1.19250000	-4.20919991
1	6.23740005	0.37630001	-2.63820004
1	5.69630003	2.52640009	-1.76849997
1	4.77199984	2.98990011	-3.22790003
1	4.40630007	-0.95700002	-3.50559998
1	3.78660011	0.38580000	-4.47270012
1	-4.19059992	0.76419997	3.68639994
1	-5.21630001	0.46390000	2.27390003

DI-1__DBP-2_Mg-2_OMe-2_GL-2

Zero-point vibrational energy	2363822.7 (Joules/Mol)
	564.96719 (Kcal/Mol)
Zero-point correction =	0.900333 (Hartree/Particle)
Thermal correction to Energy =	0.960243
Thermal correction to Enthalpy =	0.961187
Thermal correction to Gibbs Free Energy =	0.801655
Sum of electronic and zero-point Energies =	-2783.229651
Sum of electronic and thermal Energies =	-2783.169741
Sum of electronic and thermal Enthalpies =	-2783.168797
Sum of electronic and thermal Free Energies =	-2783.328329



cartesian

12	-1.44700003	-0.18860000	-0.06720000
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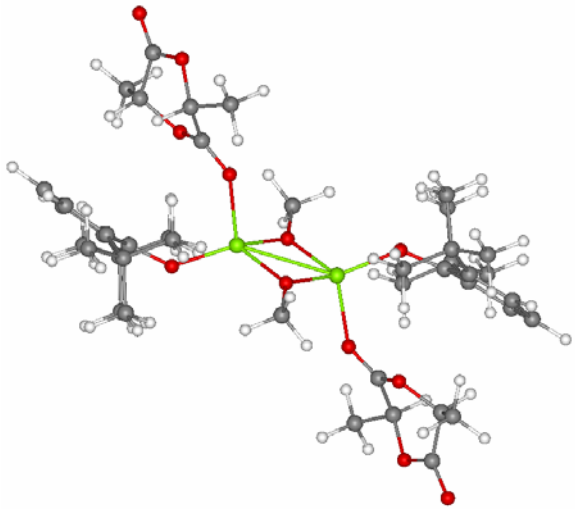
8	-2.80520010	-1.28880000	0.70620000
6	0.39179999	-2.34100008	-1.28199995
1	-0.33329999	-3.04979992	-0.86350000
1	0.29960001	-2.36820006	-2.37599993
6	-4.13089991	-1.29240000	0.69309998
6	-4.85139990	-2.05119991	-0.29010001
6	-6.23400021	-1.85839999	-0.39480001
1	-6.79710007	-2.39330006	-1.15269995
6	-6.93039989	-1.00730002	0.46090001
6	-6.24679995	-0.41740000	1.52300000
1	-6.82189989	0.14820001	2.24979997
6	-4.86590004	-0.57279998	1.69640005
6	-4.15560007	-3.11290002	-1.16589999
6	-4.18959999	-0.09040000	2.99710011
6	-3.23189998	-2.47819996	-2.22059989
1	-2.42750001	-1.89789999	-1.76820004
1	-2.76580000	-3.25589991	-2.83699989
1	-3.79310012	-1.81780005	-2.89100003
6	-3.34770012	-4.07200003	-0.26670000
1	-2.59330010	-3.53900003	0.31340000
1	-4.01300001	-4.58830023	0.43370000
1	-2.84929991	-4.83319998	-0.87910002
6	-5.17110014	-3.97819996	-1.93449998
1	-5.88630009	-4.46570015	-1.26409996
1	-5.73350000	-3.40739989	-2.68190002
1	-4.63560009	-4.76760006	-2.47289991
6	-5.21010017	0.49300000	3.99049997
1	-5.68550014	1.40660000	3.61470008
1	-5.99679995	-0.22390001	4.24599981
1	-4.69589996	0.75809997	4.92040014
6	-3.52539992	-1.30270004	3.68440008
1	-2.78110003	-1.76520002	3.03349996
1	-3.02940011	-0.98750001	4.61059999
1	-4.27500010	-2.05789995	3.94309998
6	-3.12910008	0.99970001	2.76149988
1	-3.53220010	1.84089994	2.18919992
1	-2.77430010	1.39189994	3.72199988
1	-2.25580001	0.61019999	2.23760009
12	1.45439994	0.27919999	-0.07640000
8	-0.17160000	1.15079999	0.59750003
8	2.87249994	1.39429998	-0.70789999
6	-0.37610000	2.48009992	1.03439999
1	0.38409999	3.15359998	0.61970001
1	-0.32720000	2.54769993	2.12919998
6	4.19469976	1.32900000	-0.62629998
6	4.89359999	1.96480000	0.45539999
6	6.25899982	1.69649994	0.61100000
1	6.80480003	2.13689995	1.43920004
6	6.96239996	0.89080000	-0.28250000
6	6.31080008	0.42649999	-1.42410004
1	6.89750004	-0.10260000	-2.16860008
6	4.94869995	0.66030002	-1.64900005
6	4.20170021	2.99099994	1.37650001
6	4.31790018	0.31600001	-3.01500010
6	3.14319992	2.34509993	2.28789997
1	2.32830000	1.90040004	1.71780002
1	2.70219994	3.09949994	2.95020008
1	3.58450007	1.56799996	2.92109990
6	3.54579997	4.08519983	0.50840002
1	2.82049990	3.66070008	-0.18740000
1	4.30590010	4.61810017	-0.07290000
1	3.03500009	4.81790018	1.14499998
6	5.20459986	3.69840002	2.30550003
1	6.00330019	4.19750023	1.74759996
1	5.66400003	3.01430011	3.02800012
1	4.67829990	4.46670008	2.88249993
6	5.36380005	-0.22210000	-4.00810003
1	5.78760004	-1.18320000	-3.69390011
1	6.18709993	0.48220000	-4.16450024
1	4.88579988	-0.38479999	-4.97989988
6	3.73289990	1.60640001	-3.62789989
1	2.97250009	2.04259992	-2.97760010
1	3.27579999	1.38979995	-4.60120010
1	4.52129984	2.35030007	-3.78410006
6	3.20970011	-0.74860001	-2.92149997
1	3.55209994	-1.64499998	-2.39470005
1	2.89730000	-1.05540001	-3.92680001
1	2.31900001	-0.36870000	-2.41899991
8	-5.79879999	2.24839997	-2.48760009
6	-4.99770021	1.11000001	-2.15229988
6	-3.84549999	1.44480002	-1.24329996
8	-4.05039978	2.40650010	-0.35460001
6	-5.41510010	2.84559989	-0.17200001
6	-6.14699984	3.07769990	-1.47790003
8	-2.76099992	0.88220000	-1.31289995
1	-5.94290018	2.09599996	0.42870000
1	-5.35850000	3.78209996	0.37700000
6	5.31750011	-2.87919998	0.05350000
8	3.96420002	-2.38879991	0.18230000
6	3.73720002	-1.49820006	1.13720000
6	4.83190012	-1.30320001	2.15199995
8	5.56029987	-2.50259995	2.43460011
6	5.94619989	-3.25530005	1.37940001
8	2.67840004	-0.88789999	1.18180001
1	5.25750017	-3.76390004	-0.57550001
1	5.91820002	-2.11120009	-0.44679999
1	-1.35880005	2.85319996	0.71880001
1	1.39530003	-2.70029998	-1.02090001

1	8.02140045	0.69510001	-0.13310000
1	-8.00339985	-0.87050003	0.35060000
1	-5.60559988	0.33520001	-1.66320002
1	-4.61100006	0.71319997	-3.08850002
1	5.50390005	-0.51730001	1.77980006
1	4.39340019	-0.97450000	3.09179997
8	6.72919989	-4.16060019	1.50139999
8	-6.97559977	3.93790007	-1.62279999

DI-1__DBP-2_Mg-2_OMe-2_LA-2

Zero-point vibrational energy	2656682.2 (Joules/Mol)
	634.96229 (Kcal/Mol)
Zero-point correction =	1.011877 (Hartree/Particle)
Thermal correction to Energy =	1.077874
Thermal correction to Enthalpy =	1.078818
Thermal correction to Gibbs Free Energy =	0.905852
Sum of electronic and zero-point Energies =	-2940.349349
Sum of electronic and thermal Energies =	-2940.283353
Sum of electronic and thermal Enthalpies =	-2940.282408
Sum of electronic and thermal Free Energies =	-2940.455374



cartesian

12	1.45219898	-0.16055077	-0.19066003
8	-0.17640096	-0.32075077	-1.27946007
8	2.70879889	-1.58455074	-0.36076003
6	-0.40680096	-1.08225071	-2.44656014
1	0.33019903	-1.88945067	-2.54396009
1	-0.34420097	-0.45535076	-3.34616017
6	4.02659893	-1.70685065	-0.25956002
6	4.85849905	-1.57985067	-1.42296004
6	6.24379921	-1.49245071	-1.23806012
1	6.89619923	-1.35795069	-2.09506011
6	6.83079910	-1.61775076	0.01943997
6	6.02219915	-1.93595076	1.10973990
1	6.50519896	-2.13835073	2.06033993
6	4.63029909	-2.02175093	1.00243998
6	4.27429914	-1.68275070	-2.84826016
6	3.79039907	-2.53985071	2.18874002
6	3.37149906	-0.49495077	-3.22365999
1	2.49779892	-0.42255077	-2.57666016
1	3.00779891	-0.60495079	-4.25235987
1	3.92349911	0.45004922	-3.17226005
6	3.46689892	-2.99375081	-2.95516014
1	2.65649891	-3.02055073	-2.22456002
1	4.11579895	-3.85795093	-2.77796006
1	3.03699899	-3.09495091	-3.95916009
6	5.37749910	-1.74705076	-3.91956019
1	6.06299877	-2.58465075	-3.75586009
1	5.96779919	-0.82495075	-3.97256017
1	4.91609907	-1.88945067	-4.90285969
6	4.67789888	-2.98535085	3.36473989
1	5.22799921	-2.15195084	3.81683993
1	5.39959908	-3.75385094	3.06973982
1	4.04609919	-3.41545081	4.14924002
6	2.98899889	-3.77835083	1.73433995
1	2.32939911	-3.53685093	0.89883995
1	2.37749910	-4.15865088	2.56203985
1	3.66529894	-4.58025074	1.41923988
6	2.81819892	-1.48145068	2.74283981
1	3.32929897	-0.53925079	2.96454000
1	2.36209893	-1.83935070	3.67383981
1	1.99999905	-1.27715075	2.05083990
12	-1.42450094	0.35234922	0.08173996
8	0.20929903	0.54624921	1.15903986
8	-2.76580095	1.69864929	0.23123997
6	0.45049903	1.27834928	2.34184003
1	-0.26280096	2.10554910	2.44823980
1	0.36109903	0.63774925	3.22964001
6	-4.09250116	1.73404932	0.18413997
6	-4.86440086	1.63724935	1.39103997
6	-6.24840117	1.45464933	1.27893996
1	-6.85220098	1.34084928	2.17353988
6	-6.89600086	1.45634925	0.04543997
6	-6.15640116	1.74334931	-1.10086012
1	-6.69180107	1.84744930	-2.03926015
6	-4.76970100	1.92094934	-1.06606007
6	-4.22610092	1.85674930	2.77934003
6	-4.01770115	2.39824915	-2.32586002
6	-3.27350092	0.71994925	3.18763995
1	-2.43910098	0.61434925	2.49483991
1	-2.85250092	0.91364926	4.18164015
1	-3.80610108	-0.23635076	3.23984003
6	-3.45760107	3.19504929	2.76943994
1	-2.67810106	3.19874907	2.00593996
1	-4.14070082	4.02624941	2.56483984

1	-2.99300098	3.37334919	3.74693990
6	-5.28610086	1.95804930	3.89103985
1	-6.00860119	2.75774908	3.69953990
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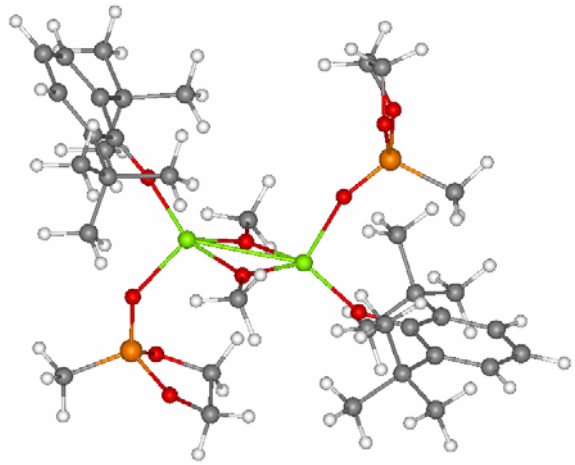
1	-4.79000092	2.18514919	4.84094000
6	-4.98050117	2.69664907	-3.48916006
1	-5.49350119	1.79864931	-3.85266018
1	-5.73740101	3.43964911	-3.21836019
1	-4.41090107	3.10364914	-4.33155966
6	-3.28110099	3.71564913	-2.00346017
1	-2.57960105	3.58504915	-1.17756009
1	-2.72380090	4.06284904	-2.88216019
1	-3.99620104	4.49804926	-1.72746015
6	-3.00410104	1.36124933	-2.84436011
1	-3.45980096	0.37234923	-2.95716000
1	-2.62050104	1.66514933	-3.82596016
1	-2.13950109	1.27194929	-2.18536019
8	5.53539896	3.57684922	-0.36946002
6	4.71569920	2.66694927	-1.12406003
6	3.81729889	1.85664928	-0.20956004
8	4.29289913	1.55064929	0.98133999
6	5.72059917	1.74714935	1.22563994
6	6.15939903	3.12244916	0.74293995
8	2.69529891	1.49584925	-0.54456002
1	6.24469900	0.97444922	0.64753997
6	5.96209908	1.54534924	2.70314002
6	-5.66270113	-1.93095076	-1.00176013
8	-4.23980093	-1.62415075	-0.87276006
6	-3.66840100	-1.81185067	0.30083996
6	-4.44870090	-2.61095071	1.32673991
8	-5.24650097	-3.62665081	0.69333994
6	-5.97000122	-3.29635072	-0.40236002
8	-2.55540109	-1.35705066	0.53403997
6	-6.01530123	-1.84505069	-2.46826005
1	-6.20110083	-1.15815067	-0.43716002
1	1.46099901	1.70944929	2.34324002
1	-1.40380096	-1.54305065	-2.43045998
1	-7.97330093	1.31914926	-0.01266004
1	7.91039896	-1.55285072	0.13323995
1	5.36819887	1.94114923	-1.63046014
6	3.94589901	3.48284912	-2.14296007
1	-5.11880112	-1.89505076	1.82393992
6	-3.56150103	-3.29665089	2.34604001
8	-6.79060078	-4.05495071	-0.85026002
8	6.99789906	3.78844929	1.29333997
1	-4.18650103	-3.83065081	3.06413984
1	-2.89620090	-4.01025105	1.85573995
1	-2.95730090	-2.55885077	2.87414002
1	-7.08030081	-2.04555082	-2.59145999
1	-5.79470110	-0.84195077	-2.83495998
1	-5.45510101	-2.58205080	-3.04776001
1	3.33299899	2.82804918	-2.76256013
1	3.29599905	4.20424938	-1.64356005
1	4.65179920	4.02174902	-2.77766013
1	7.02659893	1.66404927	2.90994000
1	5.41089916	2.28124928	3.29253983
1	5.65339899	0.53854924	2.98643994

DI-1__DBP-2_Mg-2_OMe-2_Me-EP-2

Zero-point vibrational energy	2492234.0 (Joules/Mol)
	595.65823 (Kcal/Mol)
Zero-point correction =	0.949242 (Hartree/Particle)
Thermal correction to Energy =	1.010943
Thermal correction to Enthalpy =	1.011887
Thermal correction to Gibbs Free Energy =	0.847480
Sum of electronic and zero-point Energies =	-3242.905852
Sum of electronic and thermal Energies =	-3242.844151
Sum of electronic and thermal Enthalpies =	-3242.843207
Sum of electronic and thermal Free Energies =	-3243.007614



cartesian

12	-1.68980002	0.84850001	0.03830000
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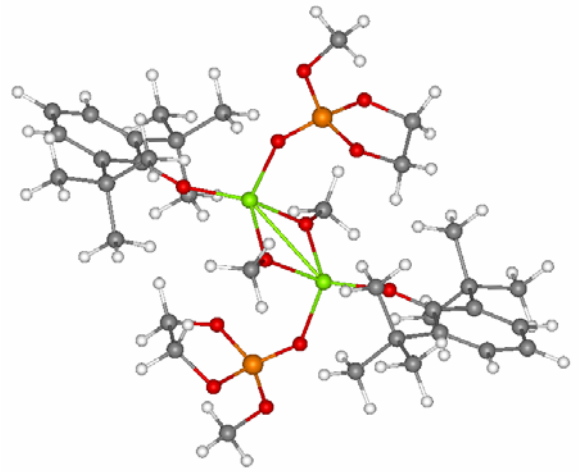
8	-3.29480004	-0.12490000	0.04970000
6	-0.18850000	0.40849999	-2.64109993
1	-0.16200000	-0.64760000	-2.94199991
1	-1.08879995	0.85430002	-3.08240008
6	-4.51060009	-0.65160000	0.08020000
6	-5.13910007	-1.09119999	-1.13110006
6	-6.42350006	-1.63859999	-1.06459999
1	-6.91419983	-1.97340000	-1.97259998
6	-7.10809994	-1.77349997	0.13830000
6	-6.49179983	-1.35529995	1.31270003
1	-7.03599977	-1.47039998	2.24419999

6	-5.20909977	-0.79960001	1.32340002
6	-4.42729998	-0.97810000	-2.49070001
6	-4.57579994	-0.36939999	2.65840006
6	-4.15080023	0.50110000	-2.82669997
1	-3.57669997	0.99559999	-2.04180002
1	-3.60139990	0.58759999	-3.77279997
1	-5.09499979	1.04639995	-2.93499994
6	-3.11989999	-1.79569995	-2.47149992
1	-2.45040011	-1.46800005	-1.67509997
1	-3.34710002	-2.85610008	-2.30890012
1	-2.59570003	-1.70690000	-3.43120003
6	-5.27139997	-1.53610003	-3.65039992
1	-5.50209999	-2.59920001	-3.52139997
1	-6.21390009	-0.99309999	-3.77839994
1	-4.70879984	-1.43579996	-4.58589983
6	-5.49209976	-0.64709997	3.86389995
1	-6.43809986	-0.09820000	3.80390000
1	-5.71859980	-1.71280003	3.97620010
1	-4.98640013	-0.32359999	4.78109980
6	-3.27719998	-1.16229999	2.91009998
1	-2.54819989	-1.02310002	2.11109996
1	-2.81760001	-0.85630000	3.85789990
1	-3.50060010	-2.23329997	2.97650003
6	-4.31090021	1.14970005	2.65879989
1	-5.25780010	1.69679999	2.58710003
1	-3.81539989	1.45650005	3.58890009
1	-3.69330001	1.46060002	1.81519997
12	1.13489997	0.01060000	0.13240001
8	-0.23450001	0.68440002	1.36819994
8	2.95889997	0.53479999	0.01670000
6	-0.25150001	0.89700001	2.76169991
1	0.56010002	1.56990004	3.06879997
1	-0.13740000	-0.04580000	3.31419992
6	4.25990009	0.27370000	0.07050000
6	4.95839977	0.29859999	1.32430005
6	6.30490017	-0.07840000	1.35020006
1	6.84469986	-0.08380000	2.29130006
6	6.99520016	-0.44270000	0.19920000
6	6.33839989	-0.38080001	-1.02499998
1	6.90399981	-0.61949998	-1.91960001
6	4.99340010	-0.01060000	-1.13129997
6	4.27309990	0.74409997	2.63080001
6	4.35129976	0.11570000	-2.52710009
6	3.22709990	-0.29449999	3.07710004
1	2.46970010	-0.47490001	2.31299996
1	2.71180010	0.03500000	3.98670006
1	3.71259999	-1.25189996	3.29979992
6	3.61940002	2.12890005	2.44860005
1	2.87479997	2.11330009	1.65199995
1	4.38070011	2.87409997	2.19079995
1	3.13549995	2.44959998	3.37919998
6	5.26809978	0.88520002	3.79740000
1	6.06629992	1.60070002	3.57369995
1	5.72900009	-0.06870000	4.07480001
1	4.73500013	1.25209999	4.68160009
6	5.37419987	-0.06350000	-3.66339993
1	5.80929995	-1.06850004	-3.68239999
1	6.19000006	0.66399997	-3.59980011
1	4.87249994	0.08760000	-4.62580013
6	3.74729991	1.52390003	-2.70129991
1	3.00379992	1.72839999	-1.92999995
1	3.27430010	1.61829996	-3.68689990
1	4.53350019	2.28410006	-2.63080001
6	3.27080011	-0.96069998	-2.73740005
1	3.71230006	-1.96319997	-2.69589996
1	2.79590011	-0.85110003	-3.71959996
1	2.48720002	-0.90149999	-1.98150003
1	0.68339998	0.90280002	-3.09200001
1	-1.19729996	1.35270000	3.08179998
1	8.04030037	-0.73799998	0.25130001
1	-8.10830021	-2.19989991	0.16040000
8	1.18710005	-2.00780010	0.29750001
15	1.76269996	-3.38179994	0.22010000
8	1.05320001	-4.40089989	1.25500000
8	1.42439997	-4.19710016	-1.13479996
6	0.40889999	-5.49030018	0.56019998
6	0.27050000	-5.03639984	-0.89429998
1	1.04170001	-6.37709999	0.65499997
1	-0.55570000	-5.66909981	1.03649998
1	-0.63709998	-4.45020008	-1.05939996
1	0.31290001	-5.86299992	-1.60329998
6	3.53309989	-3.43689990	0.45339999
1	3.90630007	-4.45219994	0.30930001
1	3.75970006	-3.09730005	1.46570003
1	4.01639986	-2.75049996	-0.24529999
8	-2.15919995	2.82680011	-0.09710000
15	-1.50209999	4.14610004	-0.34670001
8	-0.26350001	4.45900011	0.63880002
8	-0.70730001	4.30070019	-1.74210000
6	0.96850002	4.61959982	-0.10670000
6	0.69709998	4.02920008	-1.49049997
1	1.19840002	5.68779993	-0.14950000
1	1.75580001	4.08760023	0.42649999
1	0.84939998	2.94770002	-1.51279998
1	1.27079999	4.51189995	-2.28080010
6	-2.68269992	5.48839998	-0.26740000
1	-2.18880010	6.44770002	-0.42550001
1	-3.16389990	5.47209978	0.71230000
1	-3.44549990	5.33129978	-1.03260005

DI-1__DBP-2_Mg-2_OMe-2_MeO-EP-2

Zero-point vibrational energy	2523868.7 (Joules/Mol)
	603.21909 (Kcal/Mol)
Zero-point correction =	0.961291 (Hartree/Particle)
Thermal correction to Energy =	1.024826
Thermal correction to Enthalpy =	1.025770

Thermal correction to Gibbs Free Energy =	0.859127
Sum of electronic and zero-point Energies =	-3393.311863
Sum of electronic and thermal Energies =	-3393.248328
Sum of electronic and thermal Enthalpies =	-3393.247384
Sum of electronic and thermal Free Energies =	-3393.414026



cartesian

12	1.34949994	0.72420001	0.00490000
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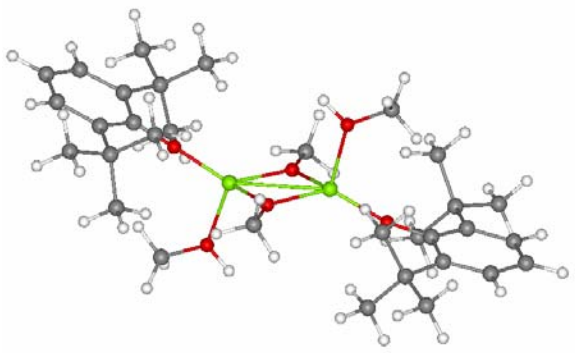
8	3.12789989	0.08530000	0.01230000
6	-0.04820000	-0.05050000	2.67569995
1	0.21320000	-1.09730005	2.88159990
1	0.69300002	0.57999998	3.18330002
6	4.45709991	0.02560000	0.07190000
6	5.12500000	-0.09550000	1.33539999
6	6.51739979	-0.22210000	1.35060000
1	7.03809977	-0.32280001	2.29660010
6	7.27479982	-0.22059999	0.18539999
6	6.62750006	-0.06980000	-1.03489995
1	7.23330021	-0.05230000	-1.93420005
6	5.23839998	0.06160000	-1.13039994
6	4.35809994	-0.06830000	2.67070007
6	4.59600019	0.25880000	-2.51620007
6	3.63800001	1.28480005	2.83550000
1	2.95639992	1.49399996	2.00970006
1	3.06629992	1.30869997	3.77130008
1	4.36709976	2.10170007	2.86579990
6	3.35960007	-1.23839998	2.74799991
1	2.62730002	-1.19830000	1.94190001
1	3.89289999	-2.19370008	2.67930007
1	2.82150006	-1.22549999	3.70350003
6	5.28660011	-0.21179999	3.89050007
1	5.82840014	-1.16380000	3.89059997
1	6.01730013	0.60100001	3.95670009
1	4.68380022	-0.18099999	4.80520010
6	5.63240004	0.25960001	-3.65499997
1	6.36299992	1.06879997	-3.55369997
1	6.17659998	-0.68870002	-3.72359991
1	5.11549997	0.40810001	-4.60990000
6	3.61719990	-0.88929999	-2.82760000
1	2.80629992	-0.92979997	-2.09929991
1	3.17939997	-0.76599997	-3.82590008
1	4.15280008	-1.84669995	-2.81229997
6	3.88120008	1.62279999	-2.58010006
1	4.60650015	2.43530011	-2.46429992
1	3.38170004	1.75390005	-3.54819989
1	3.13930011	1.74090004	-1.78999996
12	-1.34570003	-0.51539999	-0.06240000
8	0.05290000	0.06910000	-1.33029997
8	-3.17149997	-0.03250000	-0.02020000
6	0.06760000	0.17620000	-2.73790002
1	-0.76139998	0.79629999	-3.09899998
1	-0.01920000	-0.81070000	-3.21379995
6	-4.49830008	-0.12000000	-0.10010000
6	-5.15950012	-0.01300000	-1.36769998
6	-6.55530024	-0.08470000	-1.40690005
1	-7.07250023	-0.00410000	-2.35689998
6	-7.32089996	-0.25760001	-0.25999999
6	-6.67710018	-0.36260000	0.96710002
1	-7.28770018	-0.49869999	1.85329998
6	-5.28539991	-0.29830000	1.08560002
6	-4.37709999	0.16890000	-2.68169999
6	-4.64279985	-0.42359999	2.47939992
6	-3.48839998	-1.06239998	-2.94490004
1	-2.80739999	-1.26559997	-2.11710000
1	-2.89179993	-0.92580003	-3.85459995
1	-4.10839987	-1.95560002	-3.07730007
6	-3.53780007	1.46029997	-2.63450003
1	-2.79889989	1.43690002	-1.83319998
1	-4.19000006	2.32640004	-2.47199988
1	-3.01270008	1.61430001	-3.58529997
6	-5.30070019	0.30050001	-3.90660000
1	-5.96199989	1.17079997	-3.83610010
1	-5.91809988	-0.59039998	-4.06160021
1	-4.68709993	0.42940000	-4.80560017
6	-5.68419981	-0.54920000	3.60579991
1	-6.30219984	-1.44710004	3.50300002
1	-6.34679985	0.32139999	3.65849996
1	-5.16429996	-0.62349999	4.56780005
6	-3.81299996	0.83579999	2.79430008
1	-3.01760006	0.96410000	2.05929995
1	-3.36590004	0.76580000	3.79410005
1	-4.45400000	1.72549999	2.77430010
6	-3.76349998	-1.68690002	2.55119991
1	-4.37849998	-2.58400011	2.42219996
1	-3.26329994	-1.75779998	3.52530003
1	-3.00239992	-1.70319998	1.77100003
1	-1.02489996	0.14210001	3.13800001
1	1.00070000	0.63190001	-3.09170008
1	-8.40530014	-0.30960000	-0.32170001
1	8.35649967	-0.32240000	0.22880000
8	-1.14080000	-2.53929996	0.02290000
15	-0.24670000	-3.71700001	-0.08240000
8	0.35730001	-3.98049998	-1.54620004
8	1.13429999	-3.68429995	0.73060000
6	1.80490005	-4.04330015	-1.51520002
6	2.23300004	-3.41810012	-0.18300000

1	2.09610009	-5.09429979	-1.59440005
1	2.18070006	-3.48670006	-2.37260008
1	2.38579988	-2.33829999	-0.24990000
1	3.12350011	-3.88499999	0.23570000
8	-1.04439998	-4.98969984	0.40410000
8	1.30929995	2.75620008	-0.04280000
15	0.31630000	3.85089993	0.10840000
8	-1.12469995	3.56439996	-0.53070003
8	-0.16310000	4.20419979	1.59940004
6	-2.17070007	3.60750008	0.47560000
6	-1.45019996	3.57100010	1.82780004
1	-2.73320007	4.53280020	0.32730001
1	-2.81719995	2.74300003	0.32350001
1	-1.27569997	2.54909992	2.16709995
1	-1.96430004	4.14379978	2.59870005
8	0.92309999	5.16870022	-0.51069999
6	0.16440000	6.39480019	-0.54000002
6	-0.44530001	-6.30009985	0.39390001
1	-1.19920003	-6.97319984	0.79860002
1	0.44459999	-6.31629992	1.02730000
1	-0.20000000	-6.59539986	-0.62910002
1	0.81639999	7.13460016	-1.00109994
1	-0.09190000	6.70590019	0.47510001
1	-0.73559999	6.26609993	-1.14549994

DI-1__DBP-2_Mg-2_OMe-2_MeOH-2

Zero-point vibrational energy	2190791.6 (Joules/Mol)
	523.61175 (Kcal/Mol)
Zero-point correction =	0.834428 (Hartree/Particle)
Thermal correction to Energy =	0.887407
Thermal correction to Enthalpy =	0.888351
Thermal correction to Gibbs Free Energy =	0.744903
Sum of electronic and zero-point Energies =	-2103.467078
Sum of electronic and thermal Energies =	-2103.414099
Sum of electronic and thermal Enthalpies =	-2103.413155
Sum of electronic and thermal Free Energies =	-2103.556603



cartesian

12	1.38979995	-0.00030000	-0.27129999
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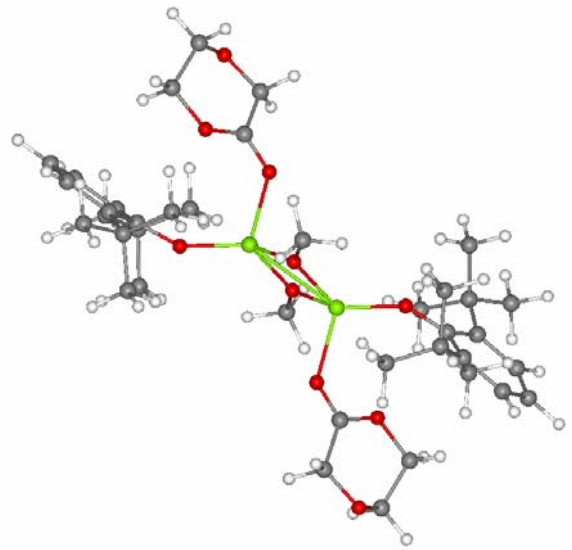
8	3.21510005	0.00180000	0.10730000
8	1.37380004	-0.00130000	-2.36669993
6	0.00050000	2.71490002	0.23029999
1	0.87800002	3.09319997	0.76819998
1	0.02310000	3.13050008	-0.78630000
6	2.47810006	-0.00020000	-3.29530001
1	2.44580007	0.89810002	-3.91720009
1	3.38509989	0.00090000	-2.69420004
1	0.53109998	-0.00310000	-2.84290004
6	4.54549980	-0.00040000	0.06580000
6	5.26809978	1.23599994	0.04890000
6	6.66009998	1.19410002	-0.07890000
1	7.22639990	2.11870003	-0.11070000
6	7.35909986	-0.00470000	-0.16069999
6	6.65670013	-1.20130002	-0.07620000
1	7.22039986	-2.12750006	-0.10600000
6	5.26450014	-1.23889995	0.05150000
6	4.55859995	2.59529996	0.20080000
6	4.55119991	-2.59599996	0.20600000
6	3.63220000	2.87339997	-0.99839997
1	2.85700011	2.11279988	-1.10319996
1	3.13750005	3.84599996	-0.88830000
1	4.20930004	2.89420009	-1.92960000
6	3.76699996	2.62930012	1.52390003
1	3.02729988	1.82860005	1.57280004
1	4.44719982	2.50819993	2.37409997
1	3.25370002	3.59200001	1.64030004
6	5.55149984	3.77110004	0.25680000
1	6.25190020	3.68149996	1.09360003
1	6.12960005	3.87299991	-0.66759998
1	4.99510002	4.70499992	0.39530000
6	5.54090023	-3.77440000	0.26539999
1	6.11940002	-3.88000011	-0.65850002
1	6.24100018	-3.68460011	1.10239995
1	4.98190022	-4.70639992	0.40570000
6	3.75860000	-2.62509990	1.52859998
1	3.02090001	-1.82229996	1.57529998
1	3.24270010	-3.58620000	1.64660001
1	4.43849993	-2.50390005	2.37890005
6	3.62529993	-2.87409997	-0.99349999
1	4.20340014	-2.89899993	-1.92410004
1	3.12730002	-3.84480000	-0.88169998
1	2.85260010	-2.11129999	-1.10130000
12	-1.43149996	0.00030000	0.61089998
8	-0.01140000	-1.30120003	0.20500000
8	-3.23079991	-0.00050000	0.12840000
6	-0.00240000	-2.71510005	0.22720000
1	-0.90460002	-3.10829997	0.71050000
1	0.86669999	-3.09439993	0.77800000

6	-4.52939987	0.00090000	-0.16270000
6	-5.23320007	-1.23580003	-0.32260001
6	-6.61079979	-1.19490004	-0.55970001
1	-7.16599989	-2.11989999	-0.67030001
6	-7.30730009	0.00340000	-0.66450000
6	-6.60900021	1.20050001	-0.55720001
1	-7.16289997	2.12649989	-0.66579998
6	-5.23140001	1.23889995	-0.31999999
6	-4.51109982	-2.59540009	-0.26499999
6	-4.50750017	2.59739995	-0.25970000
6	-3.89899993	-2.83240008	1.12909997
1	-3.17190003	-2.06089997	1.38800001
1	-3.39669991	-3.80690002	1.17100000
1	-4.68190002	-2.82629991	1.89569998
6	-3.42519999	-2.66249990	-1.35819995
1	-2.69079995	-1.86220002	-1.25320005
1	-3.88220000	-2.56929994	-2.34949994
1	-2.89800000	-3.62350011	-1.31939995
6	-5.46159983	-3.77789998	-0.52630001
1	-5.93559980	-3.71740007	-1.51129997
1	-6.24889994	-3.85630012	0.23100001
1	-4.88969994	-4.71229982	-0.49680001
6	-5.45629978	3.78180003	-0.51840001
1	-6.24340010	3.85980010	0.23920000
1	-5.93069983	3.72379994	-1.50339997
1	-4.88310003	4.71519995	-0.48719999
6	-3.42160010	2.66520000	-1.35290003
1	-2.68849993	1.86350000	-1.24989998
1	-2.89289999	3.62529993	-1.31210005
1	-3.87890005	2.57489991	-2.34439993
6	-3.89470005	2.83080006	1.13479996
1	-4.67749977	2.82410002	1.90149999
1	-3.39129996	3.80460000	1.17850006
1	-3.16840005	2.05809999	1.39199996
1	-0.89410001	3.10870004	0.72729999
1	0.03510000	-3.13030005	-0.78909999
1	-8.37959957	0.00440000	-0.84410000
1	8.44120026	-0.00630000	-0.26519999
1	2.44770002	-0.89870000	-3.91689992
8	-1.57210004	-0.00030000	2.69700003
6	-2.73869991	-0.00310000	3.54609990
1	-2.75189996	0.89429998	4.17000008
1	-3.60019994	-0.00280000	2.88140011
1	-0.76499999	0.00010000	3.23130012
1	-2.74990010	-0.90259999	4.16680002

DI-1__DBP-2_Mg-2_OMe-2_PDO-2

Zero-point vibrational energy	2462634.9 (Joules/Mol)
	588.58387 (Kcal/Mol)
Zero-point correction =	0.937968 (Hartree/Particle)
Thermal correction to Energy =	0.997102
Thermal correction to Enthalpy =	0.998047
Thermal correction to Gibbs Free Energy =	0.838564
Sum of electronic and zero-point Energies =	-2635.170683
Sum of electronic and thermal Energies =	-2635.111549
Sum of electronic and thermal Enthalpies =	-2635.110605
Sum of electronic and thermal Free Energies =	-2635.270087



cartesian

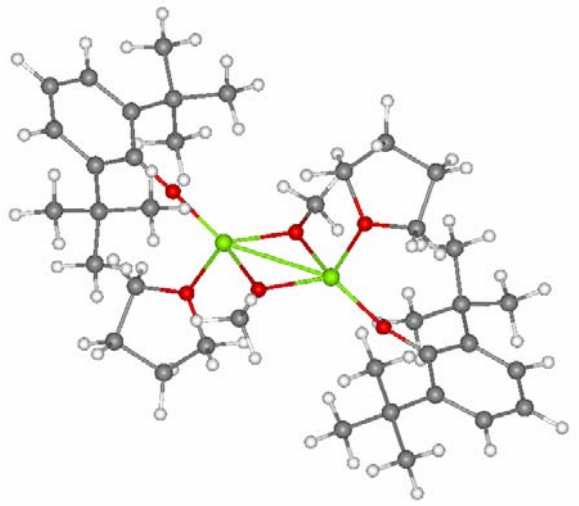
12	1.48269999	-0.07360000	-0.11350000
8	-0.01740000	-0.36620000	-1.35169995
8	3.02929997	0.77950001	-0.81970000
6	0.01360000	-0.48069999	-2.75780010
1	0.96310002	-0.11030000	-3.16319990
1	-0.10380000	-1.52620006	-3.07349992
6	4.34259987	0.90780002	-0.67839998
6	5.23750019	0.08270000	-1.43949997
6	6.59980011	0.10710000	-1.11909997
1	7.29110003	-0.53710002	-1.65279996
6	7.11530018	0.95889997	-0.14550000
6	6.26109982	1.87440002	0.46410000
1	6.69210005	2.59310007	1.15369999
6	4.88789988	1.90219998	0.19980000
6	4.75150013	-0.73600000	-2.65370011
6	4.01679993	3.02729988	0.79519999
6	3.81349993	-1.88909996	-2.25650001
1	2.89429998	-1.52919996	-1.79540002
1	3.53110003	-2.47410011	-3.14010000
1	4.31059980	-2.56920004	-1.55490005
6	4.03109980	0.21130000	-3.63619995

1	3.20510006	0.73320001	-3.15050006
1	4.72879982	0.96329999	-4.02059984
1	3.63779998	-0.35150000	-4.49209976
6	5.91930008	-1.37430000	-3.42720008
1	6.64340019	-0.62779999	-3.76889992
1	6.45279980	-2.12669992	-2.83559990
1	5.52689981	-1.88160002	-4.31570005
6	4.86549997	4.08680010	1.52209997
1	5.36460018	3.68670011	2.41199994
1	5.62669992	4.52510023	0.86849999
1	4.21360016	4.90080023	1.85850000
6	3.26970005	3.75860000	-0.33989999
1	2.63890004	3.07299995	-0.90770000
1	2.63770008	4.55499983	0.07270000
1	3.98320007	4.21990013	-1.03149998
6	3.00259995	2.49790001	1.82430005
1	3.49729991	1.90849996	2.60369992
1	2.48469996	3.33260012	2.31220007
1	2.23559999	1.87759995	1.36020005
12	-1.45210004	0.04160000	-0.06920000
8	0.04830000	0.35049999	1.16960001
8	-3.00270009	-0.88700002	0.50749999
6	0.07590000	0.50999999	2.56970000
1	-0.74790001	-0.03270000	3.04959989
1	-0.00810000	1.56900001	2.85159993
6	-4.31790018	-1.05320001	0.48230001
6	-5.14200020	-0.46090001	1.49779999
6	-6.53210020	-0.50860000	1.34420002
1	-7.17229986	-0.03770000	2.08310008
6	-7.13619995	-1.16680002	0.27669999
6	-6.33209991	-1.86360002	-0.62120003
1	-6.81930017	-2.43910003	-1.40149999
6	-4.93620014	-1.85630000	-0.53399998
6	-4.53779984	0.14710000	2.77909994
6	-4.10949993	-2.73889995	-1.48959994
6	-3.73189998	1.42700005	2.49099994
1	-2.87529993	1.23450005	1.84519994
1	-3.35039997	1.85930002	3.42409992
1	-4.36670017	2.18280005	2.01250005
6	-3.64000010	-0.90439999	3.46359992
1	-2.85299993	-1.25460005	2.79399991
1	-4.23699999	-1.77170002	3.76650000
1	-3.17709994	-0.48420000	4.36539984
6	-5.61749983	0.53789997	3.80469990
1	-6.24830008	-0.31240001	4.08339977
1	-6.26639986	1.34549999	3.44749999
1	-5.13089991	0.89709997	4.71840000
6	-4.99749994	-3.67059994	-2.33509994
1	-5.64559984	-3.12159991	-3.02749991
1	-5.62659979	-4.31629992	-1.71379995
1	-4.35799980	-4.32049990	-2.94230008
6	-3.16459990	-3.65129995	-0.67940003
1	-2.48699999	-3.07380009	-0.04930000
1	-2.56629992	-4.27390003	-1.35580003
1	-3.74349999	-4.31890011	-0.03180000
6	-3.29920006	-1.89010000	-2.48429990
1	-3.95749998	-1.24890006	-3.08030009
1	-2.74000001	-2.53480005	-3.17300010
1	-2.57699990	-1.25030005	-1.97809994
8	5.06180000	-3.61240005	2.00670004
6	3.72350001	-3.48020005	1.59010005
6	3.25760007	-2.05850005	1.35580003
8	3.93720007	-1.04700005	1.85380006
6	5.26849985	-1.26119995	2.40339994
6	5.38859987	-2.64520001	2.99259996
8	2.20560002	-1.84660006	0.75629997
1	5.97370005	-1.09370005	1.58659995
1	5.39410019	-0.47920001	3.15269995
6	-5.53770018	1.73819995	-1.77040005
8	-4.14219999	1.38740003	-1.55100000
6	-3.31500006	2.26259995	-1.02400005
6	-3.72110009	3.71639991	-0.90009999
8	-5.10330009	3.96409988	-1.00440001
6	-5.68030024	3.21180010	-2.06100011
8	-2.18470001	1.91009998	-0.68970001
1	4.74130011	-2.75860000	3.87560010
1	6.42140007	-2.83340001	3.29290009
1	-5.85780001	1.11619997	-2.60649991
1	-6.07810020	1.43490005	-0.87110001
1	-5.21210003	3.47340012	-3.02220011
1	-6.73710012	3.48289990	-2.10450006
1	1.01489997	0.12960000	2.99690008
1	-0.79310000	0.10150000	-3.22499990
1	-8.21920013	-1.18710005	0.18060000
1	8.17819977	0.95609999	0.08450000
1	3.60339999	-4.03179979	0.65679997
1	3.02530003	-3.91129994	2.32590008
1	-3.38599992	4.07670021	0.07330000
1	-3.15229988	4.25950003	-1.67240000

DI-1__DBP-2_Mg-2_OMe-2_THF-2

Zero-point vibrational energy	2536970.5 (Joules/Mol)
	606.35051 (Kcal/Mol)
Zero-point correction =	0.966281 (Hartree/Particle)
Thermal correction to Energy =	1.022842
Thermal correction to Enthalpy =	1.023787
Thermal correction to Gibbs Free Energy =	0.871566
Sum of electronic and zero-point Energies =	-2336.734811
Sum of electronic and thermal Energies =	-2336.678249
Sum of electronic and thermal Enthalpies =	-2336.677305

Sum of electronic and thermal Free Energies = -2336.829526



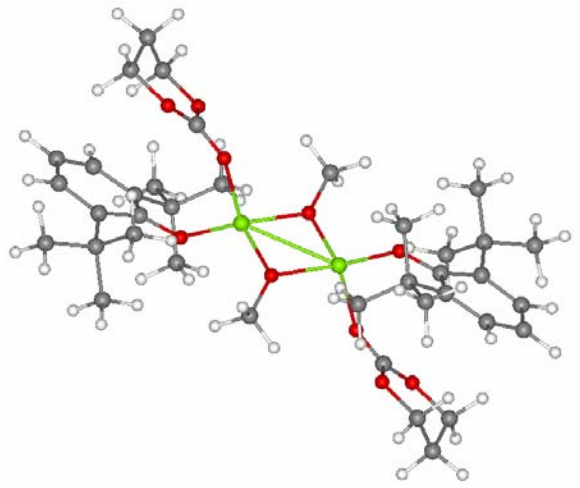
cartesian

12	1.40079999	0.11140000	-0.27370000
8	-0.01450000	-1.26040006	-0.39919999
8	3.19309998	-0.14820001	0.20200001
8	1.50909996	1.07169998	-2.12220001
6	-0.02220000	-2.50510001	-1.06659997
1	0.83510000	-3.11919999	-0.76440001
1	0.02540000	-2.37500000	-2.15680003
6	2.72370005	1.35889995	-2.86689997
1	2.88770008	0.54939997	-3.58669996
1	3.55019999	1.37829995	-2.15590000
6	2.43510008	2.67829990	-3.55949998
1	2.58690000	3.51169991	-2.86649990
1	3.07470012	2.83430004	-4.43149996
6	0.95410001	2.52839994	-3.92059994
1	0.84490001	1.93680000	-4.83479977
1	0.44929999	3.48449993	-4.07609987
6	0.38119999	1.77339995	-2.72250009
1	-0.03000000	2.44029999	-1.96099997
1	-0.37580001	1.03489995	-2.99559999
6	4.52260017	-0.16590001	0.21960001
6	5.23799992	-1.28050005	-0.32710001
6	6.63450003	-1.22329998	-0.36809999
1	7.19589996	-2.04780006	-0.79430002
6	7.34539986	-0.13760000	0.13070001
6	6.64809990	0.90740001	0.72589999
1	7.21920013	1.72839999	1.14600003
6	5.25180006	0.92079997	0.80299997
6	4.51350021	-2.54399991	-0.82990003
6	4.54260015	2.07310009	1.53910005
6	3.64350009	-2.23090005	-2.06139994
1	2.87840009	-1.48590004	-1.83879995
1	3.13940001	-3.13599992	-2.42120004
1	4.26240015	-1.84309995	-2.87820005
6	3.65700006	-3.14240003	0.30469999
1	2.91969991	-2.42729998	0.67339998
1	4.29500008	-3.43070006	1.14730000
1	3.13439989	-4.04260015	-0.04270000
6	5.49459982	-3.64849997	-1.26390004
1	6.15329981	-3.95869994	-0.44630000
1	6.11749983	-3.34529996	-2.11220002
1	4.92640018	-4.53090000	-1.57939994
6	5.53550005	3.05640006	2.18600011
1	6.16060019	3.56830001	1.44630003
1	6.19210005	2.56240010	2.90960002
1	4.97669983	3.82870007	2.72630000
6	3.67910004	1.51080000	2.68700004
1	2.93249989	0.80379999	2.32240009
1	3.16659999	2.32439995	3.21560001
1	4.31169987	0.98699999	3.41199994
6	3.68390012	2.90459991	0.56720001
1	4.31330013	3.34649992	-0.21380000
1	3.18020010	3.72280002	1.09619999
1	2.91829991	2.29870009	0.07980000
12	-1.43200004	-0.22780000	0.50139999
8	-0.00070000	1.11580002	0.68680000
8	-3.19729996	0.05250000	-0.04710000
8	-1.63989997	-1.15989995	2.35349989
6	0.03110000	2.35590005	1.36119998
1	-0.91939998	2.55629992	1.87000000
1	0.82740003	2.37709999	2.11549997
6	-2.87199998	-1.38150001	3.08920002
1	-3.01239991	-0.55100000	3.79049993
1	-3.68899989	-1.38360000	2.36759996
6	-2.64280009	-2.69650006	3.81189990
1	-2.81439996	-3.53649998	3.13190007
1	-3.30069995	-2.81259990	4.67649984
6	-1.16289997	-2.59279990	4.19460011
1	-1.04820001	-1.99489999	5.10389996
1	-0.69489998	-3.56399989	4.36959982
6	-0.54320002	-1.87199998	2.99769998
1	-0.12560000	-2.55859995	2.25769997
1	0.22040001	-1.14300001	3.27780008
6	-4.48400021	0.20800000	-0.34390000
6	-5.16739988	1.41639996	0.01160000
6	-6.53389978	1.51979995	-0.26539999
1	-7.07219982	2.42160010	0.00540000
6	-7.24179983	0.49860001	-0.88830000
6	-6.56430006	-0.65289998	-1.27170002
1	-7.12599993	-1.42999995	-1.77859998
6	-5.19820023	-0.82789999	-1.02929997
6	-4.43429995	2.60159993	0.66750002
6	-4.49679995	-2.10459995	-1.52999997
6	-3.88890004	2.20250010	2.05200005
1	-3.19269991	1.36520004	1.98339999
1	-3.37019992	3.04670000	2.52320004
1	-4.70909977	1.90090001	2.71300006
6	-3.29480004	3.09170008	-0.24869999
1	-2.57719994	2.29809999	-0.46210000
1	-3.70320010	3.44120002	-1.20340002
1	-2.76049995	3.92939997	0.21619999
6	-5.35640001	3.81250000	0.89800000
1	-5.78259993	4.19129992	-0.03680000
1	-6.17899990	3.58750010	1.58519995
1	-4.77489996	4.62709999	1.34459996
6	-5.45429993	-3.04570007	-2.28360009
1	-6.26849985	-3.40910006	-1.64760005
1	-5.89260006	-2.56920004	-3.16639996

1	-4.89690018	-3.92319989	-2.63030005
6	-3.37800002	-1.73319995	-2.52360010
1	-2.63879991	-1.07050002	-2.07080007
1	-2.86430001	-2.63380003	-2.88170004
1	-3.80229998	-1.21899998	-3.39289999
6	-3.93149996	-2.92079997	-0.35159999
1	-4.73789978	-3.21840000	0.32830000
1	-3.44339991	-3.83450007	-0.71300000
1	-3.20230007	-2.34770012	0.22360000
1	-0.93580002	-3.07010007	-0.84399998
1	0.20960000	3.18670011	0.66380000
1	-8.30539989	0.60540003	-1.08690000
1	8.43120003	-0.11820000	0.07950000

DI-1__DBP-2_Mg-2_OMe-2_TMC-2

Zero-point vibrational energy	2467157.4 (Joules/Mol)
	589.66477 (Kcal/Mol)
Zero-point correction =	0.939691 (Hartree/Particle)
Thermal correction to Energy =	0.998405
Thermal correction to Enthalpy =	0.999349
Thermal correction to Gibbs Free Energy =	0.841634
Sum of electronic and zero-point Energies =	-2635.213889
Sum of electronic and thermal Energies =	-2635.155175
Sum of electronic and thermal Enthalpies =	-2635.154231
Sum of electronic and thermal Free Energies =	-2635.311945



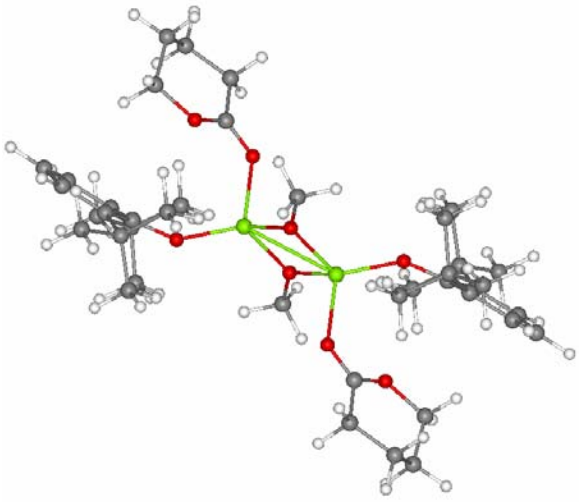
cartesian

12	-1.46490002	0.10460000	-0.02420000
8	0.07810000	0.88990003	-0.95779997
8	-2.97020006	-0.41220000	-1.08570004
6	0.14270000	1.59860003	-2.17589998
1	-0.68860000	1.32669997	-2.83909988
1	0.09770000	2.68330002	-2.00629997
6	-4.28959990	-0.48649999	-1.00469995
6	-5.10720015	0.63709998	-1.37160003
6	-6.47580004	0.58499998	-1.08029997
1	-7.10860014	1.43570006	-1.31369996
6	-7.07530022	-0.54879999	-0.53579998
6	-6.30210018	-1.69449997	-0.35490000
1	-6.79960012	-2.60019994	-0.02300000
6	-4.92579985	-1.71010005	-0.60360003
6	-4.53910017	1.81920004	-2.18740010
6	-4.14249992	-3.03600001	-0.52370000
6	-3.51220012	2.66050005	-1.40919995
1	-2.61030006	2.09500003	-1.17840004
1	-3.20379996	3.52600002	-2.00839996
1	-3.92790008	3.03679991	-0.46950001
6	-3.88429999	1.25940001	-3.46790004
1	-3.09209991	0.54879999	-3.22609997
1	-4.62830019	0.74540001	-4.08629990
1	-3.45479989	2.07459998	-4.06339979
6	-5.64519978	2.79029989	-2.63809991
1	-6.41979980	2.29060006	-3.22900009
1	-6.12779999	3.29780006	-1.79489994
1	-5.20300007	3.56850004	-3.27010012
6	-5.06990004	-4.23740005	-0.26679999
1	-5.55579996	-4.19000006	0.71460003
1	-5.84789991	-4.33169985	-1.03180003
1	-4.47770023	-5.15880013	-0.28780001
6	-3.43479991	-3.29480004	-1.87059999
1	-2.74769998	-2.48460007	-2.11929989
1	-2.86619997	-4.23180008	-1.82529998
1	-4.16890001	-3.38429999	-2.67890000
6	-3.10240006	-3.03329992	0.61119998
1	-3.56450009	-2.79559994	1.57500005
1	-2.63479996	-4.02159977	0.69819999
1	-2.30159998	-2.31680012	0.42899999
12	1.46469998	-0.10420000	0.02430000
8	-0.07820000	-0.88950002	0.95779997
8	2.97009993	0.41229999	1.08599997
6	-0.14280000	-1.59809995	2.17610002
1	0.68809998	-1.32539999	2.83960009
1	-0.09670000	-2.68280005	2.00670004
6	4.28959990	0.48649999	1.00479996
6	5.10720015	-0.63720000	1.37140000
6	6.47569990	-0.58520001	1.07990003
1	7.10850000	-1.43589997	1.31309998
6	7.07520008	0.54869998	0.53539997
6	6.30200005	1.69449997	0.35470000
1	6.79960012	2.60010004	0.02280000
6	4.92579985	1.71010005	0.60369998
6	4.53929996	-1.81930006	2.18720007
6	4.14260006	3.03609991	0.52399999
6	3.51220012	-2.66059995	1.40919995

1	2.61019993	-2.09520006	1.17869997
1	3.20400000	-3.52620006	2.00830007
1	3.92770004	-3.03670001	0.46930000
6	3.88479996	-1.25969994	3.46799994
1	3.09249997	-0.54909998	3.22650003
1	4.62890005	-0.74580002	4.08620024
1	3.45539999	-2.07509995	4.06349993
6	5.64550018	-2.79049993	2.63759995
1	6.42010021	-2.29080009	3.22849989
1	6.12809992	-3.29760003	1.79410005
1	5.20340014	-3.56890011	3.26929998
6	5.07009983	4.23740005	0.26719999
1	5.55609989	4.18989992	-0.71429998
1	5.84810019	4.33169985	1.03219998
1	4.47800016	5.15880013	0.28799999
6	3.43519998	3.29489994	1.87109995
1	2.74810004	2.48469996	2.11999989
1	2.86669993	4.23199987	1.82599998
1	4.16949987	3.38429999	2.67930007
6	3.10229993	3.03360009	-0.61059999
1	3.56430006	2.79590011	-1.57459998
1	2.63490009	4.02209997	-0.69760001
1	2.30139995	2.31730008	-0.42840001
6	-5.56449986	2.22410011	2.61840010
8	-4.19350004	2.27620006	2.15190005
6	-3.48939991	1.16869998	1.96700001
8	-3.92770004	-0.00590000	2.38890004
6	-5.28170013	-0.18510000	2.88190007
6	-5.76240015	1.06970000	3.57259989
8	-2.38490009	1.24880004	1.43840003
1	-5.89970016	-0.44980001	2.01950002
1	-5.21640015	-1.04059994	3.55439997
6	5.28170013	0.18470000	-2.88240004
8	3.92770004	0.00580000	-2.38930011
6	3.48930001	-1.16859996	-1.96689999
8	4.19329977	-2.27620006	-2.15170002
6	5.56409979	-2.22449994	-2.61859989
6	5.76200008	-1.07029998	-3.57290006
8	2.38490009	-1.24839997	-1.43820000
1	6.20039988	-2.12890005	-1.73430002
1	5.73330021	-3.19630003	-3.08270001
1	-5.73400021	3.19580007	3.08270001
1	-6.20050001	2.12849998	1.73399997
1	-5.21120024	1.23950005	4.50299978
1	-6.82350016	0.97160000	3.81920004
1	5.21649981	1.04009998	-3.55500007
1	5.89979982	0.44940001	-2.02010012
1	5.21059990	-1.24010003	-4.50330019
1	6.82299995	-0.97240001	-3.81979990
1	-1.07790005	-1.38429999	2.71190000
1	1.07739997	1.38399994	-2.71219993
1	8.14319992	0.56410003	0.32920000
1	-8.14330006	-0.56430000	-0.32990000

DI-1__DBP-2_Mg-2_OMe-2_VL-2

Zero-point vibrational energy	2588427.3 (Joules/Mol)
	618.64898 (Kcal/Mol)
Zero-point correction =	0.985880 (Hartree/Particle)
Thermal correction to Energy =	1.045870
Thermal correction to Enthalpy =	1.046814
Thermal correction to Gibbs Free Energy =	0.884258
Sum of electronic and zero-point Energies =	-2563.365317
Sum of electronic and thermal Energies =	-2563.305328
Sum of electronic and thermal Enthalpies =	-2563.304384
Sum of electronic and thermal Free Energies =	-2563.466940



cartesian

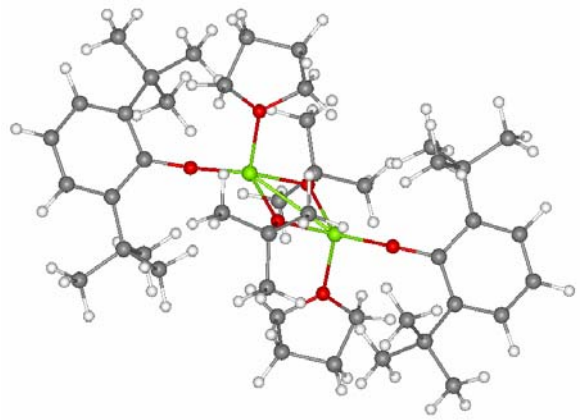
12	1.46500003	0.09220000	0.04830000
8	-0.05750000	0.26050001	1.28489995
8	2.99499989	-0.84990001	0.68610001
6	-0.07720000	0.25260001	2.69440007
1	0.80150002	-0.26370001	3.10130000
1	-0.08430000	1.27479994	3.09800005
6	4.30760002	-0.99059999	0.57150000
6	5.19360018	-0.28029999	1.45120001
6	6.56470013	-0.29499999	1.16929996
1	7.25010014	0.26740000	1.79519999
6	7.09660006	-1.03880000	0.11910000
6	6.24669981	-1.86240005	-0.61549997
1	6.68730021	-2.50749993	-1.36889994
6	4.86549997	-1.89100003	-0.39770001
6	4.68629980	0.39610001	2.74180007
6	3.99419999	-2.92219996	-1.14349997
6	3.78889990	1.61510003	2.46589994

1	2.87290001	1.34259999	1.94319999
1	3.49990010	2.09699988	3.40790009
1	4.32159996	2.36120009	1.86440003
6	3.91129994	-0.64310002	3.57839990
1	3.07459998	-1.05809999	3.01449990
1	4.57140017	-1.46840000	3.86640000
1	3.52410007	-0.18380000	4.49660015
6	5.84390020	0.90210003	3.62249994
1	6.53870010	0.10040000	3.89289999
1	6.41529989	1.70580006	3.14400005
1	5.43470001	1.30900002	4.55399990
6	4.84549999	-3.92210007	-1.94700003
1	5.38679981	-3.44490004	-2.77160001
1	5.57110023	-4.44579983	-1.31599998
1	4.18769979	-4.67840004	-2.38980007
6	3.18230009	-3.74830008	-0.12390000
1	2.55080009	-3.10899997	0.49460000
1	2.54299998	-4.47130013	-0.64569998
1	3.85450006	-4.30730009	0.53630000
6	3.04060006	-2.25189996	-2.14739990
1	3.59100008	-1.63269997	-2.86360002
1	2.48769999	-3.01169991	-2.71359992
1	2.30290008	-1.62310004	-1.65009999
12	-1.46500003	-0.09300000	-0.04820000
8	0.05750000	-0.26140001	-1.28489995
8	-2.99489999	0.84960002	-0.68559998
6	0.07730000	-0.25310001	-2.69429994
1	-0.79939997	0.26670000	-3.10109997
1	0.08050000	-1.27509999	-3.09829998
6	-4.30749989	0.99070001	-0.57160002
6	-5.19339991	0.28090000	-1.45169997
6	-6.56449986	0.29609999	-1.17019999
1	-7.24989986	-0.26600000	-1.79639995
6	-7.09660006	1.04009998	-0.12030000
6	-6.24660015	1.86329997	0.61470002
1	-6.68730021	2.50860000	1.36800003
6	-4.86530018	1.89139998	0.39739999
6	-4.68580008	-0.39590001	-2.74200010
6	-3.99379992	2.92199993	1.14370000
6	-3.78889990	-1.61510003	-2.46569991
1	-2.87290001	-1.34290004	-1.94280005
1	-3.49990010	-2.09730005	-3.40759993
1	-4.32200003	-2.36100006	-1.86409998
6	-3.91020012	0.64300001	-3.57839990
1	-3.07349992	1.05770004	-3.01419997
1	-4.56990004	1.46860003	-3.86660004
1	-3.52270007	0.18350001	-4.49639988
6	-5.84320021	-0.90149999	-3.62310004
1	-6.53770018	-0.09960000	-3.89380002
1	-6.41499996	-1.70500004	-3.14470005
1	-5.43380022	-1.30869997	-4.55439997
6	-4.84490013	3.92230010	1.94700003
1	-5.38689995	3.44530010	2.77130008
1	-5.56990004	4.44649982	1.31579995
1	-4.18680000	4.67810011	2.39030004
6	-3.18109989	3.74790001	0.12450000
1	-2.54979992	3.10829997	-0.49390000
1	-2.54159999	4.47039986	0.64670002
1	-3.85279989	4.30730009	-0.53590000
6	-3.04099989	2.25110006	2.14779997
1	-3.59200001	1.63230002	2.86400008
1	-2.48760009	3.01040006	2.71409988
1	-2.30369997	1.62160003	1.65069997
6	5.30100012	3.71830010	-1.41830003
6	3.80920005	3.62170005	-1.10730004
6	3.26160002	2.21810007	-1.12989998
8	3.86540008	1.26709998	-1.81739998
6	5.23680019	1.39670002	-2.29889989
6	5.62279987	2.82660007	-2.61179996
8	2.20330000	1.94350004	-0.56059998
1	5.86859989	0.95749998	-1.52219999
1	5.27129984	0.75190002	-3.17720008
6	-5.23789978	-1.39649999	2.29839993
8	-3.86649990	-1.26689994	1.81710005
6	-3.26230001	-2.21819997	1.13030005
6	-3.80979991	-3.62190008	1.10810006
6	-5.30159998	-3.71849990	1.41890001
6	-5.62379980	-2.82640004	2.61190009
8	-2.20379996	-1.94379997	0.56129998
1	-5.88450003	-3.39490008	0.54949999
1	-5.57149982	-4.75979996	1.61660004
1	5.57100010	4.75960016	-1.61549997
1	5.88390017	3.39420009	-0.54909998
1	5.09130001	3.17779994	-3.50460005
1	6.69250011	2.84410000	-2.84380007
1	-5.27269983	-0.75120002	3.17630005
1	-5.86959982	-0.95779997	1.52139997
1	-5.09229994	-3.17700005	3.50489998
1	-6.69350004	-2.84389997	2.84369993
1	0.97180003	0.25720000	-3.07879996
1	-0.96980000	-0.26100001	3.07900000
1	-8.16619968	1.03269994	0.07630000
1	8.16609955	-1.03100002	-0.07790000
1	3.54349995	4.05480003	-0.14120001
1	3.22530007	4.16830015	-1.85959995
1	-3.54390001	-4.05520010	0.14219999
1	-3.22589993	-4.16820002	1.86059999

DI-1__DBP-2_Mg-2_OtBu-2_THF-2

Zero-point vibrational energy	2981161.6 (Joules/Mol)
	712.51471 (Kcal/Mol)
Zero-point correction =	1.135464 (Hartree/Particle)
Thermal correction to Energy =	1.198871
Thermal correction to Enthalpy =	1.199815
Thermal correction to Gibbs Free Energy =	1.036664

Sum of electronic and zero-point Energies = -2572.364723
Sum of electronic and thermal Energies = -2572.301317
Sum of electronic and thermal Enthalpies = -2572.300373
Sum of electronic and thermal Free Energies = -2572.463524



cartesian

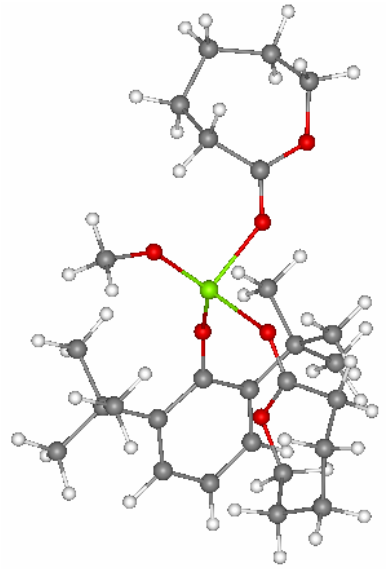
12	1.44560003	0.25420001	-0.19250000
8	-0.04360000	-0.54540002	-1.26730001
8	3.23099995	-0.20110001	0.32600001
8	1.58490002	2.12369990	-1.19630003
6	2.54410005	2.51559997	-2.21779990
1	3.52180004	2.13039994	-1.92379999
1	2.24250007	2.05570006	-3.16479993
6	2.44930005	4.03100014	-2.29209995
1	3.08489990	4.49420023	-1.53219998
1	2.75110006	4.40969992	-3.27169991
6	0.97070003	4.27519989	-1.98169994
1	0.35580000	4.09859991	-2.86969995
1	0.76709998	5.28709984	-1.62360001
6	0.68019998	3.22889996	-0.91460001
1	-0.34090000	2.84629989	-0.93860000
1	0.90369999	3.59459996	0.09220000
6	4.51000023	-0.42089999	0.00840000
6	4.93450022	-1.69560003	-0.49520001
6	6.19469976	-1.78419995	-1.09720004
1	6.51210022	-2.71919990	-1.54649997
6	7.07929993	-0.71200001	-1.12230003
6	6.75040007	0.43380001	-0.40640000
1	7.49910021	1.21399999	-0.31790000
6	5.50810003	0.59230000	0.21799999
6	4.10200024	-2.98099995	-0.29969999
6	5.31080008	1.75940001	1.21000004
6	2.85770011	-3.01970005	-1.19649994
1	2.16249990	-2.20989990	-0.97009999
1	3.14409995	-2.94079995	-2.25009990
1	2.31830001	-3.96709991	-1.06669998
6	3.68449998	-3.09929991	1.17949998
1	4.56729984	-3.15630007	1.82539999
1	3.09030008	-2.24140000	1.49530005
1	3.09549999	-4.01240015	1.33659995
6	4.91690016	-4.24730015	-0.62589997
1	5.84509993	-4.29769993	-0.04780000
1	4.32130003	-5.13189983	-0.37320000
1	5.16800022	-4.32399988	-1.68910003
6	6.61670017	2.53460002	1.46500003
1	6.43499994	3.29710007	2.23119998
1	7.41800022	1.88489997	1.83099997
1	6.97690010	3.05669999	0.57179999
6	4.87330008	1.17680001	2.56859994
1	4.71150017	1.97950006	3.29889989
1	3.95029998	0.60530001	2.47329998
1	5.64610004	0.50929999	2.96449995
6	4.28090000	2.79119992	0.72950000
1	4.13390017	3.57110000	1.48759997
1	4.63439989	3.28169990	-0.18449999
1	3.31660008	2.32769990	0.52329999
6	-0.27239999	-0.68449998	-2.67540002
6	-1.11010003	-1.94280005	-2.92350006
6	-1.01950002	0.55049998	-3.19269991
6	1.05540001	-0.82690001	-3.42459989
12	-1.44180000	-0.39820001	0.15570000
8	0.05620000	0.34230000	1.23800004
8	-3.17700005	0.25110000	-0.33730000
8	-1.67999995	-2.29390001	1.07179999
6	-2.71149993	-2.72499990	2.00379992
1	-3.65669990	-2.28649998	1.68200004
1	-2.46009994	-2.34410000	2.99909997
6	-2.65759993	-4.24230003	1.97290003
1	-3.23180008	-4.63030005	1.12650001
1	-3.05360007	-4.68330002	2.89089990
6	-1.16170001	-4.50019979	1.77620006
1	-0.62589997	-4.39519978	2.72480011
1	-0.94389999	-5.49119997	1.37109995
6	-0.76090002	-3.39409995	0.80900002
1	0.25780001	-3.02959991	0.95010000
1	-0.89300001	-3.69379997	-0.23420000
6	-4.42269993	0.50900000	0.07090000
6	-4.75519991	1.76660001	0.67699999
6	-5.95860004	1.85899997	1.38489997
1	-6.20139980	2.77440000	1.91450000
6	-6.88100004	0.81819999	1.41400003
6	-6.66279984	-0.28060001	0.58950001
1	-7.45260000	-1.01940000	0.50010002
6	-5.48140001	-0.43779999	-0.14460000
6	-3.90520000	3.03740001	0.45789999
6	-5.42089987	-1.50720000	-1.25769997
6	-2.58419991	3.02220011	1.23889995
1	-1.94470000	2.18630004	0.95050001
1	-2.77320004	2.95630002	2.31539989
1	-2.02440000	3.94989991	1.06070006
6	-3.61409998	3.19210005	-1.04859996
1	-4.54759979	3.28209996	-1.61420000
1	-3.06599998	2.33249998	-1.43710005
1	-3.02230000	4.09840012	-1.23119998
6	-4.65649986	4.30950022	0.89340001
1	-5.62830019	4.40229988	0.39809999
1	-4.06069994	5.18860006	0.62230003
1	-4.81629992	4.35340023	1.97590005
6	-6.80319977	-2.12919998	-1.53240001
1	-6.72599983	-2.80620003	-2.39089990

1	-7.55350018	-1.37030005	-1.77559996
1	-7.17469978	-2.72239995	-0.68970001
6	-4.98159981	-0.82599998	-2.56999993
1	-4.92810011	-1.55929995	-3.38429999
1	-4.00570011	-0.35150000	-2.46580005
1	-5.70370007	-0.05450000	-2.85780001
6	-4.47760010	-2.67510009	-0.93229997
1	-4.42259979	-3.37199998	-1.77820003
1	-4.85109997	-3.23600006	-0.06810000
1	-3.46690011	-2.33089995	-0.71130002
6	0.24290000	0.53479999	2.64639997
6	0.83560002	1.92770004	2.88339996
6	1.18869996	-0.54400003	3.18330002
6	-1.09619999	0.42050001	3.38120008
1	8.04220009	-0.79839998	-1.61960006
1	-7.79530001	0.90280002	1.99600005
1	1.36860001	-0.41960001	4.25699997
1	2.15229988	-0.50970000	2.66950011
1	0.75349998	-1.53659999	3.02550006
1	1.00390005	2.11360002	3.94980001
1	0.15680000	2.69880009	2.50659990
1	1.79939997	2.02970004	2.37570000
1	-0.97030002	0.61540002	4.45170021
1	-1.50329995	-0.58899999	3.28259993
1	-1.83140004	1.12930000	2.99670005
1	-1.27040005	0.45089999	-4.25460005
1	-0.40120000	1.44599998	-3.07399988
1	-1.94939995	0.69830000	-2.63660002
1	-1.29429996	-2.09369993	-3.99280000
1	-2.08330011	-1.87020004	-2.43039989
1	-0.58660001	-2.82570004	-2.54279995
1	0.89300001	-0.80760002	-4.50769997
1	1.55200005	-1.76569998	-3.17670012
1	1.73920000	-0.00840000	-3.18079996

S5.2. ROP of εCL. Mononuclear mechanism

I-1__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1784683.0 (Joules/Mol)
	426.54948 (Kcal/Mol)
Zero-point correction =	0.679750 (Hartree/Particle)
Thermal correction to Energy =	0.719103
Thermal correction to Enthalpy =	0.720047
Thermal correction to Gibbs Free Energy =	0.604580
Sum of electronic and zero-point Energies =	-1705.797246
Sum of electronic and thermal Energies =	-1705.757893
Sum of electronic and thermal Enthalpies =	-1705.756949
Sum of electronic and thermal Free Energies =	-1705.872416



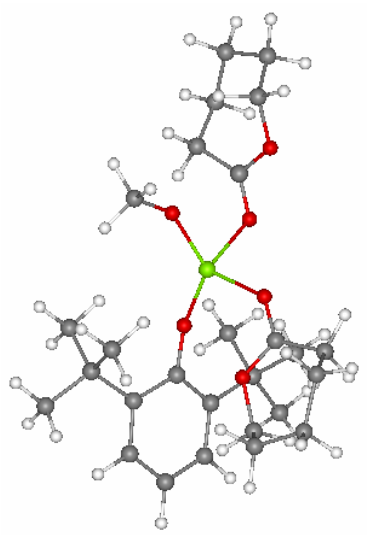
cartesian

8	-1.63320374	0.75279218	-2.54900122
6	-1.40160370	0.82269216	-3.91410136
1	-1.03700376	-0.13080782	-4.33640146
1	-0.65780371	1.59449220	-4.18610144
12	-0.80780369	0.56899220	-0.88910127
8	0.13459630	-0.89550781	-0.14480126
6	1.22249627	-1.51050782	0.28239873
6	2.20499635	-1.99840784	-0.64440125
6	3.39919639	-2.52220774	-0.13730127
1	4.16589642	-2.87290788	-0.82050127
6	3.64339638	-2.62950778	1.22909880
6	2.64119625	-2.25680780	2.12049866
1	2.82149625	-2.40140772	3.18099880
6	1.42389631	-1.72120786	1.68899870
6	1.96959639	-1.98390794	-2.16870117
6	0.32569629	-1.39340782	2.71959877
6	2.00169635	-0.54830784	-2.72600126
1	1.22779632	0.08459218	-2.29080129
1	1.84669626	-0.55240786	-3.81130123
1	2.97029638	-0.07790782	-2.52240133
6	0.62799633	-2.66250777	-2.51400137
1	-0.21590370	-2.15730786	-2.04460120
1	0.63289630	-3.70440793	-2.17460132
1	0.47189629	-2.66190791	-3.59970117
6	3.05809641	-2.76440787	-2.93000126
1	3.12749624	-3.80500793	-2.59570122
1	4.04889631	-2.30600786	-2.83710122
1	2.80979633	-2.77670789	-3.99730134
6	0.69249630	-1.87250781	4.13579845
1	1.56999624	-1.35650778	4.54119873
1	0.88229632	-2.95060778	4.16879845
1	-0.14370370	-1.66490781	4.81319857
6	-0.98840368	-2.10860777	2.34219885
1	-1.32730365	-1.81810784	1.34779871
1	-1.77440369	-1.86410785	3.06779885
1	-0.84570372	-3.19510794	2.35229874
6	0.09229630	0.12619218	2.81439877
1	1.01079631	0.63259214	3.13669872
1	-0.69010371	0.35279217	3.54929876
1	-0.22190370	0.54409218	1.85919869
8	0.18789630	2.31889224	-0.29470125
6	1.31929624	2.47839212	0.17269874
8	2.16109633	1.46659219	0.10809873
6	1.73529625	3.79649210	0.77209872
6	3.46119618	1.46709216	0.74919873
6	2.92789626	4.46169233	0.06189874
6	4.46029615	2.38929224	0.07159874
1	3.76279640	0.42199215	0.67419875
1	2.92339635	5.52069235	0.34079874
1	2.76799631	4.43219233	-1.02230132
1	1.96859622	3.64189219	1.83319879
1	0.85299629	4.43609238	0.72429872
6	4.29299641	3.86909223	0.41459873
1	3.33159637	1.70519221	1.81019878
1	4.40389633	2.22809219	-1.01120126
1	5.45969629	2.06109214	0.38019875
1	4.47169638	4.00689220	1.48959875
1	5.07019615	4.44599199	-0.09900127
8	-2.44980359	0.88429219	0.33769873
6	-3.67240381	0.92199218	0.20779873
6	-4.36730385	0.67469215	-1.10120130
8	-4.36890364	1.18019211	1.31499875
6	-5.16870356	-0.64060783	-1.11420131
1	-5.03230381	1.51969218	-1.32210124

1	-3.56980371	0.66189218	-1.85710120
6	-5.81350374	1.21099222	1.31009877
1	-4.55880356	-1.44370782	-0.68430126
1	-5.32900381	-0.91320783	-2.16200137
1	-6.16040373	1.96529222	0.59519875
1	-6.05050373	1.56709218	2.31359863
6	-6.52230358	-0.56210786	-0.40940127
1	-7.16130352	0.15109217	-0.94790125
1	-7.02310371	-1.53420782	-0.48150125
6	-6.45480347	-0.14640781	1.06049871
1	-5.91880369	-0.89490783	1.65619874
1	-7.47280359	-0.10070782	1.46559870
1	-2.32560372	1.07689226	-4.46610165
1	4.58229637	-3.04120779	1.59229875

I-1i__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1782945.7 (Joules/Mol)
	426.13425 (Kcal/Mol)
Zero-point correction =	0.679088 (Hartree/Particle)
Thermal correction to Energy =	0.718708
Thermal correction to Enthalpy =	0.719652
Thermal correction to Gibbs Free Energy =	0.602773
Sum of electronic and zero-point Energies =	-1705.793910
Sum of electronic and thermal Energies =	-1705.754291
Sum of electronic and thermal Enthalpies =	-1705.753347
Sum of electronic and thermal Free Energies =	-1705.870225



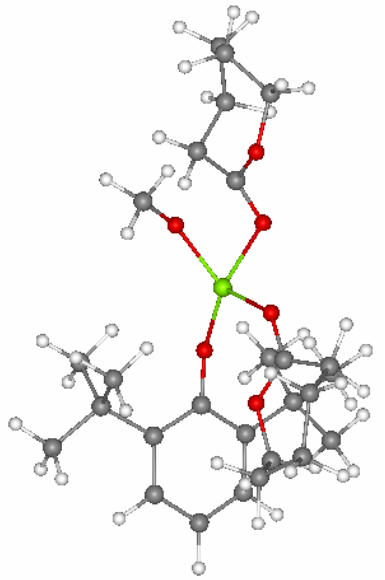
cartesian

8	0.36591670	-1.09402549	-0.04632054
6	1.62001669	-1.48082542	0.10637946
6	2.13911653	-1.74032545	1.41947949
6	3.50181651	-2.02242541	1.55687952
1	3.92011666	-2.19892550	2.54277945
6	4.35521698	-2.10502553	0.45977947
6	3.82191658	-1.96152544	-0.81842053
1	4.48731709	-2.09202552	-1.66592050
6	2.46951652	-1.67552543	-1.03402054
6	1.22561669	-1.75052547	2.66077948
6	1.92341673	-1.60882545	-2.47432041
6	0.68901670	-0.34102550	2.97387958
1	0.09571670	0.05727448	2.15177941
1	0.04891670	-0.36112550	3.86447954
1	1.51791668	0.34957448	3.17327952
6	0.04991670	-2.72562551	2.44247937
1	-0.54398328	-2.44662547	1.57187951
1	0.42561671	-3.74362540	2.29017949
1	-0.60418332	-2.73502541	3.32347941
6	1.96411669	-2.22872543	3.92407942
1	2.38351655	-3.23272538	3.80087948
1	2.77341652	-1.55202544	4.22107935
1	1.25621676	-2.26932549	4.75977945
6	2.97051668	-2.05222559	-3.51322055
1	3.83621669	-1.38162553	-3.55382061
1	3.33161664	-3.06862545	-3.32392049
1	2.51291656	-2.04652548	-4.50882053
6	0.72071666	-2.56192541	-2.63552046
1	-0.08518330	-2.31812549	-1.94332051
1	0.32861671	-2.50822544	-3.65872049
1	1.03001678	-3.59592557	-2.44682050
6	1.52031672	-0.17192551	-2.85582042
1	2.38031673	0.50307447	-2.78342056
1	1.14831674	-0.13792551	-3.88682055
1	0.73441666	0.22427449	-2.21142054
8	-2.23148346	0.40347448	-1.72542048
6	-2.38828349	0.61807448	-3.08492064
1	-2.51308346	1.68917453	-3.33202052
1	-3.28488350	0.10017449	-3.47752047
1	-1.53798330	0.25197449	-3.68702054
8	-2.53518343	-0.03042552	0.99157947
12	-0.96858335	0.20807448	-0.35082054
1	5.41121674	-2.32652545	0.59637946
6	-3.65458345	0.07807449	0.47747946
6	-4.37578297	-1.09852552	-0.12742054
8	-4.25668335	1.25627446	0.58517945
6	-5.69508314	-1.46082544	0.57547945
1	-4.53858328	-0.89222556	-1.18992054
1	-3.67168331	-1.92942548	-0.07552054
6	-5.48028326	1.54547453	-0.12582055
1	-5.55558300	-1.44022548	1.66317952
1	-5.92828321	-2.49992537	0.31997946
1	-5.35128307	1.27507448	-1.17802048
1	-5.54858303	2.63267446	-0.06542054

6	-6.88098335	-0.58352554	0.17517945
1	-7.05478334	-0.69662553	-0.90332055
1	-7.78568316	-0.95332557	0.67117947
6	-6.70978308	0.90077448	0.49587947
1	-6.67328310	1.06267452	1.57997942
1	-7.58548307	1.45047450	0.13007946
8	-0.19668330	2.05777454	0.25987947
6	0.96151668	2.42177463	0.48217946
6	1.24741673	3.73447442	1.16237950
8	1.94211674	1.63887453	0.07977946
6	2.07441664	4.71317434	0.30957946
1	1.76251674	3.53507447	2.11037946
1	0.27361670	4.16127443	1.40577948
6	3.33381653	1.86237454	0.41877946
1	1.66361678	4.74667406	-0.70662051
1	1.92911673	5.71427441	0.72897947
1	3.42251658	1.95327449	1.50647950
1	3.80191660	0.92337447	0.12277947
6	3.57321668	4.41317415	0.26947945
1	3.97541642	4.48717451	1.28897953
1	4.07381678	5.19547415	-0.31212053
6	3.94291663	3.04767442	-0.31032053
1	3.66701651	2.98367453	-1.36942053
1	5.03141689	2.92427444	-0.26802054

TS-12__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1783379.8 (Joules/Mol)
	426.23801 (Kcal/Mol)
Zero-point correction =	0.679254 (Hartree/Particle)
Thermal correction to Energy =	0.717627
Thermal correction to Enthalpy =	0.718571
Thermal correction to Gibbs Free Energy =	0.606288
Sum of electronic and zero-point Energies =	-1705.775815
Sum of electronic and thermal Energies =	-1705.737442
Sum of electronic and thermal Enthalpies =	-1705.736497
Sum of electronic and thermal Free Energies =	-1705.848780



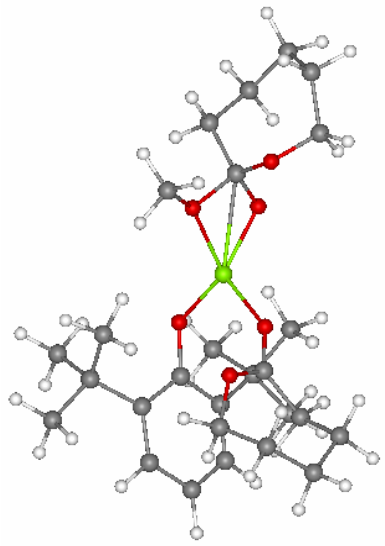
cartesian

8	0.41141027	-1.15696788	-0.07369613
6	1.69001031	-1.49026787	-0.03679613
6	2.30881023	-1.84046793	1.20880389
6	3.68981028	-2.06046796	1.22960389
1	4.18301010	-2.30446792	2.16520381
6	4.46741009	-1.99406791	0.07620387
6	3.84031034	-1.76226795	-1.14559615
1	4.44991016	-1.77586794	-2.04339623
6	2.46371031	-1.53326786	-1.24389613
6	1.48361027	-2.01206779	2.50000381
6	1.80941033	-1.37266791	-2.63079619
6	0.91351026	-0.66596794	2.98640370
1	0.25141028	-0.21386795	2.24790382
1	0.33271030	-0.80276799	3.90650368
1	1.72361028	0.04093205	3.20330381
6	0.33601028	-3.01746798	2.26750374
1	-0.32858971	-2.69306779	1.46680391
1	0.74171031	-3.99906802	1.99850392
1	-0.25518972	-3.13586783	3.18390369
6	2.32831025	-2.57186794	3.65860367
1	2.78131032	-3.53636789	3.40650368
1	3.12621021	-1.88756788	3.96840382
1	1.68311024	-2.72986794	4.53010368
6	2.79891038	-1.65776789	-3.77539635
1	3.62341022	-0.93686795	-3.81029630
1	3.22491026	-2.66426802	-3.70729613
1	2.27051020	-1.58856785	-4.73289633
6	0.65211028	-2.38096786	-2.79249620
1	-0.11508973	-2.24266791	-2.03059626
1	0.18671027	-2.26826787	-3.77949619
1	1.02981031	-3.40636802	-2.71309614
6	1.29531026	0.06283205	-2.84889627
1	2.12041020	0.78233200	-2.80179620
1	0.81961030	0.15553205	-3.83279634
1	0.55941027	0.35193205	-2.09759617
8	-2.42238975	0.30173206	-1.32939613
6	-2.89018965	1.03173208	-2.41749620
1	-3.55088973	1.85293210	-2.09219623
1	-3.45608974	0.39653206	-3.11979628
1	-2.06328964	1.48363209	-2.98629618
8	-2.59148979	-0.21696796	1.08880389
12	-0.98018974	0.10603204	-0.06809613
1	5.53981018	-2.16926789	0.12200387
6	-3.57408977	-0.00136795	0.32490388
6	-4.36918974	-1.17096794	-0.22409612

8	-4.13858986	1.23363209	0.39440387
6	-5.60708952	-1.49636793	0.62680387
1	-4.65528965	-0.97646797	-1.25979614
1	-3.67498970	-2.01206779	-0.23259613
6	-5.53198957	1.45693207	0.67950386
1	-5.38068962	-1.31876791	1.68450391
1	-5.82098961	-2.56746793	0.55030388
1	-5.63078976	2.53813219	0.56390387
1	-5.70948982	1.22123206	1.73700392
6	-6.84738970	-0.70086795	0.19940388
1	-7.33648968	-1.20586789	-0.64189613
1	-7.57548952	-0.70156795	1.01930380
6	-6.53958988	0.74493206	-0.21359614
1	-7.46748972	1.32913208	-0.19399613
1	-6.17908955	0.79373205	-1.24669611
8	-0.20808974	1.96393204	0.47260389
6	0.94761026	2.36193204	0.65290385
8	1.93371034	1.60823214	0.21490386
6	1.21631026	3.68193221	1.32550383
6	1.97771025	4.68893194	0.44520387
1	1.77321029	3.49763203	2.25290370
1	0.23911029	4.07623196	1.60690391
6	3.33221030	1.87703204	0.49130389
1	1.52491033	4.71423197	-0.55309612
1	1.81881022	5.68303204	0.87590390
1	3.46591020	1.96803212	1.57440388
1	3.81631017	0.95493203	0.16850388
6	3.48191023	4.43523169	0.34190387
1	3.92411017	4.51903200	1.34390390
1	3.93341017	5.23423195	-0.25669613
6	3.86871028	3.08373213	-0.25889611
1	3.54871035	3.01313210	-1.30499613
1	4.96131039	2.99503207	-0.26549613

I-2__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1790760.0 (Joules/Mol)
	428.00192 (Kcal/Mol)
Zero-point correction =	0.682064 (Hartree/Particle)
Thermal correction to Energy =	0.719931
Thermal correction to Enthalpy =	0.720875
Thermal correction to Gibbs Free Energy =	0.610171
Sum of electronic and zero-point Energies =	-1705.786682
Sum of electronic and thermal Energies =	-1705.748816
Sum of electronic and thermal Enthalpies =	-1705.747872
Sum of electronic and thermal Free Energies =	-1705.858576



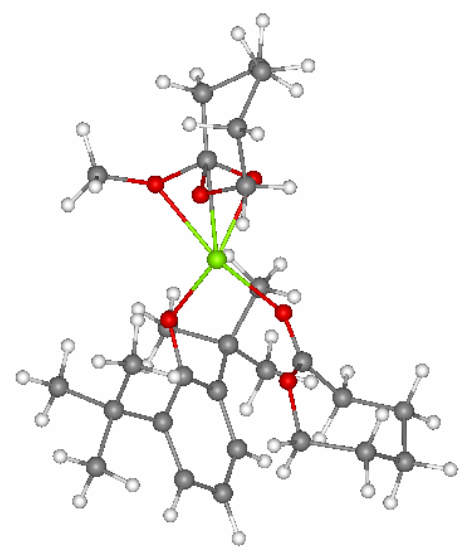
cartesian

8	0.25038970	-1.54128444	-0.52589613
6	1.55038965	-1.49038446	-0.25979611
6	2.04138970	-1.90178442	1.02160394
6	3.38618970	-1.66128445	1.32230389
1	3.77998972	-1.92938447	2.29760385
6	4.25868988	-1.09088445	0.39690387
6	3.80318975	-0.83638448	-0.89599609
1	4.51898956	-0.47988445	-1.63059604
6	2.47238970	-1.05808449	-1.26819611
6	1.14478970	-2.68048429	2.00710392
6	2.04238963	-0.95208442	-2.74569607
6	-0.09141032	-1.88158441	2.47390389
1	-0.89181030	-1.89168441	1.73110390
1	-0.52021033	-2.33808422	3.37380385
1	0.15808968	-0.84528446	2.72550392
6	0.66888970	-3.97908449	1.32170391
1	0.11828968	-3.75778437	0.40500388
1	1.52198970	-4.61748409	1.06830394
1	0.00998968	-4.54408455	1.99260390
6	1.91628969	-3.08808422	3.27440405
1	2.79738975	-3.69548440	3.04440403
1	2.23938966	-2.22208428	3.86430383
1	1.26478970	-3.69228435	3.91470385
6	3.21938968	-0.56968445	-3.65929604
1	3.61468959	0.42821556	-3.43489599
1	4.04348946	-1.28758442	-3.59569597
1	2.87978959	-0.55708444	-4.70069599
6	1.53138971	-2.33438444	-3.20529604
1	0.68218970	-2.65698433	-2.59939599
1	1.21378970	-2.29388428	-4.25479603
1	2.32318974	-3.08648443	-3.12059617
6	0.93418968	0.09231555	-2.98299599
1	1.19908965	1.06801558	-2.56409597
1	0.76808971	0.22291555	-4.05949593
1	-0.01091032	-0.23308444	-2.54619598
8	-2.51511025	0.44661555	-1.40109611

6	-2.79721022	1.37281561	-2.44719601
1	-3.59261036	0.99051553	-3.09539604
1	-1.88301027	1.47491550	-3.03479600
1	-3.08721042	2.34221578	-2.03589606
8	-3.96351027	1.47891557	0.02840389
6	-3.55441022	0.16831554	-0.34559610
8	-2.88151026	-0.48128444	0.59690386
6	-4.69181013	-0.64958447	-0.97319609
12	-1.07961035	-0.25568444	-0.06869611
1	-5.21001053	-0.06388445	-1.74139607
1	5.29918957	-0.91248447	0.65930390
6	-4.86801052	1.53341556	1.13160396
1	-4.53901052	0.83841556	1.91380394
6	-6.31771040	1.29591560	0.71040386
1	-4.76451015	2.54961562	1.52370393
1	-6.97701025	1.77911556	1.44270396
6	-6.75461054	-0.17248444	0.54540390
1	-6.46301031	1.84231555	-0.22909610
1	-4.21801043	-1.50208449	-1.46999609
6	-5.67481041	-1.16488445	0.08390389
1	-5.08111048	-1.50418448	0.93860388
1	-6.17911053	-2.05678439	-0.30569613
1	-7.59651041	-0.19698445	-0.15749609
1	-7.15621042	-0.53948444	1.49780393
8	0.05928968	1.24481559	0.70280391
6	1.14918971	1.81891561	0.66840386
8	1.43688965	2.51341558	-0.42329612
6	2.09968972	1.78121555	1.83130395
6	2.75248981	3.08281565	-0.64669609
6	2.42978978	3.15791559	2.43530393
6	3.04598975	4.29811573	0.21720390
1	2.71668959	3.36051559	-1.70069611
1	2.81878972	2.98181558	3.44340396
1	1.50578964	3.73481560	2.56270385
1	3.01308966	1.26161551	1.51130390
1	1.62688971	1.14341557	2.57770395
6	3.45868969	3.96971560	1.65070391
1	3.50038958	2.29251575	-0.52989614
1	2.16978979	4.95741558	0.20140390
1	3.85688972	4.85051584	-0.27229610
1	4.40668964	3.41641569	1.63060391
1	3.66058969	4.90341568	2.18740392

TS-23__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1788747.1 (Joules/Mol)
	427.52081 (Kcal/Mol)
Zero-point correction =	0.681298 (Hartree/Particle)
Thermal correction to Energy =	0.718427
Thermal correction to Enthalpy =	0.719371
Thermal correction to Gibbs Free Energy =	0.611018
Sum of electronic and zero-point Energies =	-1705.780691
Sum of electronic and thermal Energies =	-1705.743562
Sum of electronic and thermal Enthalpies =	-1705.742618
Sum of electronic and thermal Free Energies =	-1705.850971



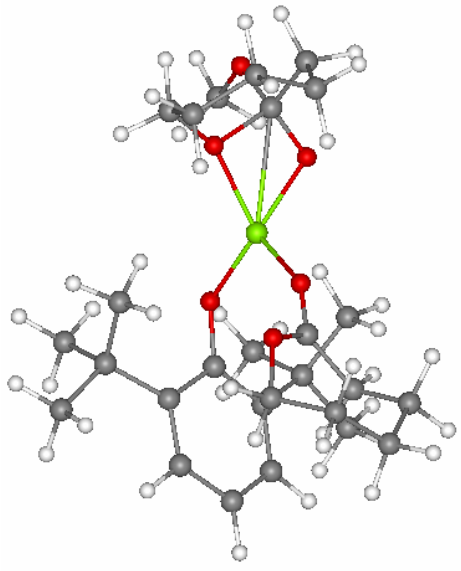
cartesian

8	0.24478835	-1.67412949	-0.32297692
6	1.54718840	-1.43452954	-0.26237693
6	2.27778840	-1.73972952	0.93122309
6	3.61268830	-1.33162951	1.01452315
1	4.18368816	-1.52022958	1.91822302
6	4.25228834	-0.68542951	-0.04217692
6	3.56978846	-0.51442951	-1.24617696
1	4.11058807	-0.08632953	-2.08467698
6	2.23468852	-0.90412956	-1.40257692
6	1.64438844	-2.59272933	2.04992318
6	1.56468844	-0.87412953	-2.79167700
6	0.33978835	-1.99292958	2.62472296
1	-0.52971166	-2.25762939	2.01732302
1	0.13608834	-2.40432930	3.61992311
1	0.39358833	-0.90442955	2.73692298
6	1.33308840	-3.99182940	1.47692311
1	0.65868837	-3.91782951	0.62072307
1	2.25298834	-4.48992920	1.15282309
1	0.85648835	-4.62072945	2.23932314
6	2.60698843	-2.78162932	3.23542309
1	3.54128838	-3.26732945	2.93682313
1	2.85348845	-1.83252954	3.72592306
1	2.13558841	-3.42522931	3.98582315
6	2.52298832	-0.35772952	-3.87887692
1	2.82088852	0.68407047	-3.71087694
1	3.42988849	-0.96622956	-3.95687699
1	2.02058840	-0.39762953	-4.85157681
6	1.17138839	-2.31702948	-3.17457700

1	0.48208833	-2.74002934	-2.44107699
1	0.68588835	-2.33132935	-4.15847683
1	2.05758834	-2.95882940	-3.22597694
6	0.31018835	0.01947048	-2.84337687
1	0.51898837	1.03187048	-2.48517704
1	-0.05021165	0.09747048	-3.87647700
1	-0.50371164	-0.39632952	-2.24847698
8	-2.91061163	-1.82912958	-0.21447693
6	-3.37271166	-2.31852937	-1.47297692
1	-4.34011173	-2.81902933	-1.35757697
1	-2.63431168	-3.04852939	-1.80907691
1	-3.45271158	-1.51352954	-2.20877695
8	-3.17851162	0.34757045	-0.68777692
6	-3.53521156	-0.62462956	0.37402308
8	-2.83101153	-0.37542954	1.45772302
6	-5.04001188	-0.79232955	0.56262308
12	-1.18441164	-0.62062955	0.38092306
1	-5.53341198	-0.97352952	-0.39847693
1	5.29098797	-0.37612954	0.05032308
6	-3.56971169	1.70197046	-0.43477693
1	-3.29821157	1.97757041	0.59212309
6	-5.04951191	1.94217050	-0.72647691
1	-2.95571160	2.29797053	-1.11557698
1	-5.18411160	2.99567056	-1.00187695
6	-6.03201199	1.60237050	0.40952307
1	-5.29131174	1.36547041	-1.62707698
1	-5.15571165	-1.69632959	1.16902304
6	-5.66531181	0.39937046	1.29302311
1	-4.96581173	0.70217049	2.07842302
1	-6.57301188	0.06577048	1.80862308
1	-7.02021170	1.43997049	-0.03827692
1	-6.14401197	2.47607064	1.06302309
8	-0.11161165	1.08457041	0.78702307
6	0.87358832	1.80287051	0.62592310
8	0.89628834	2.57047057	-0.45817691
6	1.98798847	1.86657047	1.63232303
6	2.08128834	3.30927062	-0.84657693
6	2.22078848	3.25917053	2.24472308
6	2.34998846	4.53097057	0.01702308
1	1.85418844	3.60627055	-1.87127697
1	2.77268839	3.11157060	3.17872310
1	1.25848842	3.70307064	2.52732301
1	2.90358829	1.48577046	1.16032302
1	1.72428846	1.15067041	2.41042304
6	3.00998831	4.22187042	1.35942304
1	2.93148851	2.62047052	-0.87437695
1	1.40648842	5.07177067	0.15862308
1	3.00338840	5.19577074	-0.56037694
1	4.00668812	3.79937053	1.17652309
1	3.16958833	5.15917063	1.90412307

I-3__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1789228.3 (Joules/Mol)
	427.63583 (Kcal/Mol)
Zero-point correction =	0.681481 (Hartree/Particle)
Thermal correction to Energy =	0.719233
Thermal correction to Enthalpy =	0.720177
Thermal correction to Gibbs Free Energy =	0.610751
Sum of electronic and zero-point Energies =	-1705.795191
Sum of electronic and thermal Energies =	-1705.757440
Sum of electronic and thermal Enthalpies =	-1705.756495
Sum of electronic and thermal Free Energies =	-1705.865921



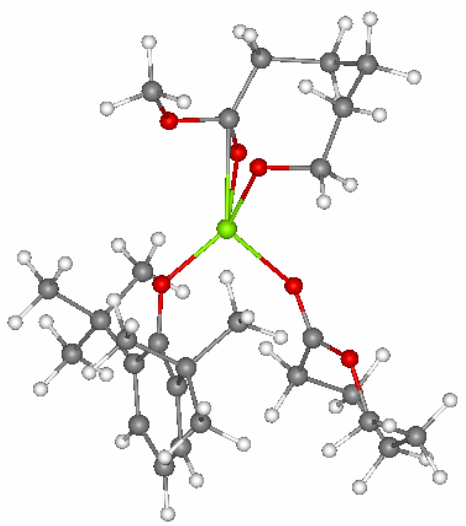
cartesian

12	-1.32603967	-0.55938852	0.35671797
8	-4.71623993	-1.63358855	0.46611795
6	-4.11123991	-2.89658856	0.21591796
1	-3.42143965	-2.85068870	-0.63568205
1	-4.92984009	-3.57638860	-0.02838204
1	-3.57683969	-3.26008868	1.09751797
8	-0.00773977	-1.66278851	-0.46178207
6	1.30666029	-1.47548854	-0.49968204
6	1.90356016	-0.80138850	-1.61558211
6	3.25946021	-0.46368855	-1.53578210
1	3.73326039	0.07141146	-2.35298204
6	4.04646015	-0.82498848	-0.44348204
6	3.48826027	-1.61348855	0.56121790
1	4.13585997	-1.95308852	1.36291790
6	2.13806033	-1.97798848	0.55391794
6	1.11556029	-0.56578851	-2.92128205
6	1.59136033	-2.96728873	1.60391796
6	-0.10053977	0.36361146	-2.74048209
1	-0.88833976	-0.12358854	-2.16378212

1	-0.52963978	0.61281145	-3.71888208
1	0.17136024	1.30241144	-2.24838209
6	0.62716019	-1.93038857	-3.45228195
1	-0.01243977	-2.42758870	-2.72028208
1	1.47666025	-2.58598852	-3.67118216
1	0.05546023	-1.79538846	-4.37898207
6	1.99446034	0.06441145	-4.01548195
1	2.86916018	-0.55048859	-4.25058174
1	2.34226036	1.06831145	-3.74498200
1	1.40946031	0.16221146	-4.93638182
6	2.69586039	-3.44798875	2.56231785
1	3.10186028	-2.63328862	3.17311788
1	3.52486038	-3.92758870	2.03181791
1	2.27756023	-4.19068861	3.25031781
6	1.04066026	-4.21328878	0.87841791
1	0.24966024	-3.94058871	0.17741796
1	0.63056022	-4.92578840	1.60491788
1	1.83736026	-4.71878862	0.32201797
6	0.47646022	-2.36618853	2.48481798
1	0.76066023	-1.39088857	2.89521790
1	0.27376026	-3.02628875	3.33641791
1	-0.46963978	-2.26688862	1.95091796
8	-2.79233980	-0.95398855	1.56241798
6	-3.83493972	-0.60638857	0.82461792
6	-4.70974016	0.52411151	1.37811792
8	-3.13833976	-0.13808854	-0.49248204
6	-4.15483999	1.94351149	1.23261797
1	-5.70673990	0.46231148	0.92911792
1	-4.82863998	0.27191147	2.43601799
6	-3.89053965	0.54091144	-1.49598205
1	-3.07163978	1.94511151	1.40541792
1	-4.58614016	2.55911136	2.03121805
1	-4.92884016	0.19221146	-1.44818211
1	-3.48633981	0.22941145	-2.46498203
6	-4.49064016	2.61881137	-0.10438204
1	-5.57764006	2.56281137	-0.25488204
1	-4.25224018	3.68751144	-0.03338205
6	-3.78433967	2.05161142	-1.33808208
1	-2.71853971	2.31041145	-1.31108212
1	-4.19553995	2.52441144	-2.23998213
8	-0.24823976	1.09011149	0.85171795
6	0.79226023	1.74681151	0.77931792
8	0.82596022	2.71761131	-0.12328205
6	1.95486021	1.51011145	1.69951797
6	2.03556037	3.47061133	-0.39678204
6	2.31036019	2.70961142	2.59651804
6	2.40736032	4.44751120	0.70651793
1	1.78336024	4.00291157	-1.31458211
1	2.90166020	2.32081127	3.43161798
1	1.39566028	3.12281132	3.03861785
1	2.81986022	1.19611144	1.10011792
1	1.67886031	0.65101147	2.30941796
6	3.11096025	3.81011128	1.90301788
1	2.84346032	2.76741147	-0.62218207
1	1.50166023	4.98011160	1.02041793
1	3.06866026	5.19961119	0.26011795
1	4.07066011	3.39391136	1.57021797
1	3.35196018	4.59041119	2.63341784
1	5.09935999	-0.55408859	-0.40948203

TS-34__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1786096.1 (Joules/Mol)
	426.88722 (Kcal/Mol)
Zero-point correction =	0.680288 (Hartree/Particle)
Thermal correction to Energy =	0.717896
Thermal correction to Enthalpy =	0.718841
Thermal correction to Gibbs Free Energy =	0.609286
Sum of electronic and zero-point Energies =	-1705.777674
Sum of electronic and thermal Energies =	-1705.740065
Sum of electronic and thermal Enthalpies =	-1705.739121
Sum of electronic and thermal Free Energies =	-1705.848676



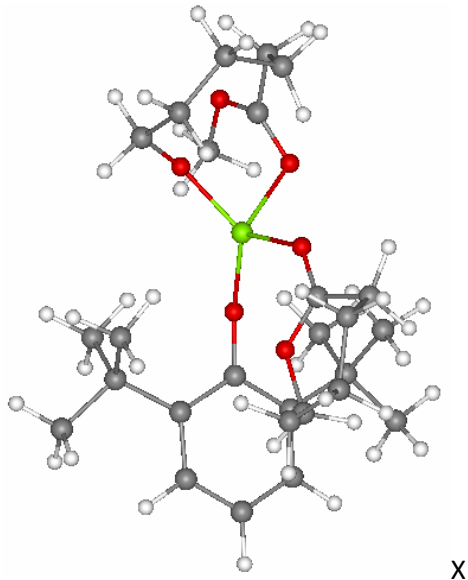
cartesian

8	0.05624477	-1.57122314	-0.39618218
6	1.37754476	-1.45982313	-0.42278218
6	2.17114472	-1.98902309	0.64811784
6	3.53784466	-1.69412315	0.66631782
1	4.15784454	-2.05532289	1.48061776
6	4.14734459	-0.94912302	-0.34208214
6	3.39364481	-0.57122302	-1.45228219
1	3.90454483	-0.07602306	-2.27248216
6	2.02414465	-0.84532303	-1.54648221
6	1.56134474	-2.92422295	1.71291780
6	1.27204478	-0.61362302	-2.87488222
6	0.53204477	-2.21162295	2.61091781
1	-0.37365526	-1.93732309	2.06961775
1	0.21684477	-2.87582302	3.42471790
1	0.95464474	-1.31182313	3.07161784
6	0.88294476	-4.12022305	1.01161778
1	0.09744477	-3.78632307	0.33181781
1	1.61744475	-4.69512320	0.43711782
1	0.43584475	-4.79092312	1.75561774
6	2.63744473	-3.50162292	2.64991784
1	3.41394472	-4.04512310	2.10171771
1	3.12154484	-2.72942305	3.25911784
1	2.16844463	-4.20982313	3.34151769
6	2.20404482	-0.06312306	-3.96858239
1	2.58974481	0.93377697	-3.72438216
1	3.05534482	-0.72442305	-4.15958214
1	1.64584470	0.02707694	-4.90678215
6	0.73364478	-1.97232306	-3.37228227
1	0.05994476	-2.41722298	-2.63718224
1	0.18374476	-1.84152305	-4.31278181
1	1.55724478	-2.67072296	-3.55558228
6	0.09504475	0.37497693	-2.75848222
1	0.39314476	1.31187689	-2.27808213
1	-0.28235525	0.62177694	-3.75858212
1	-0.74295521	-0.05692307	-2.20898223
8	-3.47085524	-1.95982313	0.29901785
6	-4.32905531	-2.35782290	-0.76918215
1	-5.33185530	-2.60052299	-0.40168220
1	-3.87985539	-3.25822306	-1.19058216
1	-4.37425518	-1.57902312	-1.53418219
8	-2.96445537	0.19687694	-0.64928216
6	-3.60495520	-0.69972306	0.84801787
8	-2.68215537	-0.44902307	1.69331777
6	-5.01335526	-0.20202306	1.10591781
12	-1.25645530	-0.36332306	0.27131784
1	-5.68015528	-0.45692307	0.27911782
1	5.21164465	-0.72922307	-0.29788220
6	-3.21575522	1.56867695	-0.91658217
1	-2.77495527	2.21737695	-0.14088216
6	-4.70205545	1.88307691	-1.07418227
1	-2.69615531	1.80627692	-1.85488224
1	-4.81645536	2.74487710	-1.74368227
6	-5.44525528	2.18587708	0.23511782
1	-5.16145515	1.03587687	-1.59728217
1	-5.34085512	-0.79462302	1.96971774
6	-5.08565521	1.29307687	1.43031776
1	-4.12705517	1.59347689	1.86421776
1	-5.83135509	1.45707691	2.21591783
1	-6.52445507	2.12237692	0.04461783
1	-5.25455523	3.22717690	0.52411783
8	-0.09695524	1.24047685	0.77591783
6	0.98724478	1.82047689	0.70571786
8	1.11084473	2.75087690	-0.23328216
6	2.10854483	1.54397690	1.66541779
6	2.37964463	3.39537692	-0.51068217
6	2.53144479	2.75407696	2.51761770
6	2.80394483	4.39097691	0.55671787
1	2.18824482	3.90377712	-1.45628226
1	3.07084465	2.36207700	3.38581777
1	1.64034474	3.25537705	2.91441774
1	2.96204472	1.14247692	1.10251784
1	1.75554478	0.73607695	2.30501771
6	3.43004465	3.75827694	1.79781783
1	3.13574481	2.62367702	-0.68698215
1	1.93604469	5.00587654	0.82391787
1	3.53104472	5.06857681	0.09331783
1	4.36224461	3.25577712	1.50871778
1	3.71384478	4.55097675	2.49901772

I-4_DBP_Mg_OMe_eCL-2

Zero-point vibrational energy	1785379.5 (Joules/Mol)
	426.71594 (Kcal/Mol)
Zero-point correction =	0.680015 (Hartree/Particle)
Thermal correction to Energy =	0.718940
Thermal correction to Enthalpy =	0.719884
Thermal correction to Gibbs Free Energy =	0.606721
Sum of electronic and zero-point Energies =	-1705.795516

Sum of electronic and thermal Energies = -1705.756591
Sum of electronic and thermal Enthalpies = -1705.755647
Sum of electronic and thermal Free Energies = -1705.868810



X

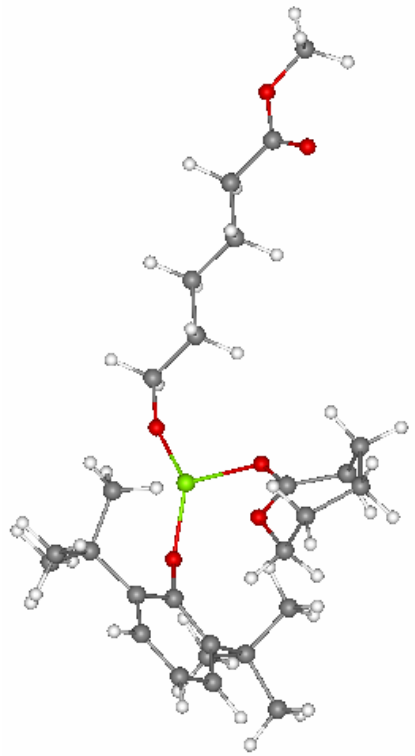
cartesian

12	-1.31694233	-0.37061539	0.06525776
8	-4.11644220	-2.53401542	0.44225776
6	-3.08504224	-3.52941537	0.32925773
1	-2.35734224	-3.21721530	-0.42234224
1	-3.59404230	-4.43581533	0.00475775
1	-2.59114242	-3.68531537	1.28935766
8	0.29085767	-1.35411537	-0.04504225
6	1.60835767	-1.38961542	-0.16484225
6	2.23075771	-1.23641539	-1.44854224
6	3.62595773	-1.14701545	-1.50544226
1	4.11855745	-1.00551534	-2.46184206
6	4.42395735	-1.25001538	-0.36894226
6	3.81735778	-1.51241541	0.85625780
1	4.45565748	-1.65471542	1.72255766
6	2.42895770	-1.61201537	0.99135774
6	1.41225767	-1.20921540	-2.75604224
6	1.81855774	-1.99531543	2.35415792
6	0.56825763	0.07378461	-2.87534213
1	-0.19644235	0.14078462	-2.10044217
1	0.04755765	0.09988461	-3.84004211
1	1.20115769	0.96528459	-2.80724216
6	0.50065762	-2.45101547	-2.83864212
1	-0.18944235	-2.49651551	-1.99614227
1	1.10365772	-3.36561537	-2.83794212
1	-0.08524235	-2.43131542	-3.76554227
6	2.31595778	-1.24731541	-4.00314236
1	2.97025776	-2.12531543	-4.01004219
1	2.94025779	-0.35171539	-4.09834194
1	1.68835771	-1.29841542	-4.89964199
6	2.89535761	-2.35411549	3.39385772
1	3.53945780	-1.50351536	3.64385772
1	3.53195763	-3.18001533	3.05975795
1	2.40715766	-2.67161536	4.32215786
6	0.92315763	-3.24171543	2.19795775
1	0.11915766	-3.06381536	1.48345768
1	0.48095763	-3.51541543	3.16415787
1	1.51495767	-4.09321547	1.84435773
6	1.00145769	-0.83561540	2.95365787
1	1.63455772	0.04908461	3.09485793
1	0.59645766	-1.11561537	3.93375778
1	0.16045766	-0.56181538	2.31735778
8	-2.63994241	-1.15431535	1.43725777
6	-3.75714231	-1.34901536	0.92015779
6	-4.93104267	-0.41631538	1.03005779
8	-2.81434226	-0.38061538	-1.08194232
6	-4.64674234	1.09118462	0.94165778
1	-5.68024254	-0.72811538	0.29905778
1	-5.35644245	-0.65131539	2.01625776
6	-3.49894238	0.36258462	-2.03124213
1	-3.60854220	1.29068458	1.22495770
1	-5.26184273	1.57818460	1.70725775
1	-4.39934254	-0.18531539	-2.36784220
1	-2.88744235	0.51458460	-2.93974209
6	-4.98244238	1.75928462	-0.40544224
1	-5.91834259	1.33058465	-0.79064220
1	-5.21224260	2.81228471	-0.19624224
6	-3.92484236	1.73968458	-1.51574230
1	-3.02454233	2.26438451	-1.16584229
1	-4.31594276	2.32548451	-2.36054206
8	-0.88794237	1.52528465	0.82615775
6	0.17585765	2.15278459	0.88395774
8	1.19855773	1.69108462	0.19675776
6	0.28685766	3.42208457	1.68575776
6	2.54085779	2.23448467	0.29915774
6	0.65885764	4.65878439	0.84745777
6	2.68005776	3.59928465	-0.35244226
1	3.13985777	1.47878456	-0.20944224
1	0.38035762	5.54238462	1.43105769
1	0.03975765	4.68448448	-0.05704224
1	1.02575767	3.27288461	2.48315787
1	-0.68324238	3.55868459	2.16525793
6	2.14005780	4.76078463	0.48205775
1	2.83755779	2.24498463	1.35305774
1	2.19925761	3.56588459	-1.33704233
1	3.74875760	3.75808454	-0.53714222
1	2.72835779	4.83808470	1.40625775
1	2.30405760	5.69788456	-0.06144224
1	5.50635767	-1.17701542	-0.44584227

I-5__DBP_Mg_OMe_eCL-2

Zero-point vibrational energy 1783528.2 (Joules/Mol)
426.27347 (Kcal/Mol)

Zero-point correction =	0.679310 (Hartree/Particle)
Thermal correction to Energy =	0.719268
Thermal correction to Enthalpy =	0.720212
Thermal correction to Gibbs Free Energy =	0.600374
Sum of electronic and zero-point Energies =	-1705.785721
Sum of electronic and thermal Energies =	-1705.745763
Sum of electronic and thermal Enthalpies =	-1705.744819
Sum of electronic and thermal Free Energies =	-1705.864657



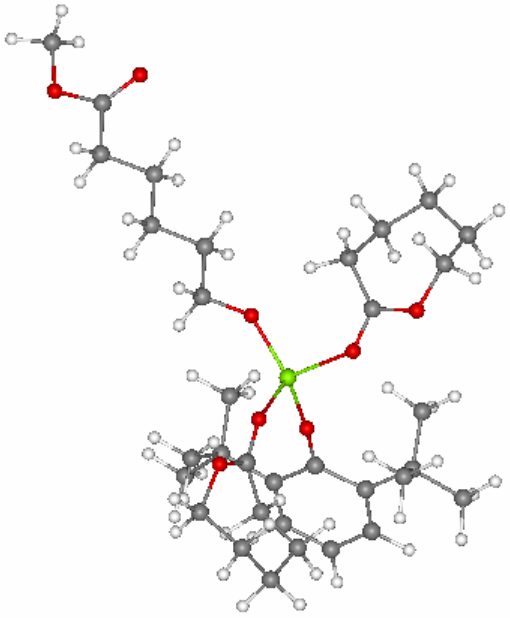
cartesian

8	1.27109492	-2.23759246	-0.31333464
6	2.60169506	-2.59969234	-0.41193464
6	3.56399488	-1.41969228	-0.24203461
6	5.03909492	-1.81049228	-0.33473465
6	5.98759508	-0.62299228	-0.16173463
6	7.45579481	-1.02429235	-0.25423464
1	5.22829485	-2.29119229	-1.30483460
1	2.80499506	-3.07659245	-1.38893461
1	2.84939504	-3.36109233	0.35086536
1	5.26289511	-2.57049251	0.42706537
1	3.36479497	-0.94869226	0.73036534
1	3.33029485	-0.66649228	-1.00673461
1	5.80669498	-0.13949229	0.80486536
1	5.77329493	0.13810770	-0.92053461
12	-0.19880506	-1.18599224	-0.31313464
8	-2.02980494	-1.44849229	-0.62623465
6	-3.20260501	-1.00439227	-0.19033462
6	-3.57290506	-1.18959224	1.17836535
6	-4.76120520	-0.61009228	1.63366532
1	-5.05350494	-0.71519226	2.67346549
6	-5.60620499	0.09640770	0.78046536
6	-5.28530502	0.18340771	-0.57233465
1	-5.98460484	0.68710774	-1.23223460
6	-4.10940504	-0.36599228	-1.09383464
6	-2.72410512	-2.07629251	2.10946560
6	-3.82980514	-0.31789228	-2.60793447
6	-1.25290501	-1.58399224	2.22976542
1	-0.55770504	-2.21649241	1.66076541
1	-0.89470506	-1.65589225	3.26256537
1	-1.15180504	-0.52839231	1.94946539
6	-2.73950505	-3.52309251	1.57076538
1	-2.35860515	-3.56799245	0.54816538
1	-3.76000500	-3.91969252	1.57416534
1	-2.12000513	-4.17429209	2.19966555
6	-3.29660511	-2.11849236	3.53786540
1	-4.31740522	-2.51209235	3.56146550
1	-3.29610515	-1.13149226	4.01476526
1	-2.68140507	-2.78279233	4.15436506
6	-5.00010490	0.29640773	-3.39523458
1	-5.18060493	1.34440768	-3.12993455
1	-5.93150520	-0.26009229	-3.24803448
1	-4.76910496	0.26930773	-4.46583462
6	-3.62400508	-1.74839222	-3.14903450
1	-2.79270506	-2.24779248	-2.64993453
1	-3.42030501	-1.72039223	-4.22663498
1	-4.52730513	-2.34789228	-2.99343443
6	-2.58620501	0.53690773	-2.92003441
1	-2.72850513	1.56860769	-2.57383442
1	-2.40620494	0.57280773	-4.00143480
1	-1.69390500	0.12770770	-2.44443440
8	0.20239493	0.83510774	-0.41953462
6	-0.49130508	1.82250774	-0.14733462
8	-1.55840504	1.62990773	0.60006535
6	-0.10790507	3.19690752	-0.62033463
6	-2.55170512	2.66230750	0.84946537
6	0.13789493	4.20400763	0.51816535
6	-2.05760503	3.74600768	1.79126537
1	-3.37780499	2.09530759	1.27856541
1	0.72529495	5.02740765	0.09966538
1	0.76979494	3.74020767	1.28476536
1	-0.89320505	3.56870770	-1.29043460
1	0.79359496	3.06500769	-1.21983469
6	-1.13140500	4.77860785	1.14756536
1	-2.88560510	3.06300759	-0.11243462
1	-1.57460499	3.26750755	2.65156555
1	-2.94510508	4.25670767	2.18276548
1	-1.69060504	5.32740784	0.37796536
1	-0.84540510	5.51990795	1.90166533
6	8.41199493	0.13160770	-0.07813462
1	7.70859480	-1.77979231	0.49976534
1	7.67939472	-1.49439228	-1.21953464
8	9.69679451	-0.28499228	-0.17363462
8	8.10559464	1.28910768	0.12346537
6	10.68679428	0.74110770	-0.01803462

1	11.64809418	0.23880769	-0.12203462
1	10.57159424	1.50770772	-0.78773463
1	10.60519409	1.20930767	0.96556538
1	-6.52680492	0.53580773	1.15726531

I-5m_DBP_Mg_OMe_eCL-3

Zero-point vibrational energy	2200979.7 (Joules/Mol)
	526.04676 (Kcal/Mol)
Zero-point correction =	0.838309 (Hartree/Particle)
Thermal correction to Energy =	0.887169
Thermal correction to Enthalpy =	0.888113
Thermal correction to Gibbs Free Energy =	0.747361
Sum of electronic and zero-point Energies =	-2090.672967
Sum of electronic and thermal Energies =	-2090.624107
Sum of electronic and thermal Enthalpies =	-2090.623163
Sum of electronic and thermal Free Energies =	-2090.763914



X

cartesian

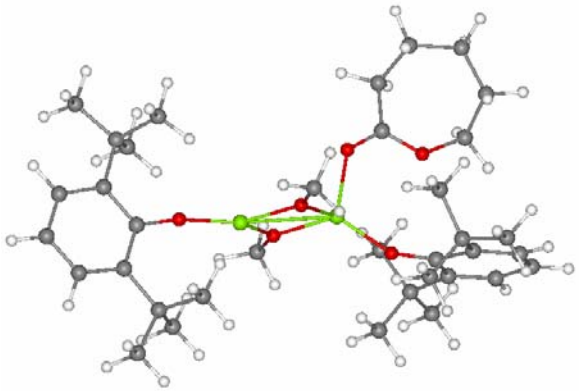
8	-1.25303173	0.46260831	-0.91945100
6	-2.31623173	-0.32219172	-1.34725094
6	-3.63003159	0.06570829	-0.66225100
6	-4.82033205	-0.79089171	-1.09295106
6	-6.13663197	-0.37349170	-0.43515098
6	-7.30663204	-1.25789165	-0.85415095
6	-8.63063145	-0.83559173	-0.26265097
8	-9.58473110	-1.76839173	-0.49635097
1	-2.14063168	-1.39809167	-1.15685105
1	-2.45823169	-0.23199171	-2.44215107
1	-3.48663163	-0.00929171	0.42344904
1	-3.83713174	1.12320828	-0.87745100
1	-4.61243200	-1.84419167	-0.85795099
1	-4.92963171	-0.74169171	-2.18585110
6	-10.88983154	-1.44729173	0.00434902
12	0.57596827	0.37700829	-0.56125098
8	1.06506824	2.38550806	-0.53875101
6	0.46066827	3.45830822	-0.55155098
6	-1.03763175	3.55460835	-0.57595098
8	1.21646833	4.55430841	-0.52225101
6	-1.62233174	4.11240864	0.73474902
1	-1.34573174	4.18380833	-1.42095089
1	-1.39723170	2.53350830	-0.75925100
6	0.63196826	5.87720823	-0.49725097
1	-1.13893175	3.62210846	1.58774900
1	-2.67433167	3.81350851	0.77374899
1	-0.00253175	6.01190853	-1.38015103
1	1.50166833	6.52620840	-0.60745096
6	-1.53173172	5.63130856	0.86954904
1	-2.13903165	6.09420824	0.07974902
1	-1.98383164	5.93690825	1.81974912
6	-0.11243175	6.19640827	0.79124904
1	0.49536824	5.85000849	1.63574910
1	-0.15833175	7.28900862	0.87234902
1	-6.36563206	0.66840827	-0.68395096
1	-6.03283215	-0.40499172	0.65564901
1	-7.13383198	-2.30629158	-0.58665097
1	-7.42783213	-1.25289166	-1.94535089
8	-8.85013103	0.19820829	0.33494902
1	-11.52273178	-2.29269171	-0.26415098
1	-10.86513138	-1.31809175	1.08874893
1	-11.26413155	-0.52939171	-0.45475098
8	1.49596834	-0.52699172	0.81274903
6	2.10396838	-1.27949166	1.71854901
6	1.72176826	-2.64909172	1.90644908
6	2.46516824	-3.43399191	2.79384899
1	2.20576835	-4.47759151	2.93744898
6	3.53486824	-2.92119169	3.51984906
6	3.85036826	-1.57279170	3.39174891
1	4.65946817	-1.17689168	3.99624896
6	3.15536833	-0.72649169	2.52264905
6	0.49376822	-3.25419188	1.19834900
6	3.50556827	0.77320832	2.47344899
6	0.68556821	-3.28739166	-0.33005098
1	0.85546821	-2.28999186	-0.73745096
1	-0.20013174	-3.70659161	-0.82265097
1	1.54656827	-3.91279173	-0.59415096
6	-0.77013177	-2.44969177	1.56464911
1	-0.69683176	-1.40429175	1.26234913
1	-0.93383175	-2.47749186	2.64744902
1	-1.65303171	-2.88319159	1.07914901
6	0.22676824	-4.70809174	1.62934899
1	0.04166825	-4.79279137	2.70524907

1	1.05096829	-5.38069153	1.36754894
1	-0.66793174	-5.07649136	1.11474895
6	4.59316826	1.15640831	3.49334908
1	5.54676819	0.65420830	3.29634905
1	4.29316807	0.93280828	4.52264929
1	4.77766800	2.23520851	3.43304896
6	2.26036835	1.61260831	2.82554889
1	1.42876828	1.39430833	2.15494895
1	2.49066830	2.68340826	2.75934887
1	1.93516827	1.39760828	3.84944892
6	4.04736805	1.16900826	1.08664894
1	4.97326803	0.62250829	0.87244904
1	4.27406788	2.24180841	1.05214906
1	3.32676840	0.95480829	0.29784903
8	1.67166829	-0.03809170	-2.27645111
6	2.59546828	-0.70059168	-2.74295115
8	2.68436837	-0.72869170	-4.07065105
6	3.59966826	-1.42799175	-1.89015102
6	3.68036819	-1.52029169	-4.75895071
6	5.03696823	-0.89369172	-2.03445101
6	5.09836817	-0.99479175	-4.60405064
1	3.35866833	-1.45909166	-5.79925060
1	5.58996820	-1.22489166	-1.15055108
1	5.02446795	0.20120829	-1.99075103
1	3.57056832	-2.49759150	-2.13305116
1	3.25776839	-1.32359171	-0.85955095
6	5.77266788	-1.37129176	-3.28545094
1	3.59416819	-2.56529188	-4.44165087
1	5.08116817	0.09320830	-4.74055099
1	5.68516827	-1.40139174	-5.43645096
1	5.87846804	-2.46359158	-3.24065113
1	6.79066801	-0.96629167	-3.27635098
1	4.09686804	-3.55799150	4.19894934

S5.3. ROP of εCL. Binuclear mechanism

DI-1__DBP-2_Mg-2_OMe-2_eCL-1

Zero-point vibrational energy	2324642.7 (Joules/Mol)
	555.60294 (Kcal/Mol)
Zero-point correction =	0.885410 (Hartree/Particle)
Thermal correction to Energy =	0.938485
Thermal correction to Enthalpy =	0.939429
Thermal correction to Gibbs Free Energy =	0.794792
Sum of electronic and zero-point Energies =	-2257.023297
Sum of electronic and thermal Energies =	-2256.970222
Sum of electronic and thermal Enthalpies =	-2256.969278
Sum of electronic and thermal Free Energies =	-2257.113915



cartesian

12	2.15292025	-0.09183032	-0.08794509
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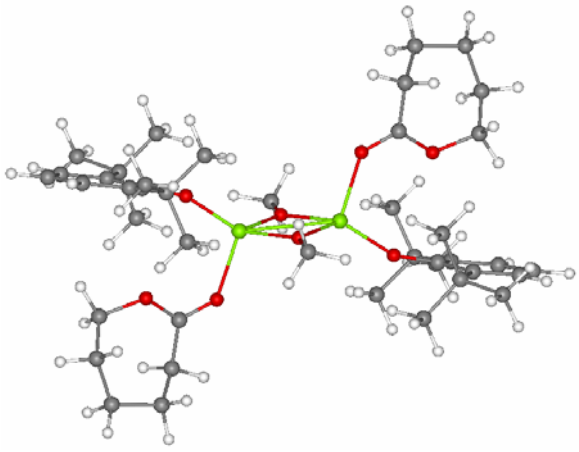
8	3.96892023	0.08726969	-0.09234509
6	0.77062023	0.21656968	2.60745502
1	1.80612028	0.27026969	2.96785498
1	0.27952024	-0.62023032	3.11765504
6	5.29252005	-0.03533031	0.00095491
6	5.88441992	-1.32203031	0.18225491
6	7.27782011	-1.40273035	0.27035493
1	7.75661993	-2.36663032	0.40705490
6	8.08612061	-0.27443030	0.18785492
6	7.49702024	0.97356969	0.01305491
1	8.14512062	1.84116960	-0.04794508
6	6.11151981	1.13086963	-0.08424509
6	5.02761984	-2.59803033	0.28335491
6	5.50012016	2.53096986	-0.28014508
6	4.21941996	-2.81533027	-1.01314509
1	3.60242033	-1.95183039	-1.27374506
1	3.56822038	-3.69303036	-0.92344505
1	4.89531994	-2.98223019	-1.85834503
6	4.09692001	-2.52763033	1.51215494
1	3.47772026	-1.62673032	1.52065492
1	4.68631983	-2.50673032	2.43475485
1	3.43662024	-3.40203023	1.55265498
6	5.88051987	-3.86623025	0.46915492
1	6.47332001	-3.83513021	1.38905489
1	6.55942011	-4.03413057	-0.37314507
1	5.22151995	-4.73913050	0.53575492
6	6.57261992	3.63336968	-0.33674508
1	7.26531982	3.49616981	-1.17374504
1	7.15642023	3.69176984	0.58795494
1	6.08432007	4.60456944	-0.47504508
6	4.57202005	2.88596964	0.89995492
1	3.76222038	2.16306973	1.01225495
1	4.13051987	3.87976980	0.75435495
1	5.13532019	2.90226984	1.83935499
6	4.72792006	2.59876966	-1.61364508
1	5.40362024	2.41876984	-2.45674515
1	4.27992010	3.59146976	-1.74674511
1	3.93392038	1.85156965	-1.65994501
12	-0.75857979	-0.04293031	-0.11724509
8	0.75152022	-0.22433032	-1.40334511
8	-2.23447967	-1.20303035	-0.05044509
6	0.80952024	-0.36663032	-2.80994511
1	0.27822024	-1.26873040	-3.13474512
1	0.35492024	0.49736971	-3.31214499
6	-3.53557968	-1.45493031	-0.01494509
6	-4.26208019	-1.68163037	-1.23044503
6	-5.65117979	-1.83193040	-1.16234505
1	-6.22238016	-1.98413038	-2.07204509
6	-6.34007978	-1.80753040	0.04655492
6	-5.61677980	-1.68373036	1.22905493
1	-6.16137981	-1.72263038	2.16655493
6	-4.22677994	-1.52873039	1.23925495
6	-3.55017972	-1.79353034	-2.59254503
6	-3.47917962	-1.46193039	2.58545494
6	-2.94627976	-0.44133031	-3.01664495
1	-2.21507978	-0.07643032	-2.29414511
1	-2.44297981	-0.52923030	-3.98704505
1	-3.73177981	0.31696969	-3.11344504
6	-2.45487976	-2.87753034	-2.53244495
1	-1.71357977	-2.66163015	-1.76234508
1	-2.90027976	-3.85243034	-2.30634499
1	-1.94587970	-2.95893025	-3.50114512
6	-4.51208019	-2.20713019	-3.72224498
1	-4.99597979	-3.16793013	-3.51904511
1	-5.29247999	-1.46033037	-3.90534496

1	-3.94637966	-2.31653023	-4.65434551
6	-4.40288019	-1.75723040	3.78205490
1	-5.19218016	-1.00703037	3.90265489
1	-4.87417984	-2.74223018	3.70235491
1	-3.81067967	-1.75033033	4.70405483
6	-2.35867977	-2.52093029	2.63305497
1	-1.63577974	-2.38713026	1.82805490
1	-1.83067977	-2.47173023	3.59345484
1	-2.78417969	-3.52573013	2.53765488
6	-2.90307975	-0.05363031	2.82105494
1	-3.70867968	0.68816972	2.85805488
1	-2.35957980	-0.00923031	3.77235484
1	-2.21667981	0.24486969	2.02705503
1	1.84822023	-0.44413030	-3.15694499
1	0.26562023	1.14396966	2.90775490
1	-7.42047977	-1.92813039	0.06965491
1	9.16712093	-0.36673030	0.25875491
8	-3.56057978	1.67046964	-0.19074509
6	-2.51937962	2.44226980	-0.41284508
6	-2.68367982	3.90696979	-0.71624506
1	-3.26577973	4.01476955	-1.64014506
6	-4.93737984	2.11136985	-0.32984510
1	-5.49098015	1.17706966	-0.23394509
6	-5.36028004	3.11566973	0.72805494
1	-5.08158016	2.49436975	-1.34614503
1	-5.03717995	2.74506974	1.70755494
6	-4.87128019	4.54496956	0.49285492
1	-6.45637989	3.11146975	0.74625492
1	-1.68077970	4.28706932	-0.91464508
6	-3.35287976	4.70256948	0.41925490
1	-2.89247966	4.42926931	1.37595499
1	-3.11627960	5.75946951	0.25885493
1	-5.31207991	4.92456961	-0.43884510
1	-5.25347996	5.18786955	1.29325497
8	-1.39577973	1.92826962	-0.34394509

DI-1__DBP-2_Mg-2_OMe-2_eCL-2

Zero-point vibrational energy	2741870.0 (Joules/Mol)
	655.32265 (Kcal/Mol)
Zero-point correction =	1.044323 (Hartree/Particle)
Thermal correction to Energy =	1.106188
Thermal correction to Enthalpy =	1.107132
Thermal correction to Gibbs Free Energy =	0.939188
Sum of electronic and zero-point Energies =	-2641.906101
Sum of electronic and thermal Energies =	-2641.844236
Sum of electronic and thermal Enthalpies =	-2641.843292
Sum of electronic and thermal Free Energies =	-2642.011236



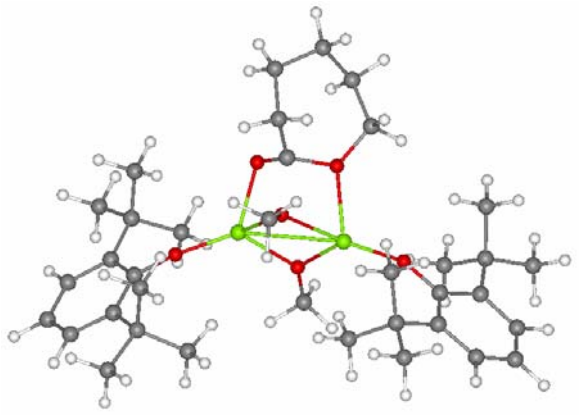
cartesian

12	1.47032356	-0.02421751	-0.07869257
8	-0.05907640	0.31048250	-1.27439260
8	2.96052361	1.13318241	0.04100743
6	-0.12177639	0.70638245	-2.62499261
1	0.86982358	0.97638249	-3.00679278
1	-0.51787639	-0.09921751	-3.25829268
6	4.23312330	1.48518252	0.12660743
6	4.96702337	1.84628248	-1.05359256
6	6.33652353	2.10598254	-0.94189256
1	6.91072321	2.36038256	-1.82679260
6	7.00102329	2.06548238	0.28000745
6	6.26622343	1.80888247	1.43350744
1	6.78662348	1.83368242	2.38530731
6	4.89442348	1.53808248	1.39970744
6	4.27832317	1.98258245	-2.42479277
6	4.13322353	1.31778252	2.72090721
6	3.79252362	0.61218244	-2.93269277
1	3.09382367	0.14838248	-2.23569274
1	3.29182363	0.71078247	-3.90389276
1	4.64212322	-0.06861752	-3.06319261
6	3.10102367	2.97468257	-2.32799268
1	2.36782360	2.66198254	-1.58409250
1	3.46852350	3.96688247	-2.04309273
1	2.59962368	3.06948256	-3.29949260
6	5.22502327	2.53468251	-3.50629258
1	5.62832355	3.51658249	-3.23749256
1	6.06522322	1.86268246	-3.71369267
1	4.66912317	2.65398240	-4.44319248
6	5.00402355	1.61428249	3.95620728
1	5.85522318	0.93068248	4.04620743
1	5.38572359	2.64068246	3.95300722
1	4.39732313	1.49178243	4.86060762
6	2.91932368	2.26558256	2.81080723
1	2.22622371	2.12088251	1.98220742
1	2.37992358	2.10298252	3.75230742
1	3.25312352	3.30898237	2.79150724
6	3.68672371	-0.15021752	2.84630728

1	4.55922318	-0.81291753	2.86650729
1	3.12002349	-0.30821750	3.77160740
1	3.06062365	-0.45731750	2.00780725
12	-1.46877635	-0.02241751	0.06220743
8	0.06092360	-0.37221751	1.25400746
8	-2.97617650	-1.15701759	-0.05989257
6	0.12542361	-0.78351754	2.59980726
1	-0.85647643	-1.10741758	2.96420741
1	0.47392359	0.03108249	3.24970722
6	-4.25717640	-1.48041749	-0.13669257
6	-4.98737669	-1.83891749	1.04650748
6	-6.36317682	-2.06721759	0.94550747
1	-6.93427658	-2.31911755	1.83320749
6	-7.03847647	-1.99801755	-0.26919255
6	-6.30927658	-1.74461758	-1.42699254
1	-6.83937645	-1.74711752	-2.37379265
6	-4.93157673	-1.50441754	-1.40369260
6	-4.28877640	-2.00571752	2.40930724
6	-4.17857647	-1.28621757	-2.72989273
6	-3.76967645	-0.65171754	2.92840743
1	-3.06817651	-0.19371752	2.23040724
1	-3.26177645	-0.77211756	3.89330721
1	-4.60367680	0.04478249	3.07510734
6	-3.13377643	-3.02131748	2.28950739
1	-2.40127635	-2.71541762	1.54200745
1	-3.52497649	-4.00191736	1.99660742
1	-2.62547636	-3.13841748	3.25490737
6	-5.23667669	-2.55061746	3.49330735
1	-5.66317654	-3.52051759	3.21690726
1	-6.06027651	-1.86361754	3.71700740
1	-4.67447662	-2.69291759	4.42330742
6	-5.06767654	-1.54961753	-3.95959258
1	-5.90437651	-0.84641755	-4.03379250
1	-5.47217655	-2.56731749	-3.96389270
1	-4.46717644	-1.43061757	-4.86869240
6	-2.98717642	-2.25981760	-2.84209275
1	-2.28277636	-2.13951755	-2.01889277
1	-2.45367646	-2.09961748	-3.78729272
1	-3.34417629	-3.29561758	-2.83019257
6	-3.70067644	0.17278248	-2.84419274
1	-4.55847645	0.85488248	-2.84689260
1	-3.14147639	0.32868248	-3.77439260
1	-3.05797648	0.45678249	-2.01009274
1	0.81422359	-1.63091755	2.72750735
1	-0.76987642	1.58478248	-2.75599265
1	-8.10947609	-2.18061757	-0.31849256
1	8.06712341	2.27208257	0.33750746
8	4.35762358	-1.67631757	-0.21999258
6	3.34922361	-2.39571762	-0.67029256
6	3.57172370	-3.76491761	-1.25679255
1	4.20562315	-3.67031765	-2.14759278
6	5.74662352	-2.06221747	-0.36949256
1	6.27482319	-1.16011751	-0.06019257
6	6.13592339	-3.25531745	0.48670745
1	5.95502329	-2.23081756	-1.43169260
1	5.74102354	-3.10111761	1.49750745
6	5.70182323	-4.61121750	-0.06989257
1	7.22832346	-3.23941755	0.57770747
1	2.59152365	-4.10851717	-1.58939254
6	4.19512320	-4.77131748	-0.27319255
1	3.67102361	-4.71261740	0.68810743
1	3.99832368	-5.77451706	-0.66529256
1	6.20872355	-4.78091717	-1.02949250
1	6.05262327	-5.40181732	0.60270745
8	2.21352363	-1.92091751	-0.57709253
8	-4.33187675	1.67188251	0.24670742
6	-3.30607629	2.37648249	0.68100744
6	-3.49877644	3.74988246	1.26820743
1	-4.12257671	3.66688251	2.16730738
6	-5.71227646	2.08078241	0.41280743
1	-6.25907660	1.18708241	0.11150743
6	-6.09287643	3.27868247	-0.44089255
1	-5.90467644	2.25478244	1.47710741
1	-5.71317673	3.11618257	-1.45619261
6	-5.63007641	4.62848282	0.10740743
1	-7.18647671	3.28018236	-0.51829255
1	-2.50887632	4.07808256	1.58750749
6	-4.11847687	4.76478291	0.29100743
1	-3.60787630	4.69628286	-0.67669255
1	-3.90067649	5.76518250	0.67910743
1	-6.12177658	4.80788279	1.07310748
1	-5.97687674	5.42328262	-0.56219256
8	-2.17927647	1.88398242	0.57240742

DTS-12_DBP-2_Mg-2_OMe-2_eCL-1

Zero-point vibrational energy	2323698.0 (Joules/Mol)
	555.37715 (Kcal/Mol)
Zero-point correction =	0.885050 (Hartree/Particle)
Thermal correction to Energy =	0.936814
Thermal correction to Enthalpy =	0.937758
Thermal correction to Gibbs Free Energy =	0.796554
Sum of electronic and zero-point Energies =	-2256.996350
Sum of electronic and thermal Energies =	-2256.944586
Sum of electronic and thermal Enthalpies =	-2256.943642
Sum of electronic and thermal Free Energies =	-2257.084846

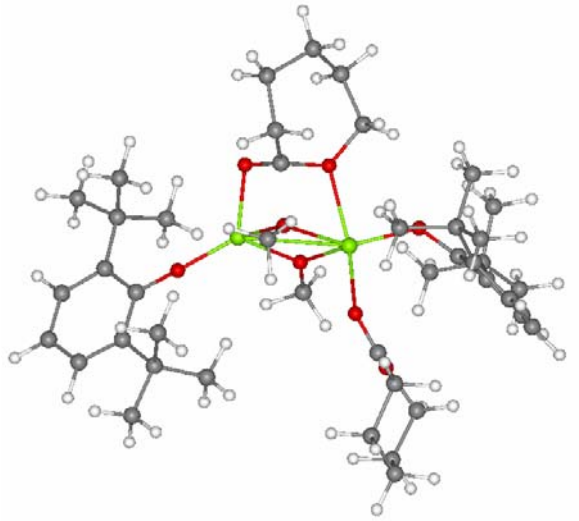


cartesian

12	1.62262011	0.52389312	-0.09829409
8	0.10242005	0.06559312	-1.24839401
8	3.29452014	-0.23970687	-0.05799409
6	0.12692004	-0.37260690	-2.60019398
1	0.07322004	0.47919312	-3.28959417
1	-0.71927994	-1.03680682	-2.81129408
6	4.46891975	-0.74270689	-0.43789408
6	5.38681984	0.05399312	-1.18979406
6	6.60401964	-0.51820689	-1.57259405
1	7.31751966	0.06359312	-2.14629412
6	6.94161987	-1.82490683	-1.23819411
6	6.04761982	-2.58680701	-0.49359408
1	6.33071995	-3.60170698	-0.23519409
6	4.81311989	-2.08140683	-0.07569409
6	5.06891966	1.51229322	-1.57119405
6	3.86302018	-2.95920706	0.76020586
6	4.84301996	2.36379313	-0.30469409
1	4.58951998	3.39619303	-0.57539409
1	5.75761986	2.38929296	0.29760590
1	4.04651976	1.96909320	0.32680592
6	3.84622002	1.57329321	-2.50949407
1	2.97602010	1.05229318	-2.10219407
1	4.07441998	1.09079313	-3.46569395
1	3.55832005	2.61149311	-2.71199417
6	6.22211981	2.18369317	-2.33979416
1	6.44121981	1.68099320	-3.28759408
1	7.14261961	2.22109294	-1.74829412
1	5.94461966	3.21719313	-2.57629395
6	4.45511961	-4.34940672	1.05270588
1	5.39222002	-4.29040718	1.61610591
1	4.63831997	-4.92280674	0.13790591
1	3.74541998	-4.92360687	1.65910590
6	2.54112005	-3.19880700	0.00370591
1	2.03292012	-2.26310706	-0.23529409
1	1.86112010	-3.81790686	0.60220587
1	2.72862005	-3.72380686	-0.93909413
6	3.59391999	-2.29780698	2.12750602
1	4.52511978	-2.20900702	2.69780588
1	2.89582014	-2.90570688	2.71730590
1	3.17892003	-1.29530680	2.01040602
12	-1.39847994	0.35209310	-0.05069409
8	0.07002004	0.40279311	1.44540596
8	-3.16817999	-0.16920689	-0.09099409
6	0.09792005	-0.30730689	2.68610597
1	1.02491999	-0.10340688	3.23070598
1	-0.76197994	-0.04200688	3.30880594
6	-4.21878004	-0.91360688	-0.45329410
6	-4.46388006	-2.16810703	0.18510590
6	-5.55938005	-2.92760706	-0.23809409
1	-5.76468039	-3.88680696	0.22490591
6	-6.41188002	-2.49280691	-1.24589407
6	-6.18478012	-1.25590682	-1.83799410
1	-6.87158012	-0.92580688	-2.61009407
6	-5.11298037	-0.44000688	-1.46319401
6	-3.56148005	-2.69450688	1.31720591
6	-4.94418001	0.94629312	-2.11219406
6	-2.14748001	-2.99440694	0.78290588
1	-1.66807997	-2.11750698	0.34020591
1	-1.49767995	-3.36820698	1.58350599
1	-2.18657994	-3.75860691	0.00010591
6	-3.51437998	-1.68580687	2.48320603
1	-3.17227983	-0.70210689	2.15680599
1	-4.51388025	-1.55930686	2.91320586
1	-2.85218000	-2.04940701	3.27890587
6	-4.07818031	-4.01660681	1.91370595
1	-5.08558035	-3.91320705	2.32960606
1	-4.08828020	-4.83000708	1.18100595
1	-3.41768003	-4.32670689	2.73130584
6	-6.04958010	1.25769317	-3.13659406
1	-6.04368019	0.56009310	-3.98069406
1	-7.04688025	1.24529314	-2.68549395
1	-5.88998032	2.26229310	-3.54439402
6	-5.03198004	2.03599310	-1.02489412
1	-4.31558037	1.85179317	-0.22299409
1	-4.84568024	3.02849317	-1.45599401
1	-6.03258038	2.04779315	-0.57929415
6	-3.61087990	1.04439318	-2.87879395
1	-3.56767988	0.29459313	-3.67549396
1	-3.50187993	2.03349304	-3.33989406
1	-2.74927998	0.87989312	-2.22919416
1	0.05582004	-1.37730682	2.46920586
1	1.04892004	-0.92700690	-2.81099415
1	-7.25238037	-3.10710692	-1.55909407
1	7.89511967	-2.24390697	-1.55019403
8	1.18552005	2.34799314	0.63160586
6	0.17482004	2.19039297	1.37270594
6	0.20182003	2.70359302	2.79470587
8	-1.09287989	2.30219316	0.69330591
6	0.50222003	4.20979309	2.83800602
1	-0.72767991	2.46539307	3.32150602
1	1.01662004	2.17639303	3.29620600
6	-1.96687996	3.43219304	0.95660585
1	1.37572002	4.40079308	2.20660591
1	0.79202008	4.46599293	3.86260605
1	-2.54577994	3.22499299	1.86430597
1	-2.65427995	3.41689301	0.11120591
6	-0.66477996	5.10059309	2.41670585
1	-1.46277988	5.03549290	3.16860604
1	-0.32857996	6.14339304	2.42210603
6	-1.26257992	4.77899313	1.04470599
1	-0.50597996	4.84399319	0.25480592
1	-2.02027988	5.53619289	0.81090587

DTS-12_DBP-2_Mg-2_OMe-2_eCL-2

Zero-point vibrational energy	2743388.9 (Joules/Mol)
	655.68569 (Kcal/Mol)
Zero-point correction =	1.044902 (Hartree/Particle)
Thermal correction to Energy =	1.104986
Thermal correction to Enthalpy =	1.105930
Thermal correction to Gibbs Free Energy =	0.948895
Sum of electronic and zero-point Energies =	-2641.876207
Sum of electronic and thermal Energies =	-2641.816123
Sum of electronic and thermal Enthalpies =	-2641.815178
Sum of electronic and thermal Free Energies =	-2641.972214



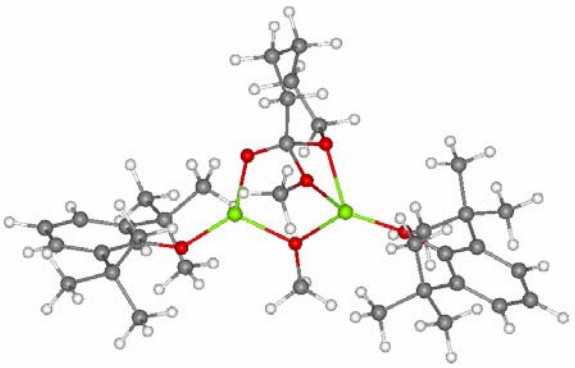
cartesian

12	-2.17877817	-0.80065995	-0.17020410
8	-0.70437819	-0.15536001	-1.27220404
8	-3.76337814	0.12093999	0.09129591
6	-0.88157821	0.64484000	-2.42550397
1	-0.63707817	0.08514000	-3.33790398
1	-0.24337818	1.53634000	-2.38990402
6	-4.93657827	0.72883999	-0.06240410
6	-5.98737860	0.10444000	-0.80610406
6	-7.19737816	0.78934002	-0.95370406
1	-8.00747776	0.33783999	-1.51640403
6	-7.40757847	2.04574013	-0.39630407
6	-6.38747835	2.63813996	0.34029591
1	-6.57287836	3.61464000	0.77579594
6	-5.15157843	2.01324010	0.53039593
6	-5.81637859	-1.29306006	-1.42960405
6	-4.06147814	2.70293999	1.37119591
6	-5.51637840	-2.33635998	-0.33360407
1	-4.63857841	-2.08125997	0.25989592
1	-5.35217857	-3.32525992	-0.77810407
1	-6.36717844	-2.41095996	0.35239592
6	-4.70847845	-1.27366006	-2.50280404
1	-3.76577806	-0.87105995	-2.12510419
1	-5.00407839	-0.63685995	-3.34350419
1	-4.51857853	-2.28185987	-2.88950419
6	-7.08917856	-1.77936006	-2.14650416
1	-7.37487841	-1.12866008	-2.97980404
1	-7.94137859	-1.86036003	-1.46370411
1	-6.90847826	-2.77765989	-2.56110406
6	-4.52357817	4.05843973	1.93389595
1	-5.39617825	3.95864010	2.58789587
1	-4.76647854	4.77683973	1.14369595
1	-3.71567822	4.49423981	2.53339601
6	-2.81317806	2.98593998	0.51159590
1	-2.39697814	2.07294011	0.08439590
1	-2.03547812	3.47034001	1.11689591
1	-3.06397820	3.65934014	-0.31570408
6	-3.69417810	1.82524002	2.58449602
1	-4.56187820	1.70143998	3.24159598
1	-2.89237809	2.29414010	3.16979599
1	-3.36767817	0.83324003	2.27059603
12	0.88692182	-0.62575996	-0.18740410
8	-0.57657820	-1.13036001	1.27919590
8	2.74482179	-1.13206005	-0.46020409
6	-0.69367820	-0.75635999	2.64909601
1	-1.67957807	-1.02326000	3.04709601
1	0.08352183	-1.23236001	3.25509596
6	3.84932184	-0.39206001	-0.41940409
6	4.57112169	-0.22556001	0.81039590
6	5.58402157	0.73824000	0.86239594
1	6.11422157	0.91554004	1.79259586
6	5.96052170	1.47433996	-0.25870410
6	5.38392162	1.16393995	-1.48880410
1	5.76242161	1.66813993	-2.37240410
6	4.36382151	0.21463999	-1.61310410
6	4.34882164	-1.17176008	2.00879598
6	3.89712191	-0.24006002	-3.01070404
6	2.91962194	-1.12406003	2.57719588
1	2.20282197	-1.54436004	1.87049592
1	2.86342192	-1.71516001	3.50009584
1	2.61272192	-0.10096000	2.81329584
6	4.65772152	-2.60965991	1.54039598
1	4.03462172	-2.88145995	0.68589592
1	5.70662165	-2.70025992	1.23939598
1	4.47582150	-3.32685995	2.35119581
6	5.29762173	-0.86096001	3.17939591
1	6.35102177	-0.92395997	2.88899589
1	5.11742163	0.13113999	3.60929585
1	5.13782167	-1.59446001	3.97729611
6	4.67942142	0.45914000	-4.13650417
1	4.50142145	1.54064000	-4.15920448

1	5.75832176	0.28983998	-4.06140423
1	4.35392141	0.05894000	-5.10280418
6	4.15952158	-1.75476003	-3.14650416
1	3.62802196	-2.31125998	-2.37170410
1	3.82262182	-2.11555982	-4.12630415
1	5.22892141	-1.97276008	-3.05470419
6	2.40612197	0.03743999	-3.26790404
1	2.14962196	1.07913995	-3.05330420
1	2.15832186	-0.15936001	-4.31810427
1	1.76952183	-0.60815996	-2.66210413
1	-0.57467818	0.32804000	2.71749592
1	-1.92137814	0.98804003	-2.51200414
1	6.74862146	2.22074008	-0.19030410
1	-8.35887814	2.55534005	-0.52900410
8	-1.94057810	-2.75515985	0.16989590
6	-0.81437820	-2.81835985	0.75549591
6	-0.68757820	-3.69355989	1.98439598
8	0.31302184	-2.77385998	-0.11130410
6	-1.02837813	-5.15795994	1.66609597
1	0.30442184	-3.60275984	2.43839598
1	-1.41957808	-3.31866002	2.70349598
6	1.21642184	-3.90046000	-0.18810409
1	-1.96637809	-5.17305994	1.10149586
1	-1.22267818	-5.67476034	2.61239600
1	1.85992193	-3.91265988	0.69869590
1	1.84602189	-3.64845991	-1.04100406
6	0.06252183	-5.91276026	0.90759593
1	0.93482178	-6.04266024	1.56269586
1	-0.30047816	-6.92206001	0.68209594
6	0.52852184	-5.24486017	-0.38850409
1	-0.30147818	-5.12215996	-1.09360409
1	1.25742185	-5.90336037	-0.87600410
8	1.82372189	2.64614010	-0.81740409
6	1.88472188	2.25134015	0.44669592
6	2.60272193	3.07974005	1.47729588
1	3.66412187	3.12163997	1.20249593
6	2.57202196	3.78824019	-1.30750406
1	2.46162176	3.70004010	-2.38870406
6	2.02922177	5.12254000	-0.82250410
1	3.62962198	3.64514017	-1.06630409
1	0.93712181	5.11123991	-0.91970408
6	2.44852185	5.50004005	0.59719592
1	2.39302182	5.88823986	-1.51790404
1	2.53872180	2.51294017	2.40639591
6	2.03172183	4.49584007	1.67039597
1	0.93872184	4.44463968	1.74029589
1	2.38192177	4.85753965	2.64279580
1	3.53992176	5.61764002	0.62599593
1	2.02782178	6.48083973	0.84509593
8	1.31322193	1.20333993	0.74879593

DI-2__DBP-2_Mg-2_OMe-2_eCL-1

Zero-point vibrational energy	2329379.0 (Joules/Mol)
	556.73493 (Kcal/Mol)
Zero-point correction =	0.887214 (Hartree/Particle)
Thermal correction to Energy =	0.938840
Thermal correction to Enthalpy =	0.939784
Thermal correction to Gibbs Free Energy =	0.800201
Sum of electronic and zero-point Energies =	-2257.002940
Sum of electronic and thermal Energies =	-2256.951314
Sum of electronic and thermal Enthalpies =	-2256.950370
Sum of electronic and thermal Free Energies =	-2257.089953



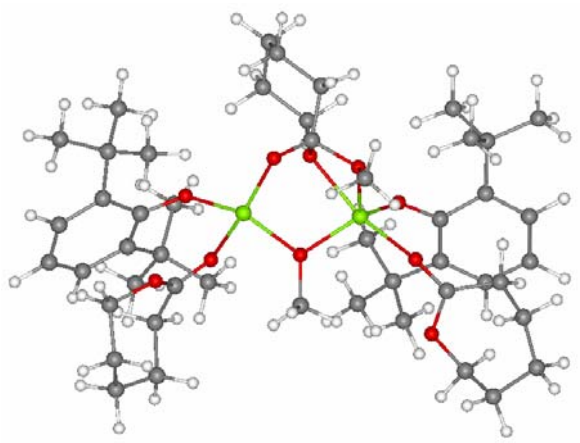
cartesian

12	1.69027424	0.10028534	0.03642142
8	-0.06322573	-0.10871466	-0.80457860
8	3.21057439	-0.59091467	-0.76437861
6	-0.18542573	-0.46501467	-2.18487859
1	0.62137425	-1.14411473	-2.48267865
1	-0.13822573	0.42648533	-2.82147861
6	4.53737450	-0.42741469	-0.78727859
6	5.08767462	0.77838534	-1.31207860
6	6.47527456	0.94838536	-1.28547859
1	6.92057419	1.86298525	-1.66277862
6	7.31947422	-0.03731467	-0.78587860
6	6.77437449	-1.23071468	-0.32167858
1	7.45267439	-1.99571466	0.04092142
6	5.39577436	-1.46331465	-0.31247857
6	4.18007421	1.83988535	-1.95947862
6	4.83517456	-2.80781460	0.18622142
6	3.03997445	2.30168533	-1.00587869
1	2.07377434	1.86558533	-1.30327868
1	2.87887430	3.38318539	-1.07047868
1	3.26647449	2.08888531	0.04592142
6	3.56827450	1.25818527	-3.25167871
1	3.01327443	0.33988532	-3.04477859
1	4.35797453	1.01948535	-3.97097850
1	2.89017439	1.98148525	-3.72267866
6	4.96317434	3.10508537	-2.35377860

1	5.74877453	2.88918543	-3.08347869
1	5.42317438	3.59308553	-1.48737860
1	4.28257418	3.82578540	-2.82037854
6	5.94887447	-3.79881454	0.56592143
1	6.56487417	-3.43871450	1.39692140
1	6.60727453	-4.02141476	-0.28017858
1	5.49657440	-4.74481440	0.88362139
6	3.99597430	-3.48131466	-0.91937858
1	3.17017436	-2.84481454	-1.23987865
1	3.58707428	-4.43361473	-0.55897856
1	4.61877441	-3.69491458	-1.79477859
6	3.97967434	-2.60041451	1.45162141
1	4.57077456	-2.14261460	2.25192142
1	3.59677434	-3.56101465	1.81822133
1	3.12517428	-1.94971466	1.25302136
12	-1.60602570	0.04908533	0.39602143
8	-0.68562573	-0.55791461	2.13102126
8	-3.36772561	-0.21421467	-0.02467858
6	-0.13452573	-1.75861466	2.67802143
1	0.95697427	-1.74311471	2.61262131
1	-0.44682574	-1.87751472	3.71902132
6	-4.55902576	-0.46431467	-0.56517857
6	-5.11632538	-1.77721465	-0.48437858
6	-6.36242580	-2.00541449	-1.07617867
1	-6.80822563	-2.99351454	-1.03477859
6	-7.06582546	-0.99651462	-1.72497869
6	-6.52292538	0.28248534	-1.77997863
1	-7.09172583	1.05838525	-2.28137875
6	-5.28232574	0.58488536	-1.21057868
6	-4.38612556	-2.92331457	0.24162142
6	-4.73322582	2.02278543	-1.27727866
6	-3.04402566	-3.23941469	-0.44917858
1	-2.38262558	-2.37041450	-0.48247856
1	-2.52062559	-4.04971457	0.07362141
1	-3.20872569	-3.55971456	-1.48337865
6	-4.16322565	-2.56301451	1.72502136
1	-3.59492564	-1.63861465	1.84052134
1	-5.12462568	-2.42361450	2.23062134
1	-3.62892556	-3.37171459	2.24012136
6	-5.19412565	-4.23331451	0.22732142
1	-6.16252565	-4.12581444	0.72672141
1	-5.36912584	-4.60311460	-0.78817856
1	-4.63562584	-5.00851440	0.76382142
6	-5.69972563	2.98698545	-1.98827863
1	-5.88142538	2.70008540	-3.02927876
1	-6.66482544	3.05668545	-1.47607863
1	-5.26382542	3.99248552	-1.99997854
6	-4.52622557	2.58238530	0.14512143
1	-3.85642552	1.95718527	0.73802143
1	-4.11552572	3.59948540	0.10012142
1	-5.48272562	2.63238549	0.67622143
6	-3.41642570	2.06648540	-2.07887864
1	-3.58602571	1.74788535	-3.11287856
1	-3.01182556	3.08608532	-2.10307860
1	-2.65562558	1.40468526	-1.65947866
1	-0.52252573	-2.59081459	2.08982134
1	-1.14102578	-0.96641463	-2.37497854
1	-8.03222561	-1.20371473	-2.17777872
1	8.39547443	0.11708534	-0.77157855
8	1.27357423	0.67558533	1.84162140
6	0.08487427	0.70878536	2.38072133
6	-0.00022573	1.02678525	3.86862135
8	-0.88192570	1.56028533	1.64152133
6	0.63587427	2.35298538	4.27832174
1	-1.05702567	1.00288534	4.15202141
1	0.50657427	0.21758533	4.40462160
6	-0.44712573	2.85378551	1.15762138
1	1.71597421	2.30338550	4.09962177
1	0.50497425	2.45928550	5.36132145
1	-1.39002573	3.37698531	0.97942144
1	0.05237427	2.72608542	0.18992142
6	0.07047427	3.59328532	3.58172131
1	-1.01842570	3.64278531	3.71102142
1	0.47977427	4.47948551	4.07952166
6	0.43807426	3.66388535	2.09652138
1	1.48287427	3.36358547	1.97502136
1	0.36897427	4.69988537	1.74262142

DI-2__DBP-2_Mg-2_OMe-2_eCL-3

Zero-point vibrational energy	3162763.5 (Joules/Mol)
	755.91862 (Kcal/Mol)
Zero-point correction =	1.204633 (Hartree/Particle)
Thermal correction to Energy =	1.273903
Thermal correction to Enthalpy =	1.274847
Thermal correction to Gibbs Free Energy =	1.096406
Sum of electronic and zero-point Energies =	-3026.763182
Sum of electronic and thermal Energies =	-3026.693912
Sum of electronic and thermal Enthalpies =	-3026.692968
Sum of electronic and thermal Free Energies =	-3026.871409



cartesian

12	-1.71478331	-0.29982904	0.72950435
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6	-0.08328332	2.17087102	0.35070437
1	-0.55648333	2.57347107	1.25790441
1	-0.64198333	2.54767108	-0.51829565
6	-4.18598366	-0.58272898	-0.98469561
6	-4.25558329	0.08447098	-2.25549579
6	-5.44928360	0.71997100	-2.61039567
1	-5.51118326	1.26867092	-3.54479575
6	-6.58388329	0.66637099	-1.80319560
6	-6.56158352	-0.14762902	-0.67179567
1	-7.48588324	-0.27572903	-0.11729562
6	-5.40708351	-0.82562900	-0.26239562
6	-3.07438326	0.06007098	-3.24559569
6	-5.50448322	-1.90992904	0.83440435
6	-2.60888338	-1.39492905	-3.45999575
1	-2.29398346	-1.85112906	-2.52079582
1	-1.76798332	-1.42292905	-4.16399574
1	-3.42048311	-1.99902904	-3.88049579
6	-1.89128327	0.91387099	-2.75669575
1	-1.47818327	0.55067098	-1.81469560
1	-2.19298315	1.96047091	-2.62959576
1	-1.07928336	0.89637101	-3.49379563
6	-3.47168350	0.60657102	-4.62889576
1	-3.71928310	1.67377090	-4.60549593
1	-4.32228327	0.06537098	-5.05659580
1	-2.62728310	0.48927099	-5.31719589
6	-6.95708323	-2.12262893	1.29920447
1	-7.62748337	-2.37782884	0.47190440
1	-7.36318350	-1.24492908	1.81560445
1	-6.98548365	-2.95422888	2.01200438
6	-4.68008327	-1.60502911	2.09750438
1	-3.60748339	-1.64562905	1.91490436
1	-4.89588356	-2.35622883	2.86790419
1	-4.92808342	-0.62552899	2.51680422
6	-5.02768326	-3.24702883	0.22930437
1	-5.66448355	-3.54242897	-0.61199564
1	-5.07058334	-4.04272890	0.98350435
1	-4.00038338	-3.16652894	-0.12969562
12	1.60001671	-0.31282902	0.58680439
8	1.14051664	-1.30452907	2.38260436
8	2.98961687	-0.97332901	-0.59359562
6	0.99481666	-0.72512901	3.67800426
1	0.01541668	-0.25072902	3.77530432
1	1.11751664	-1.48792911	4.45470428
6	4.22521639	-0.61272901	-0.91129559
6	5.35921669	-1.21282899	-0.26069564
6	6.62121677	-0.64532900	-0.46319562
1	7.48461676	-1.05632901	0.05030437
6	6.82111645	0.43027097	-1.32559562
6	5.74911642	0.87447101	-2.09719563
1	5.94101667	1.63317096	-2.84949565
6	4.46051645	0.34767097	-1.95459569
6	5.22991657	-2.50912905	0.56480438
6	3.36481667	0.71487099	-2.97769570
6	4.45601654	-2.29622889	1.87600446
1	3.44431686	-1.93522906	1.70220447
1	4.38231659	-3.23962903	2.43180418
1	4.97191668	-1.57662904	2.52200437
6	4.52041674	-3.57602882	-0.29459566
1	3.54341650	-3.22412896	-0.62769562
1	5.11801672	-3.81312895	-1.18179560
1	4.38731670	-4.50212908	0.27890438
6	6.60181665	-3.09142900	0.95050436
1	7.23091650	-3.28332901	0.07510437
1	7.15551662	-2.44102883	1.63710439
1	6.45301676	-4.04732895	1.46510446
6	3.91991663	1.58147097	-4.12299585
1	4.24931669	2.56907105	-3.77929568
1	4.75691652	1.10047090	-4.63969564
1	3.12951660	1.74687099	-4.86329556
6	2.82541656	-0.58162898	-3.61769581
1	2.41211653	-1.24922907	-2.85979581
1	2.03721666	-0.34722903	-4.34369564
1	3.62471676	-1.11312902	-4.14529562
6	2.19761658	1.50157094	-2.35809565
1	2.55411673	2.37517118	-1.80469561
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1	1.78591669	0.01917098	3.77980423
1	0.92881668	2.58727098	0.29360437
1	7.81311655	0.85597098	-1.45919561
1	-7.49668360	1.17977095	-2.09699559
8	-1.17298329	-1.54732907	2.16440439
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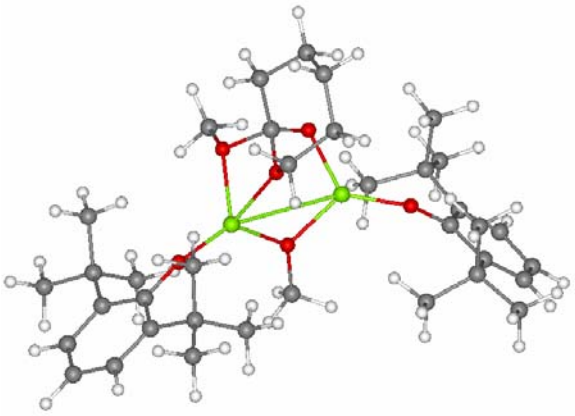
6	0.13291667	-3.53622890	2.47900438
8	0.26881668	-2.00842905	0.46140438
6	-0.98978335	-4.50322914	2.09630442
1	1.12011671	-3.93242884	2.21820426
1	0.12611668	-3.40262890	3.56540418
6	0.43301669	-3.16452885	-0.38769561
1	-1.94498336	-3.97812891	2.19810438
1	-1.00478339	-5.32352877	2.82390428
1	1.33661664	-3.70792890	-0.09069563
1	0.62371665	-2.72862887	-1.36999559
6	-0.85878330	-5.10322905	0.69660437
1	0.03761668	-5.73862886	0.66040438
1	-1.71078336	-5.76922894	0.51520437
6	-0.77958333	-4.08272886	-0.43949562
1	-1.68488336	-3.46792889	-0.48439562
1	-0.72588331	-4.62472916	-1.39209557
8	-4.68058348	2.02687097	2.47830439
6	-3.86798334	1.92207098	1.42910445

6	-4.14298344	2.69967103	0.17270437
1	-5.07978344	2.34097099	-0.27429563
6	-5.95878363	2.70017099	2.38740420
1	-6.45908356	2.39267111	3.30670428
6	-5.84858322	4.21527100	2.32100439
1	-6.51908350	2.28737116	1.54230440
1	-5.12048340	4.54347086	3.07280421
6	-5.49178362	4.76167107	0.93940437
1	-6.81808329	4.62377119	2.63030434
1	-3.35198355	2.42887115	-0.52519566
6	-4.18048334	4.22597122	0.36890435
1	-3.33628321	4.54027128	0.99490434
1	-4.01608324	4.68037128	-0.61369562
1	-6.30438328	4.52117109	0.24160437
1	-5.44218349	5.85547113	0.98860437
8	-2.87758350	1.20737100	1.56970441
8	3.51871681	2.92347097	0.58280438
6	3.78911686	1.87397099	1.35320437
6	5.13851643	1.73287094	2.00140429
1	5.88801670	1.59087098	1.21140444
6	4.55101633	3.84307098	0.14690438
1	4.05111647	4.40967083	-0.63989562
6	5.04021645	4.77337122	1.24500442
1	5.36101675	3.26967096	-0.31409562
1	4.16931677	5.16297102	1.78610444
6	6.04391670	4.14207125	2.20790434
1	5.50821638	5.63427114	0.75270438
1	5.09671640	0.79787099	2.55940437
6	5.53041649	2.89667106	2.92890429
1	4.68261671	3.15447116	3.57580423
1	6.31841660	2.52917099	3.59450436
1	6.95291662	3.87917113	1.65150440
1	6.34421635	4.88807106	2.95240426
8	2.88631678	1.06037092	1.54480445

DI-3__DBP-2_Mg-2_OMe-2_eCL-1

Zero-point vibrational energy	2328198.2 (Joules/Mol)
	556.45273 (Kcal/Mol)
Zero-point correction =	0.886764 (Hartree/Particle)
Thermal correction to Energy =	0.938528
Thermal correction to Enthalpy =	0.939472
Thermal correction to Gibbs Free Energy =	0.798094
Sum of electronic and zero-point Energies =	-2257.003950
Sum of electronic and thermal Energies =	-2256.952186
Sum of electronic and thermal Enthalpies =	-2256.951242
Sum of electronic and thermal Free Energies =	-2257.092620



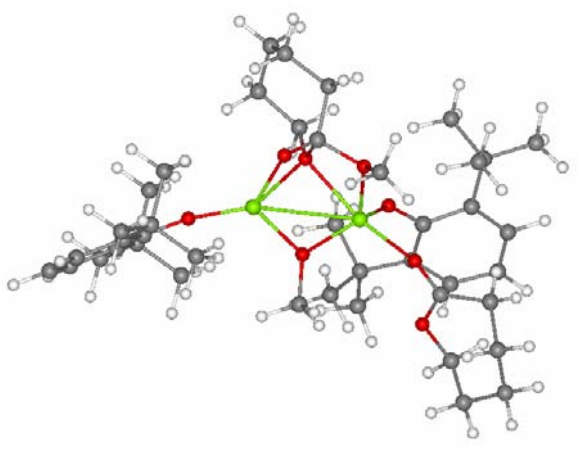
cartesian

12	-1.70097935	-0.78970581	0.00465687
8	-0.06237935	-0.35970584	0.98875690
8	-3.30567932	0.12999418	0.05375687
6	-0.06037936	0.20589417	2.29955673
1	-0.94157940	0.83969420	2.45315695
1	0.82902062	0.82689422	2.45705676
6	-4.35607958	0.47409418	0.80125690
6	-4.76427937	1.83959413	0.87345690
6	-5.84947968	2.15889406	1.69505680
1	-6.17797947	3.18949413	1.77755690
6	-6.53697968	1.19169414	2.42285681
6	-6.15317965	-0.14080583	2.31715679
1	-6.71207952	-0.88430578	2.87615681
6	-5.07897949	-0.52960581	1.51185679
6	-4.04947948	2.93489408	0.06115688
6	-4.71647930	-2.01540589	1.34605682
6	-4.11947966	2.60749412	-1.44474316
1	-3.66677928	1.63869417	-1.66184318
1	-3.59937930	3.37889409	-2.02674317
1	-5.16127968	2.57799411	-1.78234315
6	-2.57947922	3.06969404	0.50615686
1	-2.02897930	2.13929415	0.35635686
1	-2.51847935	3.33509421	1.56735682
1	-2.07707930	3.85939407	-0.06614313
6	-4.69827938	4.31689453	0.24995688
1	-4.64907932	4.66149426	1.28845680
1	-5.74607944	4.32789421	-0.06784313
1	-4.16427946	5.05289459	-0.36134312
6	-5.56877947	-2.92580581	2.24805689
1	-6.63457966	-2.85410595	2.01135683
1	-5.43567944	-2.69630575	3.31085682
1	-5.27357960	-3.96990585	2.09375691
6	-3.22527933	-2.28540587	1.71675682
1	-2.73427916	-1.39710581	2.13115692
1	-2.66187930	-2.69250584	0.86195689
1	-3.13447928	-3.05460596	2.49075675
6	-4.99167967	-2.44560575	-0.11164314
1	-6.05607939	-2.33330584	-0.34084314
1	-4.72207928	-3.49830580	-0.26374313
1	-4.43137932	-1.83660591	-0.82474309

12	1.53542066	-0.60690582	-0.10944313
8	1.12402058	-2.41080594	-1.03444314
8	3.25242066	-0.03290582	0.18385687
6	0.93262064	-3.71450591	-0.47614315
1	-0.09127936	-3.82710576	-0.11194313
1	1.15312064	-4.48230553	-1.22334313
6	4.38572073	0.46079418	0.68355691
6	5.20062065	-0.34430584	1.53715682
6	6.37552071	0.21309417	2.05145693
1	7.01192045	-0.37380582	2.70505691
6	6.76852036	1.51189411	1.74935687
6	5.97882032	2.27969408	0.90075690
1	6.30782032	3.28689408	0.66795689
6	4.79162073	1.78909409	0.34885687
6	4.82282066	-1.79680586	1.88435686
6	3.96682072	2.66799402	-0.60954309
6	3.49612069	-1.84150589	2.66895676
1	2.67352080	-1.37890589	2.11865687
1	3.21612072	-2.87680578	2.90005684
1	3.59062076	-1.30010581	3.61615682
6	4.72942066	-2.64740586	0.60095692
1	4.00882053	-2.24020576	-0.11034313
1	5.70182037	-2.68220592	0.09825687
1	4.44382048	-3.67880583	0.84435689
6	5.87212038	-2.47760582	2.78185678
1	6.85522032	-2.52740598	2.30275679
1	5.98352051	-1.97330582	3.74725676
1	5.55792046	-3.50710583	2.98785686
6	4.61352062	4.04379416	-0.84914309
1	4.69762039	4.62979460	0.07195687
1	5.60912037	3.96029401	-1.29684317
1	3.99132085	4.61899424	-1.54414320
6	3.86202073	1.98789406	-1.98984313
1	3.42662072	0.98969418	-1.91624320
1	3.25142074	2.59399414	-2.67164326
1	4.85602045	1.88139415	-2.43724322
6	2.56582069	2.94719410	-0.02934313
1	2.64232063	3.49309421	0.91675693
1	1.97442067	3.55849409	-0.72214311
1	2.01182079	2.02789402	0.17285687
1	1.63652062	-3.81430578	0.35065687
1	-0.06307936	-0.58230579	3.06265688
1	7.68642044	1.91959417	2.16545677
1	-7.37297964	1.47389412	3.05795693
8	-1.15417933	-2.04520583	-1.37964320
6	0.01642065	-1.91730583	-1.93544316
6	0.18232064	-2.57220578	-3.30134320
8	0.44992065	-0.48950583	-1.89094317
6	-0.92577940	-2.22330594	-4.29734325
1	1.17922068	-2.35850596	-3.70144320
1	0.14712064	-3.64870596	-3.10804319
6	0.54392064	0.32549417	-3.08344316
1	-1.88837934	-2.30930591	-3.78294325
1	-0.92597938	-2.97920585	-5.09054327
1	1.43082058	0.02529418	-3.65314317
1	0.72852063	1.32649410	-2.68914318
6	-0.78997940	-0.84520578	-4.94224310
1	0.10252064	-0.83060580	-5.58284330
1	-1.64387941	-0.68120581	-5.60934305
6	-0.70077938	0.32329416	-3.95984316
1	-1.59327936	0.37549418	-3.32624316
1	-0.67767936	1.25839412	-4.53254318

DI-3__DBP-2_Mg-2_OMe-2_eCL-2

Zero-point vibrational energy	2744777.8 (Joules/Mol)
	656.01764 (Kcal/Mol)
Zero-point correction =	1.045431 (Hartree/Particle)
Thermal correction to Energy =	1.106132
Thermal correction to Enthalpy =	1.107076
Thermal correction to Gibbs Free Energy =	0.947427
Sum of electronic and zero-point Energies =	-2641.887355
Sum of electronic and thermal Energies =	-2641.826654
Sum of electronic and thermal Enthalpies =	-2641.825710
Sum of electronic and thermal Free Energies =	-2641.985358



cartesian

12	-2.18133903	0.51806909	-0.65682006
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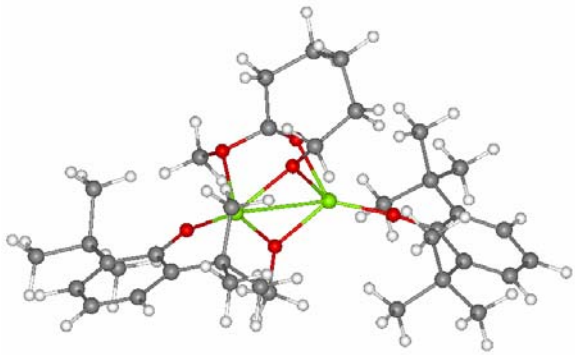
6	-0.60783887	-1.84073091	-1.62812006
1	-1.55073893	-2.37023091	-1.44082010
1	0.20766111	-2.47843075	-1.26622009
6	-4.95783901	-0.83563089	-0.05002006
6	-5.28573895	-1.62383091	1.09767997
6	-6.51003885	-2.29813075	1.11567998
1	-6.77913904	-2.90533090	1.97347987
6	-7.41203880	-2.21863079	0.06007994
6	-7.09163904	-1.43953097	-1.04592001
1	-7.81123877	-1.38263094	-1.85592008
6	-5.88523912	-0.73783094	-1.13522005
6	-4.32893896	-1.73673093	2.29898000
6	-5.58833885	0.12246910	-2.37732005
6	-4.07453871	-0.34413087	2.90968013
1	-3.66963887	0.34376907	2.16668010
1	-3.36863899	-0.41473091	3.74708009
1	-5.00843906	0.08386910	3.29048014
6	-2.99833894	-2.38723087	1.87227988
1	-2.49663901	-1.81423092	1.09147990
1	-3.17303896	-3.39843082	1.48827994
1	-2.31933904	-2.46563077	2.73047996
6	-4.90273905	-2.61233091	3.42718005
1	-5.07333899	-3.64553070	3.10637999
1	-5.84283876	-2.21483088	3.82448006
1	-4.18663883	-2.64413071	4.25617981
6	-6.74283886	0.10596910	-3.39581990
1	-7.66913891	0.50946909	-2.97381997
1	-6.94783878	-0.89923090	-3.77911997
1	-6.47563887	0.73336911	-4.25402021
6	-4.35563898	-0.42273092	-3.12831998
1	-3.49283886	-0.56323093	-2.47221994
1	-4.06293869	0.24856910	-3.94452000
1	-4.57663870	-1.40573096	-3.55841994
6	-5.39333916	1.59876907	-1.97512007
1	-6.31513882	1.98756909	-1.52892005
1	-5.15803909	2.21096921	-2.85391998
1	-4.59463882	1.73356903	-1.24582005
12	1.00016105	0.49066907	-0.51322007
8	0.48796108	2.28636909	-1.47062004
8	2.23476100	0.58426911	0.95227993
6	0.52206111	2.56316924	-2.87432003
1	-0.41793889	2.25906920	-3.34042001
1	0.70016110	3.62956929	-3.04641986
6	3.43486118	0.09536910	1.25297987
6	4.62406111	0.84266907	0.95427990
6	5.86156130	0.19926910	1.07977998
1	6.77206087	0.72856909	0.81807995
6	5.97566128	-1.09893095	1.56827998
6	4.83096123	-1.73983097	2.03597999
1	4.94616127	-2.70863080	2.51118016
6	3.56036115	-1.16603088	1.92837989
6	4.58296108	2.34756923	0.61077994
6	2.35466099	-1.84893095	2.60598016
6	3.98796129	2.62706923	-0.77982008
1	2.94636106	2.31686926	-0.84922010
1	4.02596092	3.70166922	-0.99912006
1	4.55846119	2.11106920	-1.56012011
6	3.75806117	3.08736920	1.68407989
1	2.74176097	2.69446921	1.73427999
1	4.21866131	2.96916914	2.67077994
1	3.71356106	4.16006899	1.45787990
6	5.98736095	2.97986913	0.62107992
1	6.50076103	2.83316922	1.57687998
1	6.62966108	2.59226918	-0.17762005
1	5.89416122	4.05966902	0.46037996
6	2.77446103	-3.07753086	3.43368006
1	3.17546105	-3.88653088	2.81227994
1	3.51956105	-2.82753086	4.19587994
1	1.89636111	-3.47743082	3.95228028
6	1.70136106	-0.85453093	3.58768010
1	1.39996111	0.05946910	3.07368016
1	0.81716108	-1.30343091	4.05697966
1	2.40426111	-0.58253092	4.38247967
6	1.30746102	-2.34233069	1.59257996
1	1.75866103	-3.00853086	0.85017991
1	0.51406109	-2.90013075	2.10328007
1	0.82636106	-1.51943088	1.06367993
1	1.35126102	1.98856914	-3.28681993
1	-0.49243888	-1.72673094	-2.71551991
1	6.95076084	-1.57263088	1.65697992
1	-8.35723877	-2.75463080	0.10137994
8	-1.84593892	2.31376910	-1.41482008
6	-0.77873886	2.69966912	-0.78052008
6	-0.66843891	4.18396902	-0.45432007
8	-0.61483884	1.78286910	0.41467994
6	-1.86463892	4.75986910	0.30587992
1	0.27766111	4.38876915	0.05747994
1	-0.60593891	4.67166901	-1.43232012
6	-0.52963889	2.29116917	1.77107990
1	-2.78313899	4.34516907	-0.12332006
1	-1.89933896	5.84056902	0.12777993
1	0.38206109	2.88826919	1.86727989
1	-0.39263889	1.38926911	2.36948013
6	-1.82023895	4.52186918	1.81467998
1	-0.94943893	5.04326916	2.23578000
1	-2.70183897	4.98386908	2.27408004
6	-1.76253891	3.05436921	2.23487997
1	-2.66243887	2.52166915	1.90567994
1	-1.76723897	3.00226927	3.33068013
8	3.11666107	-2.03873086	-1.43102002

6	3.22066116	-0.92853093	-2.13922000
6	4.38406086	-0.71313089	-3.07062006
1	5.30346107	-0.67773092	-2.47341990
6	4.18876123	-3.01563072	-1.35422003
1	3.86716104	-3.65723085	-0.53462005
6	4.36446095	-3.81483078	-2.63452005
1	5.10336113	-2.50913072	-1.03322005
1	3.37576103	-4.13073111	-2.98842001
6	5.13356113	-3.08973074	-3.73751998
1	4.90336084	-4.73163080	-2.36791992
1	4.24056101	0.27946907	-3.49871993
6	4.51086092	-1.76763093	-4.18472004
1	3.52786112	-1.94203091	-4.63842010
1	5.13626099	-1.33453095	-4.97222042
1	6.15756130	-2.89913082	-3.39041996
1	5.22306108	-3.75123072	-4.60612011
8	2.31846118	-0.09373090	-2.03801990

DTS-34__DBP-2_Mg-2_OMe-2_eCL-1

Zero-point vibrational energy	2323877.1 (Joules/Mol)
	555.41996 (Kcal/Mol)
Zero-point correction =	0.885118 (Hartree/Particle)
Thermal correction to Energy =	0.936717
Thermal correction to Enthalpy =	0.937661
Thermal correction to Gibbs Free Energy =	0.798530
Sum of electronic and zero-point Energies =	-2257.001126
Sum of electronic and thermal Energies =	-2256.949528
Sum of electronic and thermal Enthalpies =	-2256.948584
Sum of electronic and thermal Free Energies =	-2257.087714



cartesian

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8	-3.08695459	0.16062261	0.31355390
6	0.12094536	-0.07807740	2.82345390
1	0.42334536	-0.93887740	3.43395376
1	-0.86365467	0.25552261	3.17125392
6	-4.27925491	0.68242264	0.60735393
6	-4.45425463	2.10102272	0.60095394
6	-5.71975470	2.61492252	0.89995396
1	-5.88005447	3.68762255	0.90085393
6	-6.79835463	1.79152262	1.20295393
6	-6.61675453	0.41352260	1.21135390
1	-7.46855450	-0.21337740	1.45185399
6	-5.38075447	-0.17277738	0.92115396
6	-3.29345465	3.06302261	0.28335389
6	-5.23645449	-1.70607734	0.94225395
6	-2.75135469	2.80432272	-1.13644612
1	-2.41235471	1.77372265	-1.24984610
1	-1.91305459	3.47792268	-1.35504603
1	-3.53185463	2.98402262	-1.88374603
6	-2.16815472	2.90862250	1.32565391
1	-1.77445459	1.89152265	1.34975398
1	-2.54005480	3.14792252	2.32775378
1	-1.33895457	3.59112263	1.10225391
6	-3.72655463	4.53932238	0.32445389
1	-4.08695459	4.83852243	1.31425393
1	-4.50765467	4.76382256	-0.40954611
1	-2.86505461	5.17372227	0.08765391
6	-6.55545473	-2.41717744	1.29765391
1	-7.34525490	-2.20967746	0.56835395
1	-6.92285490	-2.14157748	2.29165387
1	-6.39115477	-3.50067735	1.29975390
6	-4.21995449	-2.13837743	2.01935387
1	-3.25485468	-1.63877738	1.90555394
1	-4.05085468	-3.22107744	1.98465395
1	-4.59125471	-1.88317740	3.01745391
6	-4.82885456	-2.22647738	-0.45094609
1	-5.61415482	-2.00077748	-1.18044603
1	-4.68645477	-3.31367731	-0.43044609
1	-3.90585470	-1.76757741	-0.80644608
12	1.51654541	-0.58257741	0.13165390
8	1.10514545	-2.63137746	-0.34134609
6	1.10754538	-3.62837744	0.70885396
1	0.37394536	-3.38187742	1.47695398
1	0.89384538	-4.61157751	0.28235391
1	2.11574531	-3.61837745	1.11985397
1	0.83234537	0.73592263	3.00585389
1	-7.77095461	2.22032261	1.43145394
8	-1.19285464	-2.64607739	-0.39054608
6	-0.13945463	-2.55177736	-1.05974603
6	0.00744536	-3.11507750	-2.44784617
8	0.00664536	-0.67807740	-1.24794602
6	-1.22085464	-2.95907736	-3.34454608
1	0.91964537	-2.72417736	-2.90744615
1	0.19944537	-4.18217754	-2.26774621
6	-0.09615464	-0.00857740	-2.51684618
1	-2.12245464	-3.08487749	-2.73594618

1	-1.21955454	-3.78417730	-4.06504631
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1	-0.09135464	1.06422257	-2.29624629
6	-1.28525460	-1.64857733	-4.13064623
1	-0.42095464	-1.59257734	-4.80664635
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6	-1.34995461	-0.35807741	-3.31024623
1	-2.21765471	-0.36517739	-2.63834620
1	-1.52195454	0.47372264	-4.00414610
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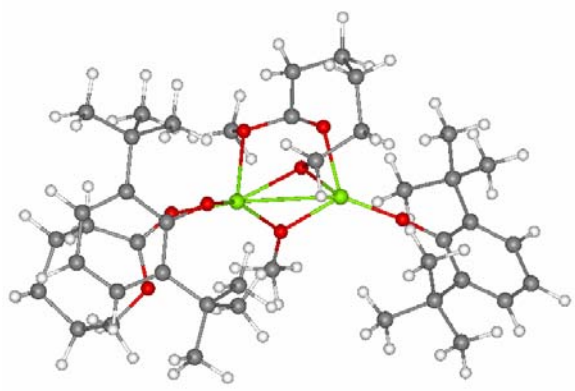
6	4.46154547	0.50472260	0.28025392
6	5.48894548	-0.18477739	0.99385393
6	6.71004534	0.46622264	1.19485390
1	7.50664520	-0.03327740	1.73565388
6	6.94714546	1.75072265	0.71915394
6	5.94614506	2.40742254	0.01285391
1	6.15264511	3.40582252	-0.35734609
6	4.70134544	1.81802261	-0.22884610
6	5.28104544	-1.61147738	1.53515399
6	3.63634539	2.57922268	-1.03934610
6	4.15694523	-1.62687743	2.59065390
1	3.21184540	-1.25487733	2.18865371
1	3.99674535	-2.64337730	2.97235370
1	4.41994524	-0.98897737	3.44105387
6	4.96494532	-2.58367729	0.38055390
1	4.08584547	-2.27307749	-0.18644610
1	5.80804539	-2.62997746	-0.31694609
1	4.79964542	-3.59757733	0.76775396
6	6.53644514	-2.16147733	2.23615384
1	7.39624548	-2.21527743	1.56055391
1	6.82064533	-1.56587744	3.10985374
1	6.33584547	-3.17947745	2.58895373
6	4.13154507	3.95542264	-1.51934612
1	4.38454533	4.62062216	-0.68744606
1	5.00524521	3.87322259	-2.17384624
1	3.33754539	4.44342232	-2.09574628
6	3.27154541	1.78382266	-2.30894613
1	2.93684530	0.77282262	-2.07064629
1	2.48274541	2.29662251	-2.87344623
1	4.14644527	1.69222260	-2.96144629
6	2.38764524	2.85282254	-0.17734610
1	2.63924527	3.50372267	0.66635394
1	1.60844541	3.35142255	-0.76624608
1	1.96254539	1.94002259	0.24705391
1	7.90554523	2.23362255	0.89285392

DTS-34__DBP-2_Mg-2_OMe-2_eCL-2

Zero-point vibrational energy	2742504.4 (Joules/Mol)
	655.47428 (Kcal/Mol)
Zero-point correction =	1.044565 (Hartree/Particle)
Thermal correction to Energy =	1.104741
Thermal correction to Enthalpy =	1.105685
Thermal correction to Gibbs Free Energy =	0.948093
Sum of electronic and zero-point Energies =	-2641.882004
Sum of electronic and thermal Energies =	-2641.821828
Sum of electronic and thermal Enthalpies =	-2641.820884
Sum of electronic and thermal Free Energies =	-2641.978475



cartesian

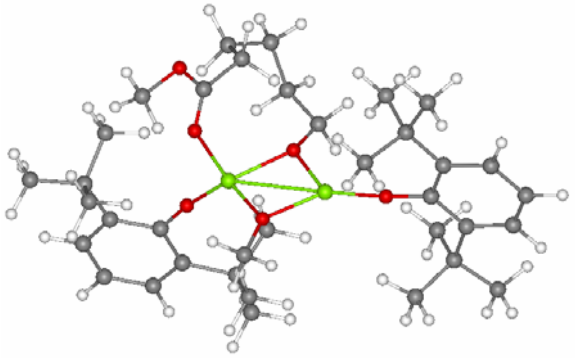
12	-2.15351391	0.45258072	-0.55202490
8	-0.61011386	-0.53921926	-1.23182487
8	-3.82531381	-0.20401928	-0.11902489
6	-0.59281385	-1.67661929	-2.07032490
1	0.29238617	-1.67381930	-2.71942472
1	-1.48201382	-1.70961928	-2.71482491
6	-5.00581408	-0.81911927	-0.08842488
6	-5.24451399	-1.85681927	0.86687511
6	-6.49501371	-2.48211908	0.87337512
1	-6.69921398	-3.27281904	1.58747518
6	-7.50401402	-2.12441921	-0.01402488
6	-7.26641369	-1.11001933	-0.93482488
1	-8.06601334	-0.83981925	-1.61642480
6	-6.04121399	-0.43931928	-0.99992490
6	-4.16481400	-2.29281926	1.87517512
6	-5.83681393	0.68598074	-2.03062487
6	-3.75281382	-1.10661924	2.76897526
1	-3.38701391	-0.26851928	2.17497516
1	-2.96631384	-1.40951931	3.47167516
1	-4.60921383	-0.75311929	3.35367513
6	-2.93851399	-2.86361909	1.13557518
1	-2.49941397	-2.13701916	0.45027512
1	-3.22181392	-3.74481916	0.54957509
1	-2.16601396	-3.16811919	1.85257518
6	-4.65711403	-3.40251923	2.82117510
1	-4.93041372	-4.31681919	2.28387523
1	-5.51671410	-3.08511925	3.42097521
1	-3.85241389	-3.66331911	3.51787519

6	-7.09211397	0.94038069	-2.88542485
1	-7.94951391	1.25028074	-2.27872491
1	-7.38351393	0.06238072	-3.47162485
1	-6.88521385	1.75058067	-3.59412479
6	-4.71691370	0.31068072	-3.02242494
1	-3.78571391	0.05208072	-2.51442480
1	-4.51061392	1.13898075	-3.71072483
1	-5.01101398	-0.56171930	-3.61602473
6	-5.52521372	2.01558089	-1.31402481
1	-6.37671375	2.31368089	-0.69252491
1	-5.34061384	2.81348085	-2.04342484
1	-4.65211391	1.93658078	-0.66642487
12	0.89908618	0.43758073	-0.36272490
8	0.37358615	2.29628086	-1.47012484
8	2.17298603	0.55588073	1.08657515
6	0.30988616	2.15898085	-2.90902495
1	-0.32681385	1.31988072	-3.18972492
1	-0.06501383	3.08498073	-3.35142493
6	3.40958619	0.10708072	1.25297511
6	4.53428602	0.99198073	1.13207519
6	5.81828594	0.43728071	1.12477517
1	6.68278599	1.08188069	1.00227511
6	6.03668594	-0.92901927	1.28707516
6	4.94928598	-1.75351930	1.57027519
1	5.14488602	-2.79711914	1.79567516
6	3.63818622	-1.26591933	1.60477519
6	4.35828590	2.52368093	1.09867513
6	2.49638605	-2.15321922	2.14447522
6	3.68598604	3.00268078	-0.19992489
1	2.70018601	2.56008077	-0.33612490
1	3.56748605	4.09368038	-0.18652488
1	4.29908609	2.75078082	-1.07252491
6	3.51468611	2.96308088	2.31317520
1	2.53668618	2.47998095	2.30547523
1	4.01948595	2.69728088	3.24837518
1	3.37308621	4.05108070	2.30467510
6	5.70368624	3.26408076	1.19987512
1	6.25718594	2.99438095	2.10537505
1	6.34978628	3.08078074	0.33397514
1	5.51818609	4.34328079	1.23807514
6	2.98718619	-3.56761909	2.50087523
1	3.34618616	-4.11801958	1.62317514
1	3.78558612	-3.55471921	3.24937510
1	2.15628600	-4.14061928	2.92597508
6	1.96378624	-1.51171923	3.44347525
1	1.60598624	-0.49691927	3.25487518
1	1.13378620	-2.10331917	3.84947515
1	2.75028610	-1.46401930	4.20407486
6	1.32328618	-2.32501912	1.15817511
1	1.66698623	-2.50031924	0.13467512
1	0.70258617	-3.18071914	1.44807518
1	0.66018617	-1.45761931	1.17027521
1	1.33628619	1.97988069	-3.22432494
1	-0.57581383	-2.60411906	-1.48292482
1	7.04648590	-1.33271933	1.27077520
1	-8.46681309	-2.62891912	0.01377512
8	-1.91561377	2.33288074	-1.40682483
6	-0.84941381	2.71168089	-0.87562490
6	-0.69061387	4.04088068	-0.18932489
8	-0.70911384	1.41798067	0.56477511
6	-1.89261377	4.49738073	0.63807511
1	0.24128616	4.04558039	0.38217509
1	-0.53091383	4.73558044	-1.02652490
6	-0.72501385	1.75038075	1.95657516
1	-2.81171393	4.14868069	0.15487511
1	-1.92771375	5.59208059	0.60587507
1	0.20698616	2.26768088	2.21377516
1	-0.71671385	0.80118072	2.50527525
6	-1.86771381	4.07428074	2.10767508
1	-0.96631384	4.48468065	2.58357525
1	-2.71641397	4.55478048	2.60907507
6	-1.93431377	2.57188082	2.39277506
1	-2.84651399	2.14058089	1.95997524
1	-2.03041387	2.43968081	3.47787523
8	3.06678605	-2.06451917	-1.88612485
6	3.32468605	-0.76631927	-1.98912489
6	4.69348621	-0.28791928	-2.38552475
1	5.39828587	-0.56871927	-1.59162486
6	4.11498594	-3.06681919	-1.93372488
1	3.60168600	-3.96531916	-1.58942485
6	4.68978596	-3.27941918	-3.32422495
1	4.87848616	-2.80951905	-1.19342482
1	3.86088610	-3.34181905	-4.03962517
6	5.70848608	-2.22641921	-3.75622487
1	5.17118597	-4.26451921	-3.32462478
1	4.63608599	0.80028075	-2.37832475
6	5.17798615	-0.79381931	-3.75592494
1	4.37408590	-0.68591928	-4.49452496
1	5.98078632	-0.12451927	-4.08212519
1	6.58028603	-2.28111911	-3.09132481
1	6.07278633	-2.47151923	-4.76012516
8	2.39418602	0.01688072	-1.79082489

DI-4__DBP-2_Mg-2_OMe-2_eCL-1

Zero-point vibrational energy	2325596.2 (Joules/Mol)
	555.83082 (Kcal/Mol)
Zero-point correction =	0.885773 (Hartree/Particle)
Thermal correction to Energy =	0.938829
Thermal correction to Enthalpy =	0.939773
Thermal correction to Gibbs Free Energy =	0.795072
Sum of electronic and zero-point Energies =	-2257.022110
Sum of electronic and thermal Energies =	-2256.969054
Sum of electronic and thermal Enthalpies =	-2256.968110

Sum of electronic and thermal Free Energies = -2257.112811

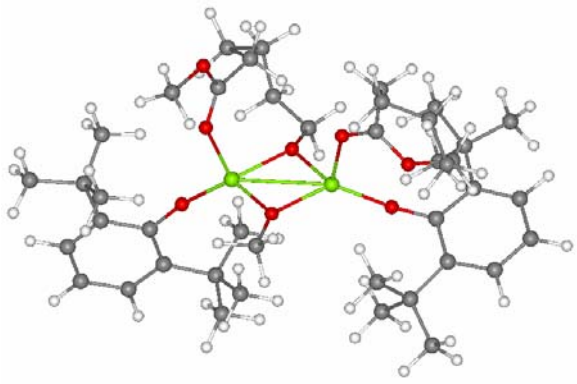


cartesian

12	-1.35846829	-0.50794321	0.26674506
8	0.06833164	-0.20824319	1.62284505
8	-2.98826838	0.37575680	0.20404504
6	-0.03556836	-0.11504319	3.03194499
1	-0.56926835	-0.98264319	3.44104505
1	-0.58126831	0.78975683	3.32594490
6	-4.07386875	1.14735675	0.23444505
6	-3.96586823	2.56425691	0.05844505
6	-5.13486862	3.33135700	0.08224505
1	-5.07666874	4.40615654	-0.05035495
6	-6.38896847	2.76345682	0.27254504
6	-6.48576880	1.38875675	0.45324504
1	-7.47116852	0.96205682	0.60664505
6	-5.36146879	0.55785686	0.44404504
6	-2.60796833	3.26135683	-0.14775495
6	-5.53346872	-0.95574319	0.66944510
6	-1.92856836	2.74585700	-1.43095493
1	-1.79606831	1.66355681	-1.41135502
1	-0.94576836	3.21595693	-1.56395495
1	-2.53866839	2.98805690	-2.30795503
6	-1.70196831	3.04235697	1.08004498
1	-1.53966832	1.98395669	1.28974497
1	-2.15716839	3.48685694	1.97154498
1	-0.72496831	3.51865697	0.92924505
6	-2.74416828	4.78575659	-0.31545496
1	-3.18236828	5.26415682	0.56664509
1	-3.34616828	5.05515671	-1.18955493
1	-1.74866831	5.22095680	-0.45975497
6	-7.00496864	-1.35954320	0.87054509
1	-7.62426853	-1.11864328	0.00014505
1	-7.44936848	-0.88574320	1.75204504
1	-7.06306839	-2.44384313	1.02024508
6	-4.78356838	-1.38984323	1.94474506
1	-3.71966839	-1.15724325	1.88754499
1	-4.89576864	-2.46964312	2.10804510
1	-5.19336843	-0.87474316	2.82014513
6	-5.02896833	-1.74124324	-0.55665493
1	-5.62136841	-1.48754323	-1.44255495
1	-5.12066841	-2.82224321	-0.38825494
1	-3.98586822	-1.50744319	-0.77175492
12	1.50833166	-0.03084319	0.36734504
8	-1.30816829	-4.76714325	0.39464504
8	3.30943155	0.22585681	0.37254503
6	-1.98546839	-4.87524319	1.66704500
1	-1.42396832	-4.34164333	2.43494511
1	-2.99156833	-4.46194315	1.59224498
6	4.63443136	0.35205680	0.28944504
6	5.46383142	-0.80684316	0.36874506
6	6.84883165	-0.63644320	0.27794504
1	7.50533152	-1.49794328	0.33434504
6	7.42563152	0.61815685	0.11574505
6	6.60633135	1.73945677	0.04134505
1	7.07623148	2.70905685	-0.08415495
6	5.21383142	1.64585674	0.12394506
6	4.86843157	-2.21544313	0.55294508
6	4.34543133	2.91485691	0.03594505
6	4.09193134	-2.30394316	1.88294506
1	3.30213165	-1.55264318	1.95044506
1	3.64093161	-3.29704309	2.00164509
1	4.76683140	-2.13844299	2.72924495
6	3.95773172	-2.57854319	-0.63845491
1	3.15663171	-1.84954321	-0.78275490
1	4.53673124	-2.60684299	-1.56765497
1	3.50683165	-3.56804299	-0.49185494
6	5.95153141	-3.30774307	0.61084509
1	6.54233122	-3.35484314	-0.30985495
1	6.63663149	-3.16634321	1.45294499
1	5.47343159	-4.28514338	0.74134505
6	5.18913126	4.19085646	-0.13465495
1	5.86543131	4.35525656	0.71064508
1	5.78313160	4.17615652	-1.05435503
1	4.52303123	5.05895662	-0.19165495
6	3.41363168	2.84505677	-1.19125497
1	2.78003168	1.95555675	-1.17465496
1	2.76773167	3.73015690	-1.23635495
1	3.99983144	2.80755687	-2.11565495
6	3.52993178	3.10415697	1.33164501
1	4.19953156	3.23985696	2.18764496
1	2.89263177	3.99375701	1.25874507
1	2.89613175	2.24225688	1.54884505
1	-2.01686835	-5.94124317	1.88234496
1	0.95603168	-0.08034319	3.50004506
1	8.50583172	0.72175682	0.04934505
1	-7.28046846	3.38575697	0.28424504
8	-1.59656835	-2.55544305	0.48994505
6	-1.16746831	-3.55104303	-0.10385495
6	-0.47476837	-3.48764300	-1.42865503
8	0.18573163	-0.43094319	-1.01425493
6	-1.44976830	-3.05994320	-2.55005503
1	0.30633163	-2.73064303	-1.31815493
1	-0.00896836	-4.44864321	-1.65345502
6	0.38093165	-0.17754319	-2.40335488
1	-2.30456829	-2.52314305	-2.12455487
1	-1.86456835	-3.96614313	-3.00335503
1	1.33723164	-0.62064320	-2.72155499
1	0.47073165	0.90615684	-2.55805492
6	-0.81776834	-2.18164301	-3.63655496
1	0.17343163	-2.56914306	-3.90735507
1	-1.43346834	-2.28794312	-4.53725481
6	-0.72756833	-0.67874318	-3.32745504
1	-1.69606829	-0.31674320	-2.95685506
1	-0.56836832	-0.16044319	-4.28195477

DI-4__DBP-2_Mg-2_OMe-2_eCL-2

Zero-point vibrational energy	2744496.9 (Joules/Mol)
	655.95050 (Kcal/Mol)
Zero-point correction =	1.045324 (Hartree/Particle)
Thermal correction to Energy =	1.106764
Thermal correction to Enthalpy =	1.107708
Thermal correction to Gibbs Free Energy =	0.945834
Sum of electronic and zero-point Energies =	-2641.905660
Sum of electronic and thermal Energies =	-2641.844220
Sum of electronic and thermal Enthalpies =	-2641.843276
Sum of electronic and thermal Free Energies =	-2642.005149



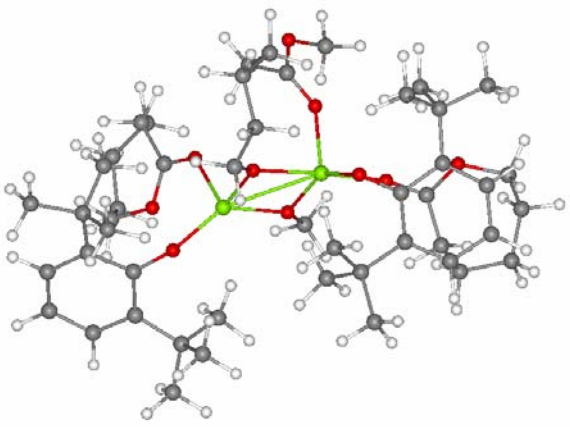
cartesian

12	1.95842278	0.42101008	0.05149665
8	0.50562274	0.13041008	1.34989655
8	3.66352272	-0.32938993	0.12109666
6	0.62322271	0.12431008	2.75429678
1	1.58762276	0.54391009	3.07329679
1	0.55802274	-0.89488995	3.15619683
6	4.78572273	-1.01928985	0.30759665
6	4.80042267	-2.44488978	0.16519664
6	6.00642300	-3.12408996	0.36379665
1	6.03852272	-4.20348978	0.26209664
6	7.18452263	-2.46358991	0.69289666
6	7.16422272	-1.08078980	0.83209664
1	8.09072208	-0.57908994	1.09079659
6	5.99652290	-0.33408993	0.65009665
6	3.53262281	-3.24248981	-0.19410336
6	6.03632259	1.19421017	0.83299667
6	2.98562288	-2.79338980	-1.56270337
1	2.77602267	-1.72368991	-1.58090341
1	2.06262279	-3.33388996	-1.80610335
1	3.71692276	-3.00058985	-2.35190320
6	2.46412277	-3.07818985	0.90499663
1	2.19092274	-2.03508997	1.07089663
1	2.83622289	-3.47418976	1.85629666
1	1.55292284	-3.62948990	0.64329666
6	3.79882288	-4.75448990	-0.31270334
1	4.14922285	-5.19128990	0.62849665
1	4.52922297	-4.98698997	-1.09490335
1	2.86472273	-5.26248980	-0.57820332
6	7.44342279	1.71341014	1.17869663
1	8.17252254	1.48921013	0.39299667
1	7.81832266	1.30531013	2.12329674
1	7.40692282	2.80371022	1.28779662
6	5.11912298	1.60861015	2.00039673
1	4.08972263	1.28901017	1.83749664
1	5.12842274	2.69881010	2.12999678
1	5.46872282	1.15701008	2.93529677
6	5.62182283	1.89991009	-0.47310334
1	6.33452272	1.66661012	-1.27190340
1	5.61232281	2.98971009	-0.33860335
1	4.63312292	1.57801008	-0.80010337
12	-0.95557725	0.02711008	0.04419665
8	1.61742282	4.67511034	0.12039664
8	-2.34937716	-1.20208991	-0.29910335
6	2.19172287	4.82671022	1.43619657
1	1.64552283	4.21641016	2.15699673
1	3.23992276	4.52661037	1.42529655
6	-3.59867716	-1.63658988	-0.20830335
6	-4.49097729	-1.50318992	-1.32530344
6	-5.83567715	-1.84758985	-1.15690339
1	-6.53007698	-1.73078990	-1.98250329
6	-6.32407713	-2.36048985	0.04099665
6	-5.43107700	-2.59378982	1.08249664
1	-5.81247711	-3.05508995	1.98759663
6	-4.07297707	-2.27058983	0.98859668
6	-3.99367714	-1.03838992	-2.70730329
6	-3.13067722	-2.62208986	2.15579677
6	-3.53127718	0.43001008	-2.66870332
1	-2.73307729	0.57961005	-1.94140339
1	-3.16207719	0.74661011	-3.65220332
1	-4.36807728	1.08761013	-2.40200329
6	-2.84417725	-1.95298982	-3.17760324
1	-2.02087712	-1.96178985	-2.46330333
1	-3.20447731	-2.98108983	-3.29190326
1	-2.46287727	-1.62028980	-4.15110350
6	-5.08837700	-1.11978984	-3.78640318
1	-5.48147726	-2.13538980	-3.89920330
1	-5.92897701	-0.44578993	-3.58640337
1	-4.66207743	-0.82608992	-4.75230312
6	-3.81627727	-3.50218987	3.21779680
1	-4.63977718	-2.98898983	3.72629666
1	-4.20177698	-4.43428993	2.79179668
1	-3.08317733	-3.77058983	3.98659682
6	-1.91837716	-3.42928982	1.64799654
1	-1.35277724	-2.88808990	0.88999665
1	-1.24547720	-3.66978979	2.47969675

1	-2.25367713	-4.37298965	1.20379663
6	-2.66927719	-1.34748983	2.88479662
1	-3.52737713	-0.82058990	3.31789660
1	-1.97827721	-1.59388983	3.69919682
1	-2.16277719	-0.65068990	2.21549678
1	2.09352279	5.88501024	1.67089665
1	-0.16857725	0.72351009	3.22619677
1	-7.37467718	-2.62148976	0.14399664
1	8.10692215	-3.02028990	0.83989668
8	2.11992288	2.50221014	0.22979665
6	1.63512278	3.45061016	-0.39160335
6	1.04252279	3.33151007	-1.75940335
8	0.50322276	0.31401008	-1.29610336
6	2.10902286	2.93961024	-2.80760336
1	0.29992276	2.53231025	-1.67910337
1	0.54152274	4.26271009	-2.03130317
6	0.44582272	-0.04228991	-2.66780329
1	2.97162271	2.47851014	-2.31480336
1	2.48762274	3.85801005	-3.26930332
1	-0.50777727	0.30071008	-3.09650326
1	0.44732273	-1.13718987	-2.75930333
6	1.60612273	1.98481011	-3.89760327
1	0.61222273	2.29901004	-4.24490309
1	2.27192283	2.10031009	-4.76130342
6	1.58622277	0.49081007	-3.53550339
1	2.54802275	0.20861009	-3.08590317
1	1.52852273	-0.07228991	-4.47660351
8	-3.83387733	1.27251017	0.88569665
6	-3.02767730	2.23131013	0.48449665
6	-3.51607728	3.64971018	0.35609666
1	-4.29007721	3.68641019	-0.42080334
6	-5.26787710	1.44201016	1.03979659
1	-5.61647701	0.41461009	1.14629662
6	-5.64087725	2.29151011	2.24209666
1	-5.67677736	1.83961010	0.10529666
1	-5.05947733	1.94771016	3.10559678
6	-5.47587729	3.79671025	2.03399682
1	-6.69037724	2.07511020	2.47249675
1	-2.66597724	4.22911024	-0.00620335
6	-4.06047726	4.24531031	1.66739655
1	-3.36577725	4.02090979	2.48569679
1	-4.05667734	5.33460999	1.55579662
1	-6.16607714	4.12501001	1.24529660
1	-5.78507710	4.32020998	2.94539666
8	-1.85177720	1.93261015	0.24289665

DI-4__DBP-2_Mg-2_OMe-2_eCL-3

Zero-point vibrational energy	3160853.9 (Joules/Mol)
	755.46221 (Kcal/Mol)
Zero-point correction =	1.203906 (Hartree/Particle)
Thermal correction to Energy =	1.274185
Thermal correction to Enthalpy =	1.275129
Thermal correction to Gibbs Free Energy =	1.092649
Sum of electronic and zero-point Energies =	-3026.770977
Sum of electronic and thermal Energies =	-3026.700697
Sum of electronic and thermal Enthalpies =	-3026.699753
Sum of electronic and thermal Free Energies =	-3026.882233



cartesian

12	-1.37429285	0.53733766	0.17748110
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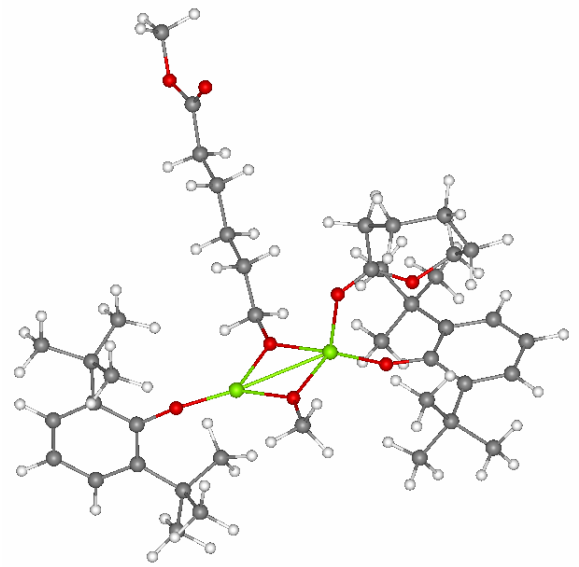
8	-2.82969284	-0.08766236	1.34488106
6	0.03070715	0.02453763	-2.51631880
1	-0.58479285	0.86023760	-2.87851882
1	-0.40029287	-0.90366238	-2.92161894
6	-3.94659305	-0.77236235	1.16358113
6	-3.92379284	-2.21006227	1.09248114
6	-5.08299303	-2.87916231	0.68918109
1	-5.07439280	-3.95936251	0.58568108
6	-6.27339315	-2.20596242	0.42118111
6	-6.33639288	-0.83696240	0.67298108
1	-7.29699278	-0.34206238	0.56848109
6	-5.21899319	-0.10216237	1.08528113
6	-2.69649291	-3.02216244	1.55718112
6	-5.39929295	1.35243762	1.56868112
6	-2.41119289	-2.67036247	3.03188109
1	-2.23319292	-1.60006237	3.14838099
1	-1.52759278	-3.21216226	3.39228106
1	-3.26079297	-2.94886231	3.66488099
6	-1.43199289	-2.75546241	0.72008109
1	-1.02109289	-1.76466238	0.91498113
1	-1.62299287	-2.85466242	-0.35381889
1	-0.64749283	-3.47636247	0.97898114
6	-2.95029306	-4.53916216	1.49508107
1	-3.10309291	-4.89536238	0.46968108
1	-3.81329298	-4.84126234	2.09728122

1	-2.07569289	-5.06536245	1.89318109
6	-6.87599277	1.78643763	1.56998110
1	-7.50069284	1.13623762	2.19158101
1	-7.30499315	1.81553757	0.56168109
1	-6.95069313	2.80023766	1.97928119
6	-4.63869286	2.37383771	0.70748109
1	-3.56839299	2.17903757	0.71218109
1	-4.80489302	3.38753772	1.09598112
1	-4.97749281	2.35163760	-0.33291888
6	-4.90659285	1.44303763	3.02798104
1	-5.49239302	0.78133762	3.67538118
1	-5.01409292	2.46803761	3.40498114
1	-3.85779285	1.15243757	3.10518122
12	1.59630716	0.05713763	0.12008111
8	-0.60909283	4.76843786	-0.31331891
8	3.03530693	-1.10156238	0.59158111
6	-1.30379283	4.82493782	-1.57491887
1	-0.87469286	4.10623741	-2.27511883
1	-2.36239290	4.60213757	-1.43461895
6	4.29750681	-1.46146238	0.41288111
6	5.32800722	-0.95126235	1.27428114
6	6.66370726	-1.20136237	0.94178110
1	7.45820713	-0.79416239	1.55898106
6	7.02040720	-1.98706245	-0.15051889
6	6.01290703	-2.61056232	-0.88191891
1	6.30500698	-3.29086232	-1.67531884
6	4.65600681	-2.40126228	-0.61221892
6	4.99610710	-0.21726239	2.58928108
6	3.59500694	-3.22706246	-1.36631894
6	4.34020710	1.15213764	2.34058118
1	3.38910699	1.05653763	1.81818116
1	4.14920712	1.66603768	3.29088116
1	4.99900723	1.79523766	1.74368107
6	4.06300688	-1.10266232	3.44128108
1	3.15100694	-1.35746241	2.90048122
1	4.57030725	-2.03506231	3.71238112
1	3.78790712	-0.58716238	4.36998129
6	6.25090694	0.05013764	3.44028115
1	6.79160690	-0.87176239	3.67718101
1	6.94820690	0.74343765	2.95628119
1	5.94990683	0.50693762	4.38998127
6	4.22980690	-4.30066252	-2.26951885
1	4.81120682	-3.86776233	-3.09171891
1	4.87900686	-4.98186255	-1.70971894
1	3.43430710	-4.90356255	-2.72151899
6	2.70470715	-3.97206259	-0.35011891
1	2.21770716	-3.27926230	0.33738109
1	1.92980719	-4.54736233	-0.87171888
1	3.30470705	-4.67316246	0.24048111
6	2.72260714	-2.34926248	-2.27981901
1	3.33840704	-1.76586235	-2.97301888
1	2.04400706	-2.97266245	-2.87471890
1	2.10320711	-1.65956235	-1.70781887
1	-1.16609287	5.84403753	-1.93291891
1	1.03160715	0.13463764	-2.96051884
1	8.06700706	-2.16316247	-0.38811889
1	-7.15799284	-2.75176239	0.10068111
8	-1.27199280	2.64393759	-0.14301889
6	-0.66479284	3.60203767	0.33158112
6	0.04350715	3.58473754	1.64708114
8	0.23880714	0.54473764	1.45958114
6	-0.94499284	3.43213773	2.82578111
1	0.68860716	2.70323753	1.60768116
1	0.65550715	4.48273754	1.75428116
6	0.36670715	0.28173763	2.84598112
1	-1.89659286	3.02403760	2.47038102
1	-1.17119288	4.43083763	3.21588111
1	1.39190722	0.51693761	3.17428112
1	0.22850715	-0.79406238	3.03068113
6	-0.43149287	2.53643751	3.96068120
1	0.62150717	2.76723766	4.17548132
1	-0.98609287	2.81063771	4.86658144
6	-0.61209285	1.02363765	3.75548100
1	-1.63209283	0.81723762	3.41198111
1	-0.52009284	0.54593766	4.74088144
8	-4.59489298	1.02363765	-2.57951880
6	-3.73699307	0.11483763	-2.09611893
6	-3.95709300	-1.34716237	-2.37411880
1	-4.87219286	-1.67706239	-1.86511886
6	-5.86889315	0.63633764	-3.14031887
1	-6.42019272	1.57773757	-3.17051888
6	-5.76469278	0.03693764	-4.53411865
1	-6.38179302	-0.03156237	-2.44071889
1	-5.07729292	0.65393764	-5.12591887
6	-5.33699274	-1.42956233	-4.55611849
1	-6.75039291	0.13153763	-5.00561857
1	-3.13329291	-1.86406243	-1.88311887
6	-4.00089264	-1.70926237	-3.86931896
1	-3.18739295	-1.19736242	-4.39811850
1	-3.78729296	-2.78036237	-3.94941878
1	-6.11539316	-2.03346229	-4.07171869
1	-5.28499317	-1.77286232	-5.59581852
8	-2.76429296	0.53943765	-1.48871887
8	4.17640686	0.98713762	-1.59631884
6	3.57080698	2.04373765	-1.08821893
6	4.17500687	3.41733766	-1.21941888
1	5.10630703	3.44683766	-0.64021891
6	5.55260706	1.01593769	-2.05941892
1	5.80020714	-0.04236237	-2.13731885
6	5.71930695	1.73333764	-3.38751888
1	6.18010712	1.43993759	-1.26971889
1	4.94250727	1.37913764	-4.07561874
6	5.70900726	3.25883770	-3.29171896
1	6.67700720	1.40753758	-3.80981898
1	3.47440696	4.09843779	-0.73451889
6	4.44580698	3.85543752	-2.66991878
1	3.57100701	3.62663770	-3.29031897
1	4.53940725	4.94653749	-2.66771889
1	6.57880688	3.58453774	-2.70551896
1	5.84260702	3.68193769	-4.29371881
8	2.48350716	1.87113762	-0.53111887

DI-5__DBP-2_Mg-2_OMe-2_eCL-2

Zero-point vibrational energy	2740824.3 (Joules/Mol)
	655.07274 (Kcal/Mol)
Zero-point correction =	1.043925 (Hartree/Particle)
Thermal correction to Energy =	1.106421
Thermal correction to Enthalpy =	1.107366
Thermal correction to Gibbs Free Energy =	0.937406
Sum of electronic and zero-point Energies =	-2641.896836
Sum of electronic and thermal Energies =	-2641.834339
Sum of electronic and thermal Enthalpies =	-2641.833395
Sum of electronic and thermal Free Energies =	-2642.003354



cartesian

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6	-0.05612016	-3.27820015	1.91197670
1	0.89617980	-3.70770001	2.24977660
1	-0.63762021	-4.07819986	1.43817675
6	4.80698013	-2.05890012	0.18247670
6	5.01397991	-2.95900011	-0.90492326
6	6.30448008	-3.09860015	-1.42382324
1	6.48638010	-3.76710010	-2.25912333
6	7.38187981	-2.39900017	-0.89102328
6	7.17587996	-1.55419993	0.19597670
1	8.03387928	-1.03369999	0.60817671
6	5.91097975	-1.36420000	0.76047671
6	3.84997988	-3.80120015	-1.45452332
6	5.72887993	-0.44219995	1.98037672
6	2.66477990	-2.90429997	-1.92502332
1	2.90827990	-1.83629990	-1.88522327
1	1.73777986	-3.12000012	-1.36952329
1	2.39717984	-3.10090017	-2.96812320
6	3.37907982	-4.78449965	-0.36022329
1	3.08917999	-4.25989962	0.55367672
1	4.18847990	-5.47440004	-0.10132329
1	2.52627993	-5.37949991	-0.71002328
6	4.26898003	-4.65329981	-2.66572332
1	5.05747986	-5.36759996	-2.41072321
1	4.61787987	-4.03769970	-3.50192332
1	3.40818000	-5.23309994	-3.01702332
6	7.06377983	0.14970005	2.46447682
1	7.53847980	0.78170007	1.70627677
1	7.77608013	-0.62739998	2.76097679
1	6.88267994	0.77770007	3.34397674
6	5.13467979	-1.23570001	3.16267681
1	4.17157984	-1.67709994	2.90277672
1	4.99597979	-0.57829994	4.03027678
1	5.81157970	-2.04430008	3.45967674
6	4.81547976	0.74910003	1.62967670
1	5.24217987	1.33520007	0.80817670
1	4.70327997	1.41260004	2.49597669
1	3.82157993	0.41370004	1.32837677
12	-1.02222013	-0.82639992	0.20947669
8	2.57268000	8.27180004	-1.30942333
8	-2.50712013	-1.16889989	-0.89462328
6	2.56868005	9.56330013	-0.68352330
1	1.54537976	9.90929985	-0.52112329
1	3.08967996	9.52670002	0.27567673
6	-3.79292011	-1.12529993	-1.21212327
6	-4.29462004	-0.07719996	-2.05352330
6	-5.67222023	-0.00189996	-2.28282332
1	-6.07352018	0.79430002	-2.90122318
6	-6.56252003	-0.93049997	-1.75232327
6	-6.05921984	-1.99680007	-1.01332331
1	-6.76041985	-2.74180007	-0.65202326
6	-4.69402027	-2.13750005	-0.74252331
6	-3.35391998	0.93770003	-2.73102331
6	-4.19672012	-3.37570000	0.02857671
6	-2.67982006	1.84840000	-1.68802333
1	-2.09342003	1.27410007	-0.96972328
1	-2.01032019	2.56709981	-2.17632318
1	-3.43232012	2.41859984	-1.13082325
6	-2.29051995	0.19680005	-3.56702328
1	-1.70242023	-0.48949993	-2.95682335
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1	-1.61232018	0.91460007	-4.04532337
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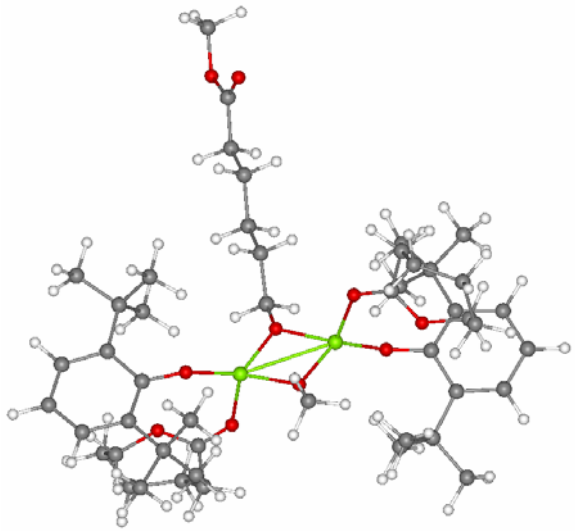
1	-4.83552027	2.50569987	-3.19272327
1	-3.37882018	2.54009986	-4.18482351
6	-5.31602001	-4.40739965	0.26167673
1	-6.11912012	-4.02119970	0.89877671
1	-5.75812006	-4.75259972	-0.67872328
1	-4.89722013	-5.28369999	0.76867670
6	-3.09581995	-4.10229969	-0.77102327
1	-2.24311996	-3.45280004	-0.96952331
1	-2.74712014	-4.98509979	-0.22082330

1	-3.49092007	-4.44299984	-1.73422325
6	-3.67902017	-2.97790003	1.42327666
1	-4.48171997	-2.52160001	2.01337671
1	-3.31642008	-3.85700011	1.96907675
1	-2.86212015	-2.25670004	1.36657667
1	3.08938003	10.22480011	-1.37512326
1	-0.60262018	-2.94220018	2.80307674
1	-7.62902021	-0.84809995	-1.94792330
1	8.37718010	-2.51980019	-1.31142330
8	1.45897985	7.46250010	0.48067671
6	1.96707976	7.28700018	-0.60822326
6	1.99947977	5.98220015	-1.36962330
8	0.70577979	-0.13299996	-0.49742329
6	1.58087981	4.78080034	-0.52842331
1	1.33577979	6.10130024	-2.23572326
1	3.00397992	5.85290003	-1.78672326
6	1.06117976	0.98050004	-1.29882324
1	0.59617978	4.97550011	-0.09012329
1	2.27038002	4.67360020	0.31667671
1	0.32887983	1.09840000	-2.10842323
1	2.03227997	0.79480004	-1.78352332
6	1.54527986	3.48169994	-1.33472323
1	0.84217983	3.59270000	-2.17162323
1	2.53027987	3.30239987	-1.78672326
6	1.14577985	2.27110004	-0.49012327
1	0.17327984	2.45469999	-0.01562329
1	1.86727977	2.13229990	0.32477671
8	-3.73932004	0.54340005	1.44607675
6	-2.66282010	0.95190006	2.08137679
6	-2.74342012	1.98950005	3.16817665
1	-3.13222003	2.92149997	2.73887682
6	-5.05802011	1.11990011	1.63487673
1	-5.63212013	0.64960003	0.83617669
6	-5.65831995	0.82330006	2.99807668
1	-5.00372028	2.19519997	1.43217671
1	-5.52831984	-0.24399996	3.21087670
6	-5.11401987	1.68110001	4.14017677
1	-6.73842001	0.98860008	2.90977669
1	-1.71532023	2.17859983	3.47937679
6	-3.60702014	1.56660008	4.37027693
1	-3.34152007	0.54560006	4.66877651
1	-3.32992005	2.21079993	5.21107674
1	-5.36362028	2.73300004	3.94627666
1	-5.63301992	1.41170001	5.06667662
8	-1.58062017	0.43990004	1.76757669

DI-5__DBP-2_Mg-2_OMe-2_eCL-3

Zero-point vibrational energy	3157909.7 (Joules/Mol)
	754.75854 (Kcal/Mol)
Zero-point correction =	1.202784 (Hartree/Particle)
Thermal correction to Energy =	1.274158
Thermal correction to Enthalpy =	1.275102
Thermal correction to Gibbs Free Energy =	1.084471
Sum of electronic and zero-point Energies =	-3026.778759
Sum of electronic and thermal Energies =	-3026.707386
Sum of electronic and thermal Enthalpies =	-3026.706442
Sum of electronic and thermal Free Energies =	-3026.897073



cartesian

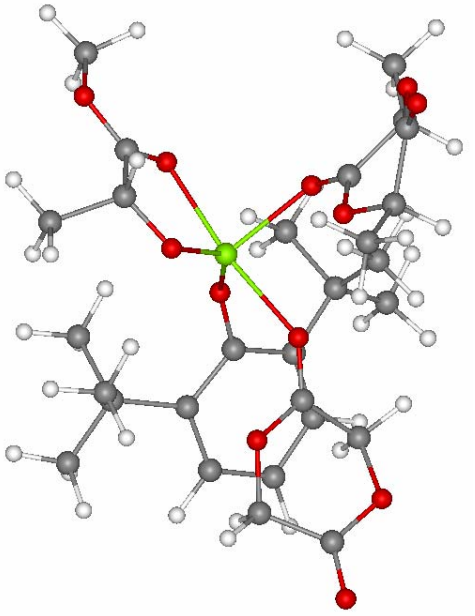
12	1.48598421	-0.80003476	0.19371514
8	-0.04101576	-1.94363487	0.69981515
8	3.03298426	-0.75833482	1.28971517
6	-0.11431575	-3.00713468	1.62131512
1	0.09848425	-2.67023468	2.64591527
1	0.60608423	-3.79773474	1.37511516
6	4.34328413	-0.71673477	1.47881508
6	5.08718443	-1.92893481	1.67781508
6	6.48268414	-1.85923481	1.73541510
1	7.06268406	-2.76813483	1.85681510
6	7.16848421	-0.65053481	1.66001511
6	6.43568420	0.53026521	1.58641517
1	6.97948408	1.46926510	1.59401512
6	5.03858423	0.53826517	1.51841509
6	4.38728428	-3.28643465	1.88261509
6	4.28888416	1.88386512	1.50431514
6	3.65658426	-3.74813461	0.60871512
1	2.87628412	-3.04903483	0.30891514
1	3.18628430	-4.72653484	0.76631510
1	4.36338425	-3.85053468	-0.22378485
6	3.39818430	-3.18163466	3.06131530
1	2.66268420	-2.39383483	2.89651537
1	3.93828416	-2.95433474	3.98701525
1	2.86978412	-4.13253450	3.20421529

6	5.37908411	-4.40863466	2.24141526
1	5.94938421	-4.18103456	3.14791536
1	6.08798409	-4.61893463	1.43261516
1	4.82168436	-5.33343458	2.42891526
6	5.22428417	3.07846522	1.76811516
1	5.97188425	3.21366525	0.97871512
1	5.74808407	2.98456526	2.72511530
1	4.63008404	3.99836516	1.80791509
6	3.22098422	1.91816521	2.61701536
1	2.49438429	1.11256516	2.51061535
1	2.68698430	2.87626529	2.60161519
1	3.69548416	1.81586516	3.59911513
6	3.64468431	2.12866521	0.12851515
1	4.41028404	2.16356516	-0.65458488
1	3.10278416	3.08196521	0.11601514
1	2.94138432	1.33766520	-0.13458486
12	-1.45331573	-0.68413478	0.13131514
8	0.07168425	0.50226521	-0.26718485
8	-2.84911585	-0.76493478	-1.16348481
6	-4.10471582	-1.09663486	-1.43188488
6	-5.13951588	-0.10093481	-1.40738487
6	-6.47171593	-0.51683480	-1.49998486
1	-7.27041578	0.21586519	-1.44408488
6	-6.81861591	-1.85163486	-1.68728483
6	-5.80331564	-2.78463483	-1.87838483
1	-6.08651590	-3.80513477	-2.11468482
6	-4.44901562	-2.44183469	-1.79678488
6	-4.81471586	1.40506518	-1.35648489
6	-3.37771583	-3.49283481	-2.15188479
6	-4.20421600	1.81956518	-0.00678485
1	-3.25421572	1.31976521	0.17891514
1	-4.02411556	2.90126538	0.01971515
1	-4.88631582	1.57836521	0.81761515
6	-3.84371567	1.75596511	-2.50268483
1	-2.93051577	1.16246510	-2.44348478
1	-4.31461573	1.56086516	-3.47238469
1	-3.57691574	2.81976533	-2.46588469
6	-6.06611586	2.27946520	-1.55468488
1	-6.57891560	2.05866528	-2.49648476
1	-6.78821564	2.17406535	-0.73708487
1	-5.76591587	3.33296537	-1.58358490
6	-3.99691582	-4.77253485	-2.74368477
1	-4.61231565	-5.31683493	-2.01868486
1	-4.60931587	-4.56433487	-3.62728477
1	-3.19241571	-5.44943476	-3.05238485
6	-2.42431569	-2.92683482	-3.22478485
1	-1.94291580	-2.00843477	-2.88688469
1	-1.64631581	-3.66233468	-3.46448469
1	-2.97501588	-2.70513463	-4.14578485
6	-2.57391572	-3.92633462	-0.91438484
1	-3.23841572	-4.30323458	-0.12898485
1	-1.87011576	-4.72703457	-1.17358482
1	-1.98541582	-3.10613465	-0.50498486
1	-1.11291575	-3.46593475	1.62031507
1	-7.86281586	-2.14923477	-1.74908483
1	8.25468445	-0.62613481	1.70811510
8	4.24668407	-0.86373478	-1.64458489
6	3.22768426	-1.43033481	-2.26058483
6	3.40488434	-2.10333467	-3.59598470
1	4.09468412	-2.94843483	-3.47848463
6	5.61828423	-0.98553485	-2.09968472
1	6.18388414	-0.59333479	-1.25428486
6	5.89848423	-0.20323482	-3.37168479
1	5.86298418	-2.04783463	-2.20408463
1	5.46698427	0.79906523	-3.26508474
6	5.41198444	-0.87463480	-4.65618515
1	6.98458433	-0.06553482	-3.42958474
1	2.42768431	-2.51293468	-3.85448480
6	3.91118431	-1.16293490	-4.70458508
1	3.34038424	-0.22723481	-4.67708492
1	3.67528415	-1.63383484	-5.66438484
1	5.95738411	-1.81833482	-4.79228497
1	5.67798424	-0.24383482	-5.51168489
8	2.11988425	-1.36823487	-1.72078490
8	-3.99261570	-1.70693481	1.73591518
6	-3.40421581	-0.74613482	2.42491531
6	-4.00141573	-0.23353481	3.70741534
1	-4.96711588	0.23706520	3.48451519
6	-5.33391571	-2.17973471	2.02871513
1	-5.58121586	-2.75773478	1.13871515
6	-5.40161562	-3.02203465	3.29091525
1	-6.01091576	-1.32073486	2.06171536
1	-4.57721567	-3.74453473	3.27261519
6	-5.39631557	-2.21943474	4.59231520
1	-6.32641554	-3.60843468	3.23701525
1	-3.33021569	0.55326521	4.05381489
6	-4.17881584	-1.31473482	4.78841496
1	-3.26371574	-1.91463482	4.85691500
1	-4.27691555	-0.80013478	5.74981499
1	-6.30471563	-1.60353482	4.63321495
1	-5.46021557	-2.91173482	5.43911505
8	-2.33461571	-0.30703482	1.99441516
8	-0.43651578	9.13496494	-0.45628488
6	-0.75031579	10.33206463	0.26971513
1	-1.81081581	10.35756493	0.53051513
1	-0.15701576	10.39366436	1.18481517
1	-0.50301576	11.15436459	-0.40088487
8	-1.11561573	7.94186544	1.33671510
6	-0.67481577	7.97866535	0.20631514
6	-0.33021575	6.78426504	-0.65208489
6	-0.42901576	5.45386505	0.08671515
1	-1.00291574	6.80376530	-1.51898491
1	0.67428422	6.94226503	-1.06138492
6	0.08308425	1.72146511	-0.98088491
1	-1.43461573	5.34876537	0.50741518
1	0.25328425	5.46546507	0.94421512
1	-0.67401576	1.69566512	-1.77868485
1	1.05378425	1.85556519	-1.48318481
6	-0.11281575	4.25806522	-0.81278485
1	-0.81401575	4.24416542	-1.65888488
1	0.88728422	4.38406515	-1.25078487
6	-0.17791575	2.92106533	-0.07428485
1	-1.16411579	2.80436516	0.39241517
1	0.55318421	2.90636516	0.74301511

S5.4. ROP of LA. Mononuclear mechanism

I-1c__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1739349.8 (Joules/Mol)
	415.71458 (Kcal/Mol)
Zero-point correction =	0.662483 (Hartree/Particle)
Thermal correction to Energy =	0.708564
Thermal correction to Enthalpy =	0.709509
Thermal correction to Gibbs Free Energy =	0.577668
Sum of electronic and zero-point Energies =	-2192.748975
Sum of electronic and thermal Energies =	-2192.702894
Sum of electronic and thermal Enthalpies =	-2192.701950
Sum of electronic and thermal Free Energies =	-2192.833790



cartesian

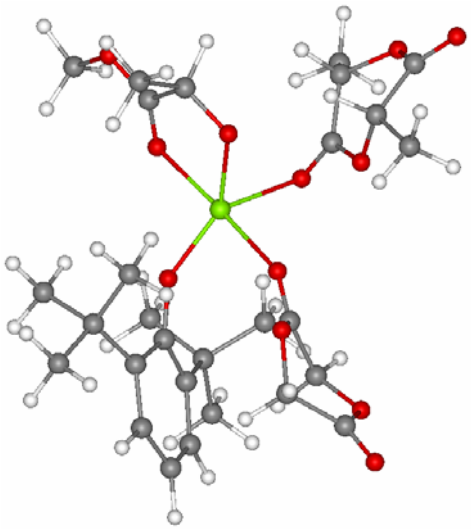
8	0.84923601	0.93898642	-0.51875049
6	2.04913592	0.44718641	-0.74535048
6	2.35563588	-0.19271362	-1.99765038
6	3.55593586	-0.90141362	-2.10775042
1	3.78943586	-1.42741358	-3.02805042
6	4.48593569	-0.95071363	-1.06995046
6	4.26783609	-0.16261362	0.05954951
1	5.05783606	-0.10661362	0.80224955
6	3.09743595	0.58588636	0.23334950
6	1.42693603	-0.06011362	-3.22105050
6	3.01233578	1.62318635	1.37554955
6	1.06773603	1.42348635	-3.44775057
1	0.55463600	1.84888637	-2.58495045
1	0.41993597	1.52338636	-4.32765055
1	1.97383606	2.01108646	-3.63165045
6	0.14033595	-0.88691360	-3.04855037
1	-0.41986406	-0.57921362	-2.16695046
1	0.37363598	-1.95461357	-2.95585036
1	-0.50886405	-0.76521361	-3.92545033
6	2.10393596	-0.55371362	-4.51285028
1	2.30313587	-1.63101363	-4.50155067
1	3.04683590	-0.03231362	-4.70815039
1	1.43913603	-0.36141360	-5.36235046
6	4.38373566	1.83818638	2.04424953
1	5.15413570	2.12468624	1.32074952
1	4.73433590	0.95328641	2.58754945
1	4.30173588	2.64748621	2.77784944
6	2.03893590	1.21788633	2.49564958
1	1.00543594	1.11218643	2.16374946
1	2.04113579	1.97918642	3.28544950
1	2.33763576	0.27198637	2.95854950
6	2.59253597	2.98918629	0.79124951
1	3.31843591	3.32568645	0.04274951
1	2.55833578	3.74178648	1.58844948
1	1.61243594	2.93908644	0.31554949
8	-5.61436415	-1.61901367	-0.93905044
6	-5.64836407	-2.41321373	0.15724951
6	-4.28496408	-2.84841347	0.68404955
8	-3.31696415	-1.77331364	0.56094950
6	-3.27456403	-1.08841360	-0.57105047
6	-4.34796429	-1.41541362	-1.59595048
8	-6.69486427	-2.74061346	0.65294951
1	-4.05176401	-2.35671377	-2.08225036
6	-4.53016424	-0.33301362	-2.63715053
6	2.56633592	-2.70021343	2.46764946
8	1.29733598	-2.08371353	2.17804956
6	0.87833595	-2.15421367	0.91684955
6	1.65003598	-3.08681345	0.01834951
8	2.08543587	-4.27441359	0.69914955
6	2.68213582	-4.10041380	1.89954948
8	-0.09246404	-1.51741362	0.54264951
1	3.36933589	-2.06841373	2.07044935
1	2.64143586	-2.74581385	3.55134964
6	-4.31736422	-3.26451349	2.13744950
1	-3.93366408	-3.68031359	0.05824951
8	-2.41056418	-0.24981362	-0.76795048
1	1.01043594	-3.41401339	-0.79775047
1	2.50923586	-2.54831362	-0.40585047
8	3.24823594	-5.00271368	2.46154952
12	-0.79086399	0.54618639	0.41564953
8	-1.59696400	0.82898641	2.13414955
6	-2.26466417	1.99928629	2.36474943

6	-2.24346399	2.86718655	1.10494947
8	-2.88116407	4.03228664	1.18184948
6	-2.85846424	4.85168648	-0.00175048
6	-1.70836401	2.79158640	3.56174946
1	-3.34556413	1.83528650	2.56494951
8	-1.67906404	2.49708652	0.07214951
1	-1.83006406	5.09308672	-0.27605051
1	-3.40866423	5.75418663	0.25984952
1	-3.34226418	4.33388662	-0.83225048
1	5.40563583	-1.52031362	-1.17785048

1	-2.28796411	3.69658661	3.76904964
1	-1.73996401	2.13938618	4.43794966
1	-0.66436404	3.06698656	3.38484955
1	-3.31736422	-3.56461382	2.45564961
1	-5.00466394	-4.10241365	2.26044941
1	-4.65686417	-2.43831348	2.76404953
1	-3.59606409	-0.17651361	-3.17775059
1	-4.82216406	0.60688639	-2.16535044
1	-5.30786419	-0.63591361	-3.34075046

I-1c__SS_DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1739725.3 (Joules/Mol)
	415.80434 (Kcal/Mol)
Zero-point correction =	0.662626 (Hartree/Particle)
Thermal correction to Energy =	0.708613
Thermal correction to Enthalpy =	0.709558
Thermal correction to Gibbs Free Energy =	0.579144
Sum of electronic and zero-point Energies =	-2192.751010
Sum of electronic and thermal Energies =	-2192.705023
Sum of electronic and thermal Enthalpies =	-2192.704079
Sum of electronic and thermal Free Energies =	-2192.834492



cartesian

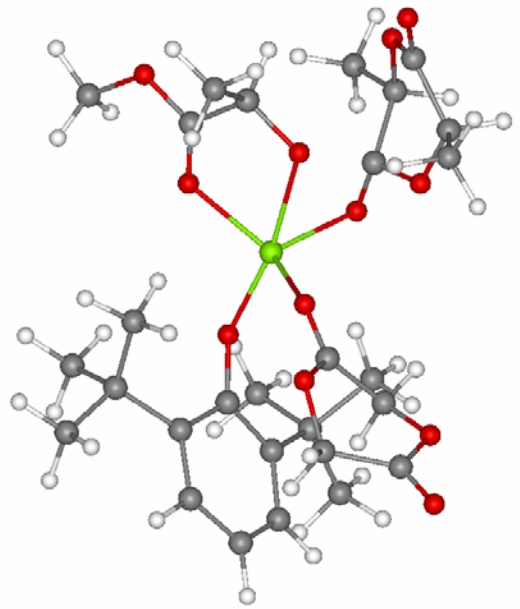
8	1.06640005	-1.48220003	0.24470000
6	2.33669996	-1.13820004	0.33149999
6	2.96740007	-0.98089999	1.61370003
6	4.24529982	-0.41440001	1.66020000
1	4.72749996	-0.25009999	2.61829996
6	4.94000006	-0.05480000	0.50590003
6	4.39319992	-0.38100001	-0.73460001
1	4.99650002	-0.20570000	-1.62039995
6	3.12639999	-0.96429998	-0.85879999
6	2.29049993	-1.46089995	2.91339993
6	2.66540003	-1.52559996	-2.22149992
6	1.79920006	-2.91400003	2.74530005
1	1.07969999	-3.00370002	1.93139994
1	1.32650006	-3.25889993	3.67309999
1	2.64380002	-3.57870007	2.53250003
6	1.11350000	-0.55080003	3.30739999

1	0.35110000	-0.50290000	2.53090000
1	1.46150005	0.46849999	3.51230001
1	0.63190001	-0.92180002	4.22030020
6	3.26869988	-1.46140003	4.10290003
1	3.59890008	-0.45429999	4.37970018
1	4.15539980	-2.07270002	3.90459991
1	2.76600003	-1.88390005	4.97989988
6	3.78419995	-1.45299995	-3.27649999
1	4.69280005	-1.96969998	-2.95079994
1	4.04920006	-0.42240000	-3.53959990
1	3.44250011	-1.93910003	-4.19680023
6	1.45850003	-0.77850002	-2.81520009
1	0.56059998	-0.88410002	-2.20600009
1	1.22080004	-1.18050003	-3.80780005
1	1.65989995	0.29040000	-2.93099999
6	2.31119990	-3.01839995	-2.04859996
1	3.18709993	-3.58489990	-1.71430004
1	1.98290002	-3.44129992	-3.00620008
1	1.51540005	-3.15499997	-1.31410003
8	-2.56760001	1.90079999	0.47260001
6	-2.83879995	0.75569999	1.07669997
6	-4.30140018	0.36300001	1.16229999
8	-5.16879988	1.51049995	1.12269998
6	-4.91440010	2.48160005	0.21220000
6	-3.56220007	2.37610006	-0.47679999
8	-1.94210005	0.07730000	1.57009995
1	-3.60739994	1.61249995	-1.26499999
6	-3.07680011	3.69320011	-1.03590000
6	2.83699989	3.13339996	-1.57509995
8	1.56019998	2.46930003	-1.50259995
6	1.23150003	1.94799995	-0.31830001
6	2.09380007	2.36579990	0.84570003
8	2.53419995	3.72939992	0.74519998
6	3.05310011	4.11479998	-0.44020000

8	0.26629999	1.21500003	-0.21879999
1	3.63170004	2.37890005	-1.57369995
1	2.84710002	3.67120004	-2.51990008
6	-4.62900019	-0.41850001	2.41980004
1	-4.49499989	-0.25150001	0.27340001
8	-5.71780014	3.35430002	0.00140000
1	1.51470006	2.29340005	1.76310003
1	2.95530009	1.68840003	0.91970003
8	3.62930012	5.16429996	-0.57110000
12	-0.66810000	-0.70150000	-0.01250000
8	-2.18149996	-0.45370001	-1.25290000
6	-2.82480001	-1.58029997	-1.70589995
6	-2.42529988	-2.77609992	-0.84069997
8	-3.06550002	-3.91230011	-1.08780003
6	-2.68120003	-5.05009985	-0.28830001
6	-2.55730009	-1.88810003	-3.18969989
1	-3.92790008	-1.50740004	-1.59309995
8	-1.56640005	-2.67659998	0.03690000
1	-1.62230003	-5.27069998	-0.43099999
1	-3.29859996	-5.87340021	-0.64310002
1	-2.87220001	-4.85169983	0.76770002
1	5.92729998	0.39550000	0.57370001
1	-3.11999989	-2.75970006	-3.53740001
1	-2.85409999	-1.01559997	-3.77699995
1	-1.49059999	-2.05979991	-3.35870004
1	-5.68100023	-0.70920002	2.40100002
1	-4.00689983	-1.31250000	2.47350001
1	-4.44670010	0.18930000	3.30859995
1	-3.79539990	4.06010008	-1.77010000
1	-2.98020005	4.44129992	-0.24620000
1	-2.11050010	3.54690003	-1.52170002

TS-12c__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1742290.6 (Joules/Mol)
	416.41746 (Kcal/Mol)
Zero-point correction =	0.663603 (Hartree/Particle)
Thermal correction to Energy =	0.707996
Thermal correction to Enthalpy =	0.708940
Thermal correction to Gibbs Free Energy =	0.583584
Sum of electronic and zero-point Energies =	-2192.739436
Sum of electronic and thermal Energies =	-2192.695044
Sum of electronic and thermal Enthalpies =	-2192.694100
Sum of electronic and thermal Free Energies =	-2192.819456



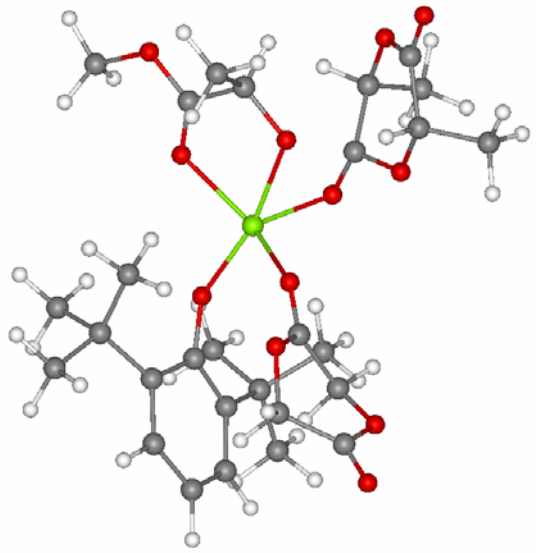
cartesian

8	-0.88305843	-1.20041120	-0.46405312
6	-2.16055846	-0.87921119	-0.34485310
6	-2.81095862	-0.95621121	0.93454689
6	-4.07715845	-0.37321126	1.06944692
1	-4.57435846	-0.37901127	2.03464699
6	-4.75515842	0.18288876	-0.01445311
6	-4.19875813	0.06188875	-1.28685308
1	-4.78465843	0.39988875	-2.13545299
6	-2.93015862	-0.49141127	-1.49495304
6	-2.21435857	-1.78081131	2.09724689
6	-2.41325855	-0.71721125	-2.93045306
6	-0.91505837	-1.19511127	2.68094683
1	-0.08505845	-1.28671122	1.97864687
1	-0.62865841	-1.75321126	3.58104682
1	-1.02665842	-0.14391124	2.96034694
6	-1.93605840	-3.21151114	1.58844697
1	-1.22965837	-3.20241117	0.75614685
1	-2.86285853	-3.68781137	1.25144696
1	-1.51685846	-3.82441139	2.39654684
6	-3.20165849	-1.90381122	3.27204704
1	-4.15925837	-2.33471131	2.96294689
1	-3.39705849	-0.94161129	3.75914693
1	-2.77545857	-2.56761122	4.03214693
6	-3.52825856	-0.52441126	-3.97515321
1	-3.88115859	0.51128876	-4.02975321
1	-4.38945818	-1.17311120	-3.78285313
1	-3.13735843	-0.77921128	-4.96625328
6	-1.91085851	-2.16811132	-3.08285308
1	-1.09875846	-2.38561130	-2.38855314
1	-1.55255842	-2.33491135	-4.10595322
1	-2.72495842	-2.87631130	-2.89265299
6	-1.28765845	0.26788875	-3.29305315
1	-1.65185845	1.30178881	-3.26275301
1	-0.93205845	0.08028875	-4.31365347
1	-0.42645845	0.18258876	-2.63135314
6	-2.77085853	3.15398884	1.99834692

8	-1.50135839	2.46948886	2.01534677
6	-1.02115846	2.08868885	0.83504689
6	-1.68425846	2.67948866	-0.38245308
8	-2.14775848	4.02018881	-0.17095309
6	-2.82985854	4.26408863	0.96904689
8	-0.07255843	1.32548881	0.78584689
1	-0.95815837	2.72538877	-1.19145310
1	-2.51245856	2.02608871	-0.68695313
12	0.79944158	-0.32531124	-0.18525311
8	2.75694156	0.40658876	0.46614692
6	3.58434153	-0.56091124	1.06004691
6	2.97754145	-1.93551135	0.82574689
8	3.75314140	-2.95141125	1.15854692
6	3.19154143	-4.27361107	0.99084687
6	3.70064139	-0.29341125	2.56684685
8	1.83974159	-2.08411121	0.37734690
1	2.29874158	-4.38131142	1.60794699
1	3.97264147	-4.95831108	1.31464696
1	2.93644142	-4.44111109	-0.05635311
1	-5.73945808	0.62618876	0.11724690
8	1.82884157	0.37528875	-1.75145304
6	2.79534149	0.99198878	-1.18975306
8	2.54654145	2.32008886	-0.92725313
6	4.20824146	0.80988872	-1.74865305
6	3.63964152	3.11608887	-0.44475311
8	5.18644190	1.23608875	-0.78055310
6	3.13474154	4.00628853	0.67434686
6	4.87934160	2.32278872	-0.03325310
6	4.55804157	-0.57831126	-2.23655295
1	-3.56285858	2.42108870	1.80684698
1	-2.89875841	3.57948875	2.99064684
8	5.62054157	2.66998887	0.85554689
8	-3.42685843	5.29538870	1.14234698
1	4.59494162	-0.55871123	0.63764685
1	4.32474184	-1.04801130	3.05334687
1	4.15904140	0.68688875	2.70854688
1	2.71214151	-0.28731126	3.03424692
1	4.25094175	1.49558878	-2.60675311
1	3.97304153	3.74218869	-1.28745306
1	3.92494154	4.68058872	1.00844693
1	2.29014158	4.59698868	0.31184691
1	2.80714154	3.39708877	1.51874697
1	5.55304193	-0.56761122	-2.68875313
1	4.55764151	-1.31751120	-1.43485308
1	3.82784152	-0.88351130	-2.98795295

TS-12c__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1741966.4 (Joules/Mol)
	416.33995 (Kcal/Mol)
Zero-point correction =	0.663480 (Hartree/Particle)
Thermal correction to Energy =	0.708099
Thermal correction to Enthalpy =	0.709043
Thermal correction to Gibbs Free Energy =	0.582584
Sum of electronic and zero-point Energies =	-2192.744211
Sum of electronic and thermal Energies =	-2192.699592
Sum of electronic and thermal Enthalpies =	-2192.698648
Sum of electronic and thermal Free Energies =	-2192.825107



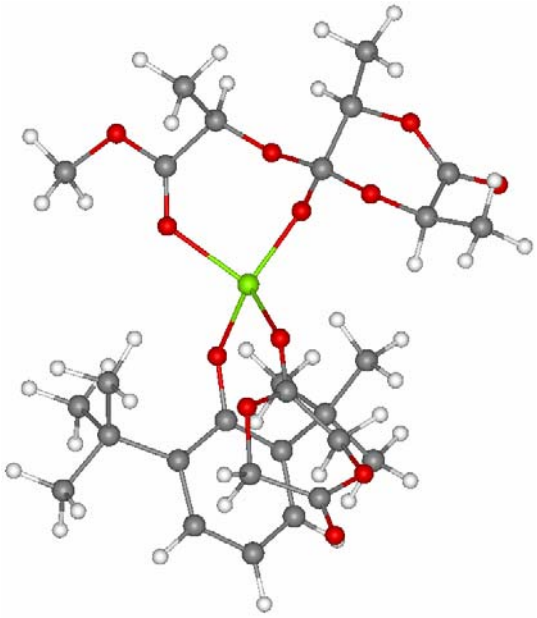
cartesian

8	0.92114705	1.16061974	-0.52918512
6	2.19074702	0.80451971	-0.45288515
6	2.90354705	0.93231970	0.78951490
6	4.16484690	0.33251971	0.89541489
1	4.71074677	0.38301975	1.83271492
6	4.77824688	-0.29508027	-0.18798514
6	4.15934706	-0.23668027	-1.43578517
1	4.69394684	-0.63878024	-2.29008532
6	2.89124703	0.32761973	-1.61328518
6	2.37734699	1.83131981	1.93101490
6	2.29954696	0.46311975	-3.03068519
6	1.06794703	1.33361983	2.57231474
1	0.22204702	1.45701981	1.89401484
1	0.84144706	1.92921972	3.46551466
1	1.12774694	0.28561974	2.87781477
6	2.14894700	3.24841976	1.36281490
1	1.42014694	3.23171973	0.55011487
1	3.08614707	3.66581988	0.97981489
1	1.77934694	3.91701961	2.15071464
6	3.40114689	1.96021986	3.07321477
1	4.36384678	2.34611988	2.72331476
1	3.57714701	1.00911975	3.58911467
1	3.02074695	2.66531968	3.82001472

6	3.34684706	0.16221973	-4.11838531
1	3.67214704	-0.88388026	-4.11428547
1	4.23274708	0.79921967	-4.02418518
1	2.90594697	0.35401970	-5.10268545
6	1.82154703	1.91141987	-3.26488519
1	1.05814695	2.20321989	-2.54318523
1	1.40534699	2.00881982	-4.27478504
1	2.66104698	2.61031985	-3.17888522
6	1.13214695	-0.51598024	-3.25278521
1	1.47174692	-1.55388021	-3.15388536
1	0.72824705	-0.40218028	-4.26618528
1	0.30924702	-0.35248029	-2.55798531
6	2.77444696	-2.89198017	2.34911466
8	1.49034703	-2.25058031	2.21051478
6	1.07144701	-2.02708030	0.96651489
6	1.82994699	-2.72908020	-0.12968515
8	2.30924702	-4.02298021	0.26421487
6	2.92554688	-4.11138010	1.46261489
8	0.10234703	-1.31518030	0.77141488
1	1.16434693	-2.88818026	-0.97518516
1	2.66244698	-2.08888030	-0.45188510
12	-0.78405297	0.38491970	-0.12598515
8	-2.65705299	-0.13118027	0.74711490
6	-3.39805293	0.92091972	1.29351485
6	-2.76715302	2.23891973	0.86411488
8	-3.46175313	3.32031989	1.17181492
6	-2.87635303	4.58921957	0.80101490
6	-3.43655300	0.82361966	2.82481480
1	-4.43685293	0.92621976	0.93411487
8	-1.68285298	2.28331971	0.28211486
1	-1.91135299	4.71461964	1.29331481
1	-3.58615303	5.34101963	1.14001489
1	-2.74515295	4.63851976	-0.28078514
1	5.75954676	-0.75098026	-0.07988514
8	-1.95385301	-0.36128026	-1.58808517
6	-2.92595291	-0.84758025	-0.93548512
8	-2.82685304	-2.16968036	-0.61978513
6	-4.32925320	-0.42278028	-1.32868516
6	-3.78425312	-2.69838023	0.30561486
8	-5.33875322	-0.89438027	-0.41558510
6	-5.12715292	-1.98078036	0.35601485
1	3.55864692	-2.16208029	2.11891484
1	2.85064697	-3.19558024	3.39021468
8	-5.99645281	-2.35608029	1.10871482
8	3.53634691	-5.09578037	1.79141486
6	-3.96475291	-4.17778015	-0.00258514
6	-4.64675283	-0.88928026	-2.74378514
1	-4.00915289	1.64681983	3.26041484
1	-3.91295314	-0.11938028	3.10051465
1	-2.42355299	0.83191973	3.23601484
1	-4.39135313	0.66661972	-1.28628516
1	-3.36315298	-2.57338023	1.30851483
1	-5.66125298	-0.58138025	-3.00798535
1	-3.93965292	-0.44268030	-3.44568515
1	-4.57675314	-1.97718024	-2.82238531
1	-4.63335323	-4.62858057	0.73211485
1	-4.38505316	-4.32258034	-1.00128508
1	-2.99425292	-4.67748022	0.04081486

I-2c__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1745899.3 (Joules/Mol)
	417.27996 (Kcal/Mol)
Zero-point correction =	0.664978 (Hartree/Particle)
Thermal correction to Energy =	0.709735
Thermal correction to Enthalpy =	0.710680
Thermal correction to Gibbs Free Energy =	0.584322
Sum of electronic and zero-point Energies =	-2192.738861
Sum of electronic and thermal Energies =	-2192.694104
Sum of electronic and thermal Enthalpies =	-2192.693160
Sum of electronic and thermal Free Energies =	-2192.819517



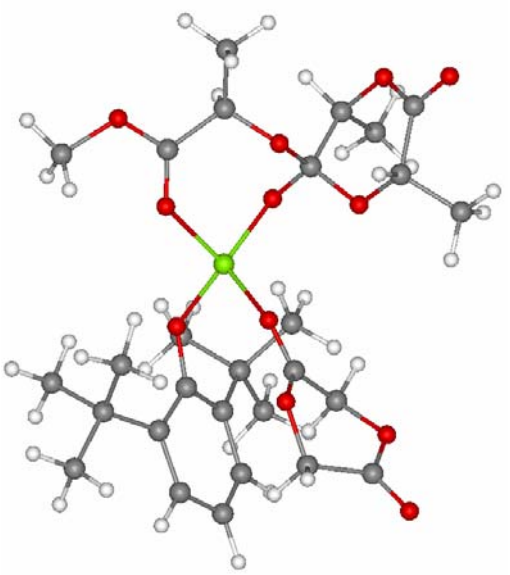
cartesian

8	0.84022111	0.76580238	-1.10614336
6	2.06202102	0.24940234	-1.12224340
6	2.33712101	-0.96099770	-1.84324336
6	3.57912111	-1.57619774	-1.65064335
1	3.80002093	-2.51409745	-2.14924335
6	4.56522131	-1.02039766	-0.83694339
6	4.35102129	0.24360234	-0.28994340
1	5.17162132	0.71680236	0.24075660
6	3.13762116	0.92430234	-0.44784337
6	1.33672106	-1.55099773	-2.85824347
6	3.02112103	2.40200233	-0.01514339
6	0.08532110	-2.13269758	-2.17534328
1	-0.54277891	-1.36389768	-1.72324336
1	-0.54587889	-2.64819765	-2.90764332
1	0.36032110	-2.86679769	-1.40924335
6	0.91872114	-0.46109766	-3.86724329
1	0.45882112	0.39250234	-3.36724329
1	1.78992105	-0.10359766	-4.42694330
1	0.20052110	-0.87069762	-4.58724356
6	1.96272111	-2.69749761	-3.67364335
1	2.87622094	-2.38439751	-4.18974352
1	2.19562101	-3.57419753	-3.05914330
1	1.24962103	-3.02429748	-4.43784332
6	4.37712145	2.97550249	0.43305659
1	4.75232124	2.50480247	1.34895658
1	5.14392138	2.87950253	-0.34224337
1	4.26102114	4.04320240	0.64875662
6	2.55842113	3.24060249	-1.22584343
1	1.58952105	2.90020251	-1.59484339
1	2.47672105	4.29730225	-0.94224334
1	3.28282094	3.16840243	-2.04414344
6	2.04282117	2.61080241	1.15385664
1	2.32952094	2.02190232	2.03075647
1	2.03802109	3.66610241	1.45435667
1	1.02242100	2.34830236	0.87935662
8	-3.36027884	0.58940232	1.51505661
6	-3.71957898	1.89620221	1.16375661
6	-4.16037893	2.60780239	2.44815660
6	-2.57687902	2.68740249	0.53085661
8	-2.45497894	-0.16469766	-0.48414338
12	-0.69537890	0.45780233	-0.02184340
1	5.51672125	-1.52809775	-0.69924337
8	-2.98027897	3.86520267	0.08755660
8	-1.39907897	2.33630252	0.46285659
6	-1.97617900	4.71640205	-0.51174337
1	-2.51047897	5.61340237	-0.81734335
1	-1.52937889	4.21760225	-1.37234342
1	-1.20347893	4.95380211	0.22015660
1	-4.54427862	1.92730224	0.44005662
1	-4.46797848	3.63590240	2.24735665
1	-4.99987888	2.05960250	2.87955666
1	-3.34477901	2.60740232	3.17575669
8	-3.07827902	-1.56909764	1.24595666
6	-3.35757899	-0.41159767	0.46005660
6	-4.77597857	-0.61049765	-0.12294339
8	-4.79757881	-1.80959773	-0.93164337
6	-3.98207903	-2.85029769	-0.67684340
6	-2.95047903	-2.73459768	0.44315660
6	-3.00767899	-3.94269753	1.36645663
1	-1.98487890	-2.72139764	-0.07984339
8	-4.05247879	-3.84749746	-1.36144340
1	-2.87277889	-4.85979795	0.79115659
1	-2.21617889	-3.86469746	2.11645651
1	-3.96867895	-3.98819757	1.88555658
6	-5.89097881	-0.69529772	0.90575659
1	-4.97747850	0.18140233	-0.84984338
1	-6.81837893	-0.99779761	0.41185659
1	-5.64697886	-1.42209768	1.68405664
1	-6.06117868	0.27130234	1.38685668
6	3.19622111	-0.84259760	3.35035658
8	1.87542105	-0.39449766	2.97885656
6	1.30382109	-1.01539767	1.95655656
6	1.97082114	-2.27809763	1.47965658
8	2.55822110	-3.03219748	2.54845667
6	3.30882096	-2.35129762	3.44105673
8	0.27202111	-0.57229769	1.47295666
1	3.91592097	-0.45769766	2.61965656
1	3.39832115	-0.40859765	4.32635641
1	1.22852111	-2.92399764	1.01645660
1	2.72862101	-2.01859760	0.72645664
8	4.00382137	-2.91199756	4.24755669

I-2c__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1746082.2 (Joules/Mol)
	417.32367 (Kcal/Mol)
Zero-point correction =	0.665048 (Hartree/Particle)
Thermal correction to Energy =	0.709698

Thermal correction to Enthalpy =	0.710643
Thermal correction to Gibbs Free Energy =	0.583946
Sum of electronic and zero-point Energies =	-2192.746538
Sum of electronic and thermal Energies =	-2192.701887
Sum of electronic and thermal Enthalpies =	-2192.700943
Sum of electronic and thermal Free Energies =	-2192.827640

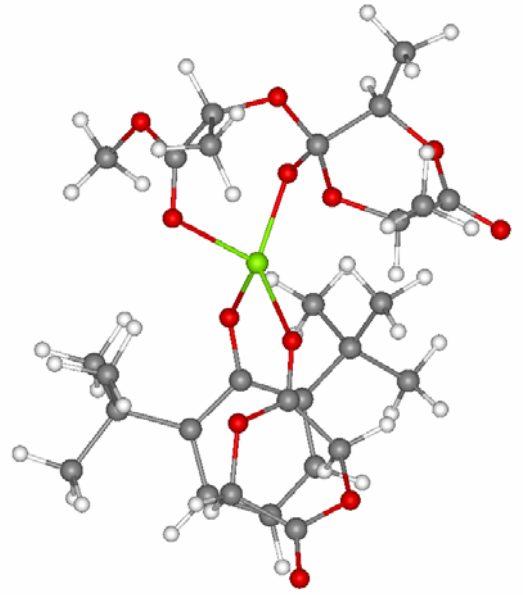


cartesian

8	1.10217416	1.19233334	-0.70712709
6	2.27817392	0.57333326	-0.70572710
6	3.21487403	0.80863327	0.35847288
6	4.31547403	-0.05006672	0.47047287
1	5.01987410	0.07933326	1.28647292
6	4.57187414	-1.04916668	-0.46762711
6	3.77037406	-1.12176669	-1.60522711
1	4.04427433	-1.83116663	-2.37892723
6	2.64507389	-0.30726671	-1.77772713
6	3.10057402	2.04403329	1.27867293
6	1.87097418	-0.34566674	-3.11202717
6	1.89587414	1.98833334	2.23467278
1	0.95007408	2.04623318	1.69747293
1	1.93037403	2.84123325	2.92427278
1	1.89757407	1.07633328	2.83917284
6	2.98907399	3.30563331	0.39617288
1	2.11377406	3.25643325	-0.25422716
1	3.87897420	3.41793323	-0.23232715
1	2.90747404	4.20023298	1.02607286
6	4.35427427	2.21723318	2.15507293
1	5.27067423	2.27983308	1.55947292
1	4.47207403	1.40833330	2.88517284
1	4.26867437	3.14983320	2.72327280
6	2.66467404	-1.08846676	-4.20422697
1	2.76757407	-2.15976667	-3.99972701
1	3.66517401	-0.66606671	-4.34422684
1	2.13127398	-0.99786675	-5.15652704
6	1.64367414	1.08813334	-3.63402724
1	1.07277417	1.69013333	-2.92682719
1	1.10027409	1.05763328	-4.58592701
1	2.60277390	1.58683336	-3.81222701
6	0.52247405	-1.07516670	-2.97362733
1	0.66727412	-2.10006666	-2.61202717
1	0.02807409	-1.14396667	-3.95022702
1	-0.17672589	-0.56716675	-2.30832720
6	2.54057407	-2.48916674	3.02877283
8	1.40897417	-1.60766673	2.86937284
6	0.87797415	-1.53686666	1.65637290
6	1.31767416	-2.58076692	0.66397285
8	1.58117414	-3.85066676	1.27547288
6	2.32687402	-3.85196686	2.40137267
8	0.05247411	-0.66896671	1.41267288
1	0.51807415	-2.74556684	-0.05552714
1	2.20687389	-2.21686673	0.13027287
12	-0.59222591	0.65463328	-0.02512714
8	-3.54802608	0.35733324	0.77517289
6	-3.85192609	1.71413326	0.57057285
6	-2.66972589	2.57233310	1.02097285
8	-3.00902605	3.77893305	1.43267286
6	-1.93122590	4.66983318	1.80137289
6	-5.16232586	2.06253314	1.26907289
1	-3.93512607	1.94093335	-0.50342715
8	-1.49042583	2.21463323	0.97867286
1	-1.36712587	4.24663305	2.63307285
1	-2.41812611	5.59753323	2.09437275
1	-1.26962590	4.82933331	0.94917285
1	5.43337440	-1.70326674	-0.35742712
8	-2.13742590	0.14293326	-1.05702710
6	-3.14712596	-0.41626674	-0.42032713
8	-2.77542591	-1.67016673	0.12817286
6	-4.36572552	-0.63966674	-1.33032715
6	-3.78492594	-2.31296682	0.90697289
8	-5.45372581	-1.27186668	-0.61672711
6	-5.21752596	-2.09326673	0.42397285
1	3.42327404	-2.01026678	2.59147286
1	2.68217397	-2.60666680	4.10017300
8	-6.14712572	-2.62446690	0.99087286
8	2.77357411	-4.86756659	2.86727285
6	-3.45732594	-3.79846692	0.96367288
6	-4.02132607	-1.44366670	-2.57142735
1	-5.43612576	3.10783315	1.11307287
1	-5.94932556	1.42273331	0.86497289
1	-5.08692598	1.87343323	2.34267282
1	-4.77552557	0.32843328	-1.63272715
1	-3.77122593	-1.89836669	1.92247283
1	-4.92172575	-1.60086668	-3.17122722
1	-3.28202605	-0.90306675	-3.16502714
1	-3.60302591	-2.41616678	-2.30022717
1	-4.18782568	-4.31766701	1.58607292
1	-3.46722603	-4.23816681	-0.03742714
1	-2.46142602	-3.93716669	1.39267290

TS-23c__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1745380.6 (Joules/Mol)
	417.15598 (Kcal/Mol)
Zero-point correction =	0.664780 (Hartree/Particle)
Thermal correction to Energy =	0.708677
Thermal correction to Enthalpy =	0.709621
Thermal correction to Gibbs Free Energy =	0.586579
Sum of electronic and zero-point Energies =	-2192.724864
Sum of electronic and thermal Energies =	-2192.680967
Sum of electronic and thermal Enthalpies =	-2192.680023
Sum of electronic and thermal Free Energies =	-2192.803066



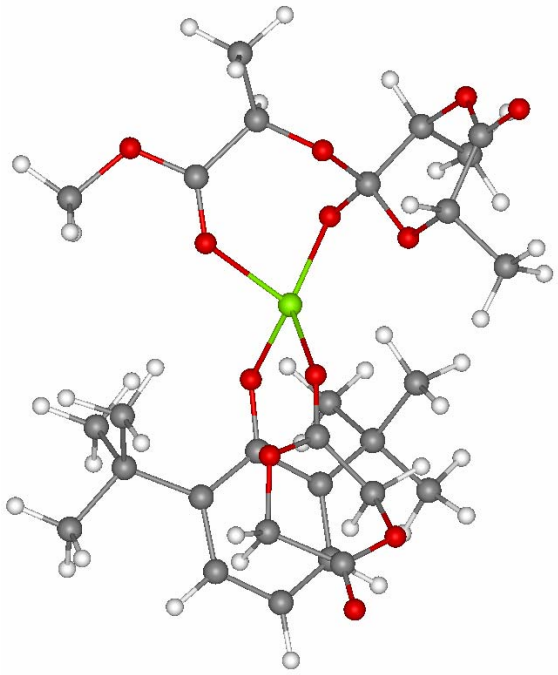
cartesian

8	-4.33981180	0.83850628	0.84513080
6	-3.75231218	1.78600621	1.72733080
6	-2.49981213	2.45280623	1.14673090
8	-2.56401229	0.61500621	-0.61266911
12	-0.78391212	0.45760626	0.16883086
8	-2.77591228	3.56030631	0.49123085
8	-1.33881211	2.07490635	1.36363077
6	-1.66711211	4.23310614	-0.14576915
1	-2.09911203	5.11840630	-0.60776913
1	-1.22771204	3.57900620	-0.90006924
1	-0.91541213	4.50560617	0.59573084
8	-2.83201218	-0.92009377	1.02863085
6	-3.50351214	-0.02649379	0.07403085
6	-4.50051212	-0.78249377	-0.83126915
8	-3.88631225	-1.97309387	-1.37366915
6	-3.22861218	-2.81379366	-0.56306911
6	-2.80711222	-2.33549380	0.82123089
6	-3.55201221	-3.07499361	1.93223083
1	-1.75491202	-2.63049364	0.88323081
8	-2.92901230	-3.92569375	-0.94066918
1	-3.43111229	-4.15319395	1.80193079
1	-3.13061213	-2.78579378	2.89823079
1	-4.61771202	-2.83899379	1.94043088
6	-5.86531210	-1.11599386	-0.25136915
1	-4.62481213	-0.14039379	-1.70396912
1	-6.41891193	-1.72219384	-0.97386920
1	-5.80031204	-1.66789389	0.68813086
1	-6.42241192	-0.19749379	-0.06156915
6	-3.47511220	1.22810614	3.11823082
1	-4.50421190	2.57680631	1.79683077
1	-3.18991208	2.03650618	3.79993081
1	-4.38811207	0.76260620	3.49653077
1	-2.68121219	0.48220623	3.10313082
8	0.74008787	1.00220621	-0.85816920
6	1.93128788	0.46220624	-1.06836915
6	3.08648777	0.97400624	-0.38076916
6	4.28178787	0.24930622	-0.46326914
1	5.16288805	0.59690624	0.06743085
6	4.39938784	-0.89529377	-1.25026917
6	3.32438779	-1.27189386	-2.05446911
1	3.46388793	-2.10839367	-2.73086929
6	2.09448791	-0.60599381	-2.01416922
6	3.06538773	2.35270619	0.31293085
6	0.98808783	-0.97089380	-3.02506924
6	2.14388776	2.39890623	1.54393077
1	1.10328794	2.21930623	1.28063083
1	2.19978786	3.38830638	2.01463079
1	2.44308782	1.66350615	2.29753089
6	2.59858775	3.40650630	-0.71396911
1	1.59848797	3.17570639	-1.08456922
1	3.28158784	3.44250631	-1.56946921
1	2.58228779	4.40210629	-0.25346914
6	4.46568823	2.77880621	0.78863084
1	5.19208813	2.80950618	-0.02986915
1	4.86078787	2.12490630	1.57493079
1	4.40878820	3.78720617	1.21243083
6	1.46288788	-2.03929377	-4.02626896
1	1.66628790	-3.00369382	-3.54696918
1	2.36008787	-1.72709382	-4.57046938
1	0.67538786	-2.20999360	-4.76746941
6	0.61548787	0.28350621	-3.84316921
1	0.26748791	1.08960617	-3.19476914
1	-0.18361211	0.04480621	-4.55506897
1	1.47928798	0.64320624	-4.41246939
6	-0.27941209	-1.53129387	-2.34926915
1	-0.03581210	-2.27509379	-1.58326924
1	-0.91901213	-2.02879381	-3.08586907
1	-0.89721215	-0.74179375	-1.91646910
6	3.22928786	-1.25009382	2.96093082
8	1.86478794	-0.87389380	2.67353082

6	1.31178796	-1.42559385	1.60463083
6	2.05768776	-2.57189369	0.97743082
8	2.73058772	-3.38709378	1.94713080
6	3.45568776	-2.74699378	2.89023089
8	0.22638792	-1.02549386	1.19903088
1	1.35698795	-3.22239375	0.45813084
1	2.77318788	-2.17299366	0.24283084
1	5.33958817	-1.43939388	-1.29666913
1	3.88958764	-0.73669380	2.25323081
1	3.43128777	-0.90239376	3.97073078
8	4.21248817	-3.33419371	3.61843085

TS-23c__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1744484.0 (Joules/Mol)
	416.94169 (Kcal/Mol)
Zero-point correction =	0.664439 (Hartree/Particle)
Thermal correction to Energy =	0.708449
Thermal correction to Enthalpy =	0.709393
Thermal correction to Gibbs Free Energy =	0.584842
Sum of electronic and zero-point Energies =	-2192.745934
Sum of electronic and thermal Energies =	-2192.701923
Sum of electronic and thermal Enthalpies =	-2192.700979
Sum of electronic and thermal Free Energies =	-2192.825530



cartesian

8	0.82245207	0.80170119	-0.98435318
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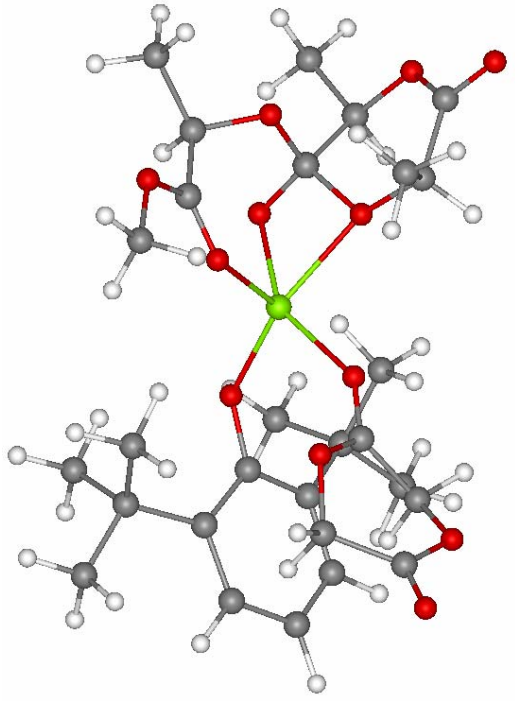
6	3.10795212	0.91480118	-0.27605316
6	4.31425190	0.21920118	-0.13245317
1	5.12625170	0.65790117	0.43924683
6	4.53285170	-1.01539874	-0.74185312
6	3.55995202	-1.52019882	-1.60375309
1	3.78555226	-2.43209887	-2.14625311
6	2.32525206	-0.88799882	-1.78575301
6	2.99015212	2.36640120	0.23544684
6	1.34635198	-1.40539885	-2.85995317
6	2.00075197	2.50590134	1.40474689
1	0.98715198	2.23430133	1.11474681
1	1.98115206	3.54610133	1.75434685
1	2.29425192	1.88240123	2.25534678
6	2.53915215	3.27290130	-0.92965317
1	1.57085204	2.95950127	-1.32335317
1	3.26755214	3.24240136	-1.74705315
1	2.46265197	4.31310081	-0.58875310
6	4.34285164	2.91130114	0.72844684
1	5.11715174	2.85850120	-0.04365316
1	4.70855188	2.38790131	1.61924684
1	4.22645187	3.96500134	1.00444686
6	1.96485209	-2.54769874	-3.68685317
1	2.13975215	-3.45089865	-3.09135318
1	2.90965199	-2.25439882	-4.15575314
1	1.27365208	-2.82209873	-4.49075317
6	1.01935208	-0.26129881	-3.84255290
1	0.58075202	0.59340119	-3.32495308
1	0.30815202	-0.60799885	-4.60185337
1	1.92595196	0.07350118	-4.35815334
6	0.03595202	-1.95449877	-2.26225305
1	0.22535200	-2.63409877	-1.42415309
1	-0.51364797	-2.52339864	-3.02125311
1	-0.64344800	-1.16409874	-1.93935323
6	3.02305198	-1.03419876	3.41924691
8	1.71025205	-0.58509880	3.02294683
6	1.19345200	-1.15179873	1.93964684
6	1.90845203	-2.37109876	1.41984689
8	2.44865203	-3.18179870	2.47344685
6	3.15005207	-2.54469872	3.43604684
8	0.16935201	-0.70299882	1.44614685
1	1.20455205	-2.99789882	0.87734687
1	2.70315194	-2.05769873	0.72794688
12	-0.78984797	0.37740117	-0.04675317
8	-3.75924802	0.50940120	0.90944684
6	-3.89804792	1.88640118	0.68624687
6	-2.57154799	2.59980130	0.95524681
8	-2.70854807	3.90440106	1.11884689
6	-1.49634802	4.66740084	1.31124687
6	-5.03214836	2.41370130	1.56264687
1	-4.11574793	2.09890127	-0.37045315
8	-1.46954799	2.05230117	1.00664687
1	-0.98474795	4.33250093	2.21414685

1	-1.82354796	5.70030117	1.41134691
1	-0.83874798	4.54920101	0.44934684
1	5.47875166	-1.53569889	-0.61315322
8	-2.48234797	0.31910118	-1.03225315
6	-3.33864808	-0.29969883	-0.24965313
8	-2.67984796	-1.41339874	0.36584684
6	-4.59114838	-0.81449884	-0.96505308
6	-3.45654798	-2.11429882	1.34164691
8	-5.43614817	-1.58189893	-0.07425317
6	-4.94224834	-2.22579885	0.99804688
1	3.76365209	-0.60359883	2.73634696
1	3.18375206	-0.64929879	4.42304659
8	-5.68504810	-2.86809874	1.70764685
8	3.81175208	-3.14289880	4.24374676
6	-2.84044790	-3.49129868	1.53694689
6	-4.26974821	-1.63549876	-2.19995308
1	-5.18904829	3.48280120	1.41014683
1	-5.94734812	1.87710118	1.30514681
1	-4.81764841	2.23330116	2.61914682
1	-5.20734835	0.04590118	-1.24305308
1	-3.42694807	-1.56019878	2.28714681
1	-5.19544840	-2.00349879	-2.65015316
1	-3.73864794	-1.01539874	-2.92445302
1	-3.63744807	-2.49029875	-1.94615316
1	-3.39924788	-4.04359865	2.29374695
1	-2.85164785	-4.05859900	0.60244685
1	-1.80424798	-3.38319874	1.86764681

I-3c__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1745241.8 (Joules/Mol)
	417.12280 (Kcal/Mol)
Zero-point correction =	0.664728 (Hartree/Particle)
Thermal correction to Energy =	0.709342
Thermal correction to Enthalpy =	0.710286
Thermal correction to Gibbs Free Energy =	0.584927
Sum of electronic and zero-point Energies =	-2192.748475
Sum of electronic and thermal Energies =	-2192.703861
Sum of electronic and thermal Enthalpies =	-2192.702916
Sum of electronic and thermal Free Energies =	-2192.828276



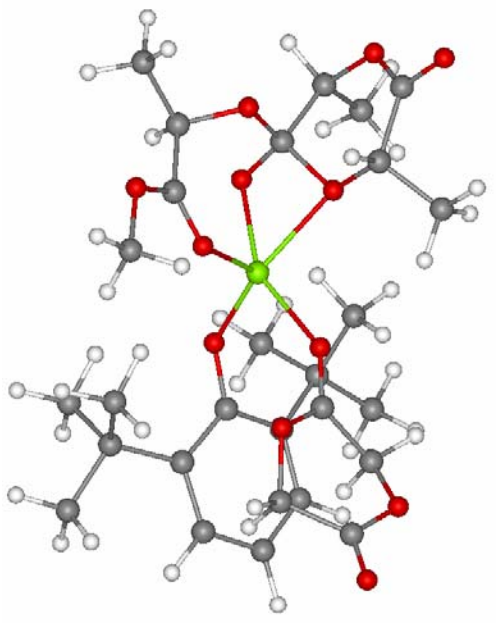
cartesian

8	0.76494312	0.53168780	1.11355686
6	2.02254319	0.81568778	0.82995683
6	3.06194305	-0.14041223	1.10315681
6	4.34314299	0.10998777	0.59785676
1	5.13994312	-0.60811222	0.76625675
6	4.65124321	1.28438783	-0.08834322
6	3.68154311	2.28278780	-0.18124323
1	3.96604300	3.22798777	-0.63184321
6	2.37794328	2.09908772	0.29185677
6	2.81584311	-1.34271216	2.03795695
6	1.39254320	3.28558779	0.33275676
6	1.83634305	-2.36861229	1.44275689
1	0.86464322	-1.92211223	1.23815680
1	1.69064319	-3.19531226	2.14995694
1	2.22114325	-2.79681230	0.51095676
6	2.25254321	-0.82021219	3.37725687
1	1.30884314	-0.29231223	3.23085690
1	2.96204329	-0.13341223	3.85105705
1	2.08224320	-1.65631223	4.06675673
6	4.11654329	-2.09891224	2.35945678
1	4.86844301	-1.45171225	2.82245684
1	4.56334305	-2.56541228	1.47365689
1	3.89764309	-2.90471220	3.06855679
6	2.02604318	4.56878757	-0.23374322
1	2.26764321	4.48018742	-1.29934323
1	2.93544316	4.85478735	0.30375677
1	1.31644320	5.39628744	-0.12934323
6	1.02504313	3.56478786	1.80605674
1	0.57244313	2.68608785	2.27035689
1	0.30894315	4.39328766	1.86885691
1	1.91534328	3.84298778	2.37985682
6	0.09384313	3.03688788	-0.46584320
1	0.28134313	2.51258779	-1.40864325
1	-0.38445687	3.99118781	-0.71574318
1	-0.64315689	2.48658776	0.12475678
6	3.17084312	-2.18861222	-2.31094313
8	1.79824317	-1.88271224	-1.98554325

6	1.43694317	-0.60881221	-2.09384322
6	2.40664315	0.30068776	-2.80084324
8	3.09114313	-0.35241222	-3.87944317
6	3.61734319	-1.56931221	-3.62034321
8	0.35474315	-0.23331222	-1.66694331
1	1.86434317	1.13598776	-3.23834324
1	3.12544322	0.69558781	-2.06794333
12	-0.79955685	0.11538778	0.08075678
8	-4.10265684	-0.54451221	0.16025677
6	-3.72825694	-1.44741225	1.18625689
6	-2.55245686	-2.31461215	0.72765678
8	-2.75075674	-3.61601210	0.84765679
6	-1.65975678	-4.47901249	0.45825678
6	-4.96315670	-2.23391223	1.59265685
1	-3.33385682	-0.87831223	2.03845692
8	-1.48805678	-1.86411226	0.29915679
1	-1.43365681	-4.33851242	-0.59954321
1	-2.01555681	-5.48991251	0.64725679
1	-0.77475691	-4.25861263	1.05575681
1	5.65434313	1.45248783	-0.47254324
8	-2.42895675	0.85658783	0.98105675
1	3.81214309	-1.84091222	-1.49304318
1	3.23014307	-3.27131224	-2.38804317
8	4.37324333	-2.11131215	-4.38424301
1	-4.73675680	-2.92831230	2.40475678
1	-5.72385693	-1.52991223	1.93605685
1	-5.36945677	-2.79991221	0.75165683
8	-2.49765682	0.48608777	-1.20854330
6	-3.30325675	0.65458781	0.02935678
6	-4.25195694	1.81868780	-0.25274321
8	-5.06275702	1.57798779	-1.43014312
6	-4.59095669	0.89488780	-2.48494315
6	-3.18005681	0.30148777	-2.45234323
1	-2.61335683	0.88428777	-3.18744326
6	-3.19765687	-1.15881217	-2.89304328
6	-5.19785690	2.11918783	0.88775676
1	-3.61325693	2.68388772	-0.45814323
8	-5.27665663	0.75938779	-3.47404313
1	-5.80885696	2.99308777	0.64805681
1	-4.62005663	2.32768774	1.79085684
1	-5.85915661	1.26908779	1.06865668
1	-3.61595678	-1.23381221	-3.89874315
1	-3.80595684	-1.76101220	-2.21544313
1	-2.17565680	-1.54621220	-2.89994311

I-3c__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1746100.9 (Joules/Mol)
	417.32813 (Kcal/Mol)
Zero-point correction =	0.665055 (Hartree/Particle)
Thermal correction to Energy =	0.709531
Thermal correction to Enthalpy =	0.710476
Thermal correction to Gibbs Free Energy =	0.585607
Sum of electronic and zero-point Energies =	-2192.748131
Sum of electronic and thermal Energies =	-2192.703654
Sum of electronic and thermal Enthalpies =	-2192.702710
Sum of electronic and thermal Free Energies =	-2192.827578



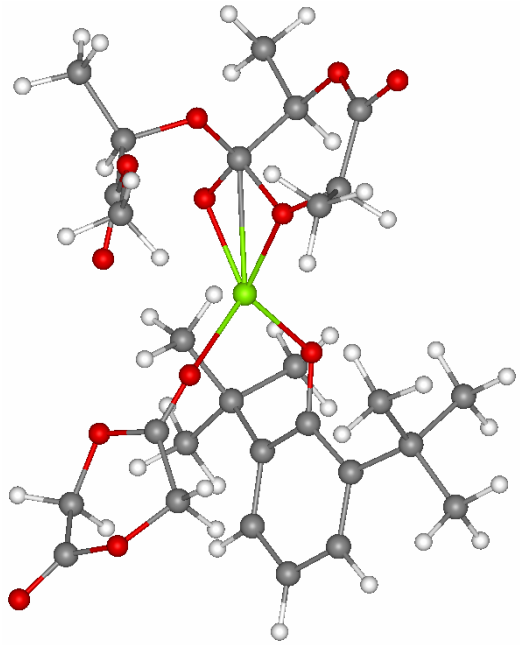
cartesian

12	0.90432960	0.01433833	0.15080622
8	-0.67747039	-0.26706165	1.20790625
6	-1.93027031	-0.59766167	0.95670617
6	-2.97667027	0.38323832	1.06830621
6	-4.24877071	0.05333833	0.58620620
1	-5.05007029	0.78473830	0.63140619
6	-4.54457045	-1.21376157	0.08470622
6	-3.57247019	-2.21096158	0.16320622
1	-3.84897017	-3.21596169	-0.13789378
6	-2.27627039	-1.95086169	0.61990619
6	-2.75287032	1.70813835	1.82630610
6	-1.29487038	-3.11406159	0.86860621
6	-1.76697040	2.64723825	1.11080623
1	-0.78467035	2.18913841	1.00660622
1	-1.65307045	3.57423830	1.68770623
1	-2.12577033	2.92143846	0.11280620
6	-2.21047020	1.38353837	3.23480630
1	-1.25887036	0.85223830	3.17920613
1	-2.92177033	0.76043832	3.78730607
1	-2.06117034	2.30913830	3.80420613
6	-4.06347036	2.49123836	2.01670623
1	-4.82077074	1.90663838	2.54880619
1	-4.49567032	2.82973838	1.06760621

1	-3.86357045	3.38723826	2.61430621
6	-1.91477048	-4.47326183	0.49840623
1	-2.13327026	-4.55656195	-0.57269382
1	-2.83527017	-4.67606163	1.05460620
1	-1.20637035	-5.27036190	0.74760616
6	-0.95897043	-3.15466166	2.37480617
1	-0.50897038	-2.21486163	2.70190620
1	-0.25127035	-3.96606183	2.58460617
1	-1.86247051	-3.33256173	2.96740627
6	0.02142961	-2.99426174	0.07060620
1	-0.14537038	-2.66686153	-0.96079379
1	0.52442962	-3.96716142	0.02580622
1	0.72832960	-2.32226157	0.56290621
8	2.71862984	-0.54966170	-0.97039378
6	3.43172979	-0.39536166	0.32020622
6	4.51812935	-1.47396159	0.34270620
8	5.36682940	-1.39806163	-0.83069378
6	4.93432951	-0.92166167	-2.00879383
6	3.51412964	-0.36736166	-2.14409375
8	2.51132965	-0.46766168	1.24460626
1	3.64592981	0.70623833	-2.32449389
6	2.79582977	-1.00176167	-3.32499385
6	-3.01717019	1.86183834	-2.64579368
8	-1.65497041	1.61023831	-2.24049377
6	-1.29667044	0.33493835	-2.13729382
6	-2.26007032	-0.67356169	-2.70399380
8	-2.91167021	-0.20436166	-3.89349389
6	-3.43447018	1.04033840	-3.84959388
8	-0.22247039	0.03133833	-1.63899374
1	-3.68117023	1.65183842	-1.79969382
1	-3.06837034	2.91793847	-2.89789367
6	3.96702981	-2.87876153	0.48230624
1	5.19032955	-1.24586165	1.17300618
1	-1.71887040	-1.57536161	-2.98089385
1	-3.00087023	-0.93196172	-1.93309379
8	-4.16587067	1.45443833	-4.71129417
8	4.13532972	0.87583834	0.23740619
6	3.66402984	1.92363834	1.06410623
6	2.49052978	2.62173843	0.37650621
8	2.61262965	3.93163848	0.25910622
6	1.51912963	4.63293791	-0.37349379
6	4.83502960	2.83553839	1.38940620
1	3.23792982	1.49633837	1.98180628
8	1.49192965	2.02743840	-0.03679380
1	1.39502954	4.28033829	-1.39829373
1	1.80702960	5.68223810	-0.35699379
1	0.59682959	4.47163820	0.18500620
1	-5.54127073	-1.44286168	-0.28419378
8	5.68102932	-0.90106171	-2.96279383
1	4.52562952	3.65383840	2.04350615
1	5.59972954	2.24723840	1.90070629
1	5.27262926	3.25843835	0.48250622
1	4.79012966	-3.59806156	0.48060620
1	3.41762972	-2.96616173	1.42180622
1	3.29052973	-3.11896157	-0.34179378
1	3.38512969	-0.85926169	-4.23209381
1	2.65232968	-2.07316160	-3.16109371
1	1.81722963	-0.53386170	-3.45399380

TS-33__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1745243.8 (Joules/Mol)
	417.12329 (Kcal/Mol)
Zero-point correction =	0.664728 (Hartree/Particle)
Thermal correction to Energy =	0.708807
Thermal correction to Enthalpy =	0.709751
Thermal correction to Gibbs Free Energy =	0.585014
Sum of electronic and zero-point Energies =	-2192.734647
Sum of electronic and thermal Energies =	-2192.690569
Sum of electronic and thermal Enthalpies =	-2192.689625
Sum of electronic and thermal Free Energies =	-2192.814362



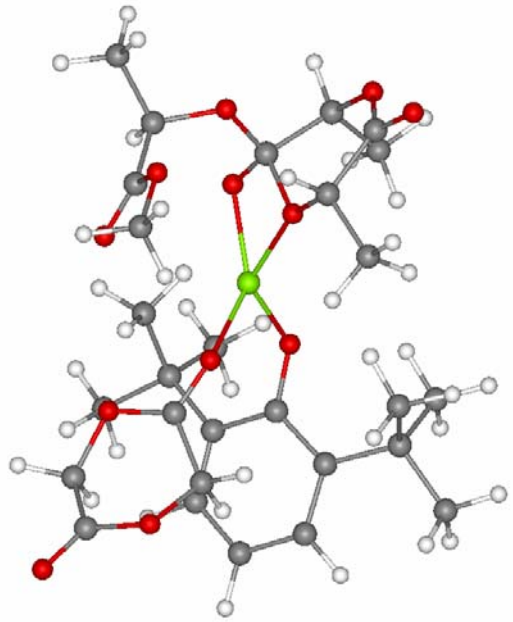
cartesian

8	0.83821988	-1.45918262	-0.36050120
6	2.13141990	-1.29438269	-0.10200121
6	3.01951981	-0.86668265	-1.14330125
6	4.33402014	-0.53018266	-0.79560119
1	5.02462006	-0.18368265	-1.55840123
6	4.81042004	-0.66588265	0.50749880
6	3.97871995	-1.22518265	1.47649872
1	4.39062023	-1.39968264	2.46509862
6	2.64971972	-1.56908262	1.20529878
6	2.58931971	-0.90998268	-2.62540126
6	1.79821992	-2.28218269	2.27409863
6	1.35671997	-0.03618264	-2.94690132
1	0.42231989	-0.53078264	-2.67270136
1	1.28761983	0.13591737	-4.02720118
1	1.41031981	0.95081735	-2.47510123
6	2.26481986	-2.37518263	-2.98850131
1	1.46881986	-2.76778269	-2.35190129
1	3.14871979	-3.00998259	-2.86740136
1	1.93761992	-2.44478273	-4.03310108
6	3.71891975	-0.44388264	-3.56070137
1	4.62412024	-1.04928267	-3.45390129
1	3.98641992	0.60791737	-3.40240121
1	3.38911986	-0.54018265	-4.60020113
6	2.61951971	-2.63068271	3.52759862
1	2.98081970	-1.74098265	4.05519915
1	3.48011971	-3.26528263	3.29289865
1	1.98731971	-3.18528271	4.22909880
6	1.26021981	-3.61028266	1.70139873
1	0.65001988	-3.44278264	0.81239879
1	0.65121990	-4.12708282	2.45289874
1	2.08821988	-4.27308273	1.42849874
6	0.62151986	-1.40748262	2.74499869
1	0.97231990	-0.45298266	3.15229869
1	0.06081988	-1.91888261	3.53659868
1	-0.07308012	-1.19958270	1.93009877
6	3.30201983	3.20371747	-0.75040120
8	1.95681977	2.67961740	-0.71680123
6	1.59471989	2.02891731	0.37649879
6	2.51261973	2.12431741	1.56349874
8	3.18191981	3.38551736	1.66349876
6	3.71181989	3.89971733	0.53179878
8	0.55331987	1.38811731	0.40339878
1	1.93161988	2.00551748	2.47539878
1	3.23811984	1.30021739	1.49709868
12	-0.50228012	-0.11698264	-0.47390121
8	-4.01507998	0.77331734	-0.82990122
6	-3.68478012	2.13841724	-1.10620129
6	-3.17318010	2.84021735	0.15419878
8	-4.15077972	3.06541729	1.04879868
6	-3.75048018	3.74851727	2.24669862
6	-4.92677975	2.80361748	-1.67640126
1	-2.86038017	2.16581726	-1.82040131
8	-2.01658010	3.17451739	0.32569879
1	-2.98768020	3.17641735	2.77849865
1	-4.65337992	3.83471727	2.84959865
1	-3.35438013	4.73751736	2.00589871
1	5.83771992	-0.40318263	0.74839878
8	-1.96468019	0.14991736	-1.73620129
1	3.99061990	2.37921739	-0.96410120
1	3.32461977	3.92011738	-1.56770122
8	4.45382023	4.84631729	0.55299878
1	-4.73767996	3.86361742	-1.87170124
1	-5.19327974	2.32081747	-2.61980128
1	-5.76698017	2.71971726	-0.98460120
8	-2.37888026	-0.45118266	0.37789878
6	-2.99788022	-0.18458265	-0.99060124
6	-3.66108012	-1.50858259	-1.38100123
8	-4.66767979	-1.90238261	-0.42170122
6	-4.46227980	-1.73548269	0.89399880
6	-3.15618014	-1.10748267	1.39259875
1	-2.55458021	-1.95568275	1.74249876
6	-3.42118025	-0.16478264	2.55709863
6	-4.33328009	-1.45888269	-2.73530126
1	-2.86938024	-2.26658273	-1.37700129
8	-5.28898001	-2.11968255	1.68979871
1	-4.74497986	-2.44028258	-2.98330116
1	-3.60068011	-1.17838264	-3.49500132
1	-5.14408016	-0.72778267	-2.72790122
1	-3.92268014	-0.70158267	3.36409879
1	-4.05607986	0.66351736	2.23679876
1	-2.47088027	0.23001736	2.92589879

TS-33__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1744870.8 (Joules/Mol)
	417.03414 (Kcal/Mol)
Zero-point correction =	0.664586 (Hartree/Particle)

Thermal correction to Energy =	0.708642
Thermal correction to Enthalpy =	0.709586
Thermal correction to Gibbs Free Energy =	0.585716
Sum of electronic and zero-point Energies =	-2192.734304
Sum of electronic and thermal Energies =	-2192.690248
Sum of electronic and thermal Enthalpies =	-2192.689304
Sum of electronic and thermal Free Energies =	-2192.813174



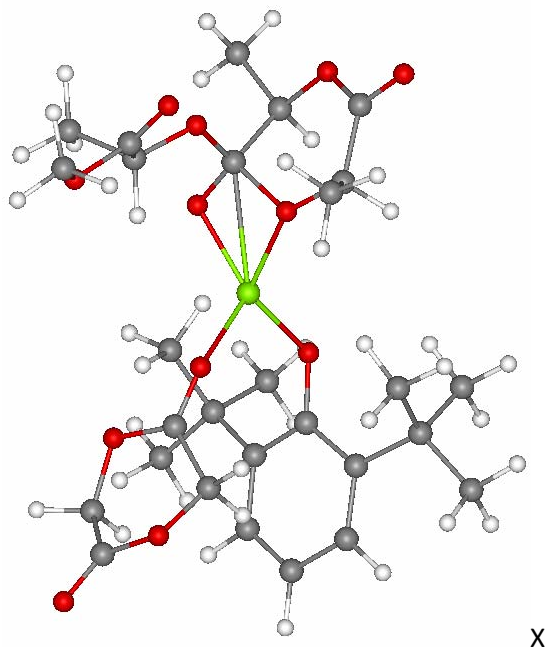
cartesian

8	0.75613952	-1.31324935	-0.68757528
6	2.04633951	-1.12144935	-0.44517529
6	2.83003950	-0.31694937	-1.33777523
6	4.13823938	0.01135060	-0.95827526
1	4.75113964	0.63255060	-1.60427523
6	4.71013927	-0.47704941	0.21552473
6	3.98903942	-1.38264942	0.99272472
1	4.48003960	-1.81894934	1.85642481
6	2.67293954	-1.74304938	0.68422472
6	2.31393957	0.04095061	-2.74837542
6	1.95113945	-2.82914925	1.50382471
6	0.96693945	0.79955059	-2.75957537
1	0.11703953	0.11585061	-2.69717526
1	0.83733952	1.32965064	-3.70987535
1	0.90933955	1.56305063	-1.97567534
6	2.13923955	-1.27684939	-3.53427529
1	1.43133950	-1.93894947	-3.03037524
1	3.09533954	-1.80144942	-3.63067532
1	1.76063955	-1.07164943	-4.54297495
6	3.32283950	0.90885061	-3.52127528
1	4.29133940	0.41415060	-3.64157534
1	3.48923945	1.88225055	-3.04447532
1	2.93613958	1.10275054	-4.52697515
6	2.87633944	-3.47254944	2.55082464
1	3.20623946	-2.76014948	3.31522465
1	3.76313949	-3.92424917	2.09442472
1	2.33363962	-4.27054930	3.06872463
6	1.47953951	-3.95634937	0.56102473
1	0.80153954	-3.57744932	-0.20507526
1	0.96073949	-4.73394918	1.13442469
1	2.33583951	-4.42294931	0.06242474
6	0.74393952	-2.25474930	2.26652479
1	1.05163956	-1.45944941	2.95522475
1	0.26263952	-3.03874922	2.86322474
1	-0.00336047	-1.85064948	1.58282471
8	-2.59126043	-0.28294939	0.47832474
6	-3.22306061	-0.25384939	-0.89467525
6	-3.97196054	-1.58714938	-1.02047515
8	-4.89806032	-1.79514945	0.07402474
6	-4.68476057	-1.31354940	1.30872464
6	-3.51016045	-0.37084937	1.57542467
8	-2.20516038	-0.09054938	-1.71287537
1	-3.96936059	0.61435062	1.71262479
6	-2.75686049	-0.76964939	2.83242464
6	2.91263962	3.35105038	0.20102474
8	1.59253955	2.77445078	0.09742474
6	1.28703952	1.82295060	0.96072471
6	2.23873949	1.61585057	2.10752463
8	2.83313942	2.83535051	2.56602478
6	3.31103945	3.68125057	1.62512469
8	0.26223955	1.16275060	0.82742476
1	3.63103962	2.64925051	-0.23637527
1	2.88673949	4.26585054	-0.38567525
6	-3.05176044	-2.78674936	-1.13987517
1	-4.61346054	-1.51454937	-1.90147519
1	1.69973946	1.19285059	2.95242476
1	3.01023960	0.89965063	1.78822470
8	3.99693966	4.62625074	1.91332483
8	-4.21036053	0.75755060	-0.90047526
6	-3.79416060	2.05305052	-1.32847524
6	-3.05246043	2.81135082	-0.22657526
8	-3.80706048	2.98535061	0.87392473
6	-3.19356060	3.73465061	1.93452477
6	-5.04166031	2.80325079	-1.77127528
1	-3.08466053	1.95145059	-2.15167522
8	-1.91826046	3.23695040	-0.33607525
1	-2.29356050	3.22865057	2.29052472
1	-3.94046044	3.78805065	2.72522473
1	-2.92836046	4.73625088	1.58952475
1	5.72993946	-0.21154940	0.48322475
8	-5.45676041	-1.58094943	2.20322466
1	-4.78306055	3.81305075	-2.10347533
1	-5.50336027	2.27075052	-2.60627532
1	-5.76286030	2.87325048	-0.95457524
1	-3.64976048	-3.69834948	-1.21637535
1	-2.43096042	-2.69444942	-2.03297544
1	-2.39936042	-2.87954950	-0.26647526
1	-3.44596052	-0.78424942	3.67822456
1	-2.31226039	-1.76204932	2.72882462
1	-1.96096051	-0.04734939	3.03242469

12 -0.69406044 -0.09974939 -0.48047525

I-3o__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1744565.1 (Joules/Mol)
	416.96107 (Kcal/Mol)
Zero-point correction =	0.664470 (Hartree/Particle)
Thermal correction to Energy =	0.709461
Thermal correction to Enthalpy =	0.710405
Thermal correction to Gibbs Free Energy =	0.582557
Sum of electronic and zero-point Energies =	-2192.734587
Sum of electronic and thermal Energies =	-2192.689596
Sum of electronic and thermal Enthalpies =	-2192.688652
Sum of electronic and thermal Free Energies =	-2192.816500



X

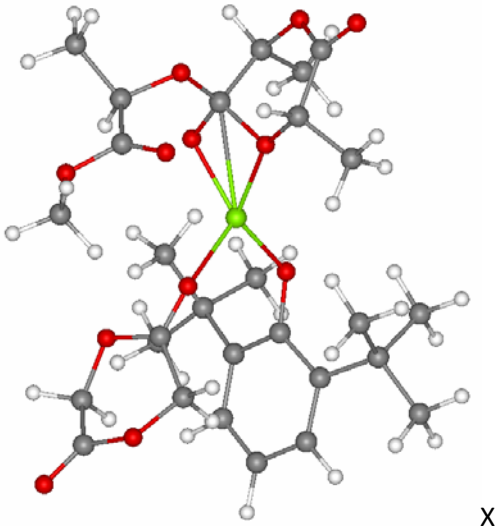
cartesian

8	1.04428279	-1.48061717	-0.38771600
6	2.30828285	-1.16281724	-0.12891598
6	3.11228275	-0.54821730	-1.14491606
6	4.38088274	-0.07311724	-0.78711599
1	5.00788260	0.41118276	-1.52941597
6	4.89758301	-0.24401726	0.49628401
6	4.16258287	-0.97261721	1.43048394
1	4.61278296	-1.16551721	2.39848399
6	2.88138270	-1.46011722	1.15008402
6	2.66598272	-0.54701728	-2.62301612
6	2.14188290	-2.34141731	2.17538404
6	1.30308282	0.13738275	-2.87041593
1	0.46588284	-0.53371727	-2.66471601
1	1.20038283	0.40868276	-3.92701626
1	1.19228280	1.06638277	-2.30061603
6	2.57278275	-2.01561713	-3.09181595
1	1.85938287	-2.57581711	-2.48281598
1	3.54788280	-2.50821710	-3.02101612
1	2.24478269	-2.06191730	-4.13731623
6	3.68908286	0.16198274	-3.52831602
1	4.67848301	-0.30291724	-3.48471594
1	3.79668283	1.22588277	-3.28491592
1	3.35348272	0.10158274	-4.56861591
6	3.02198267	-2.67301726	3.39328408
1	3.28908277	-1.78401721	3.97538400
1	3.94488287	-3.18751717	3.10628390
1	2.47078276	-3.34131718	4.06308413
6	1.75298274	-3.68291712	1.51918399
1	1.10058284	-3.53181720	0.65808403
1	1.23438275	-4.32111740	2.24458408
1	2.64728284	-4.21761751	1.18218398
6	0.88008291	-1.64371717	2.71718407
1	1.13018274	-0.69751728	3.21018386
1	0.38308287	-2.27951717	3.45918393
1	0.16098283	-1.43951726	1.92258394
6	2.98778272	3.42858291	-0.43391597
8	1.68188274	2.81038284	-0.49091595
6	1.34518278	2.02968264	0.52158403
6	2.22758269	2.07408261	1.73818398
8	2.78418279	3.37088275	1.97908401
6	3.30698276	4.02908278	0.92028403
8	0.33948284	1.33078277	0.45378405
1	1.63978279	1.81788278	2.61708403
1	3.02168274	1.32308280	1.61528397
12	-0.45931715	-0.33161730	-0.46401596
8	-4.01821709	0.39338273	-0.64111596
6	-3.70911717	1.78068280	-0.65731597
6	-4.51721716	2.45608282	0.44498402
8	-4.15911722	3.75638270	0.53898400
6	-4.87571716	4.51718235	1.52468395
6	-4.02031708	2.38468289	-2.02661610
1	-2.65081716	1.94098282	-0.42801595
8	-5.35831738	1.93868279	1.14338398
1	-5.94541740	4.51548243	1.30588400
1	-4.47431707	5.52788258	1.46198392
1	-4.71391726	4.10148287	2.52148390
1	5.88888264	0.12718275	0.74448401
8	-1.97251725	-0.03731725	-1.65061605
1	3.73758268	2.67488289	-0.69701594
1	2.97918272	4.21648264	-1.18281603
8	3.97018290	5.02298260	1.05568397
1	-3.80531716	3.45598269	-2.03551602
1	-3.40131712	1.88788283	-2.77561593
1	-5.07391739	2.23158288	-2.27661610

8	-2.26301718	-0.80551726	0.42818403
6	-2.96441722	-0.48321724	-0.89681596
6	-3.55951715	-1.81861711	-1.34861600
8	-4.46271706	-2.37111712	-0.36661595
6	-4.19971704	-2.29411721	0.94868404
6	-2.97631717	-1.52241719	1.45028400
1	-2.28851724	-2.29541731	1.81188393
6	-3.35181713	-0.60321724	2.60498405
6	-4.32851744	-1.71371722	-2.64781594
1	-2.71671724	-2.51021719	-1.46131599
8	-4.91741705	-2.85831714	1.74238396
1	-4.68641710	-2.70141721	-2.94871593
1	-3.67411733	-1.32001722	-3.42861605
1	-5.18521738	-1.04841721	-2.52561593
1	-3.78681731	-1.19111717	3.41538405
1	-4.07871723	0.14448275	2.28368402
1	-2.45181727	-0.10281725	2.97338390

I-3o__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1744552.5 (Joules/Mol)
	416.95806 (Kcal/Mol)
Zero-point correction =	0.664465 (Hartree/Particle)
Thermal correction to Energy =	0.709471
Thermal correction to Enthalpy =	0.710415
Thermal correction to Gibbs Free Energy =	0.581999
Sum of electronic and zero-point Energies =	-2192.736279
Sum of electronic and thermal Energies =	-2192.691273
Sum of electronic and thermal Enthalpies =	-2192.690329
Sum of electronic and thermal Free Energies =	-2192.818745



X

cartesian

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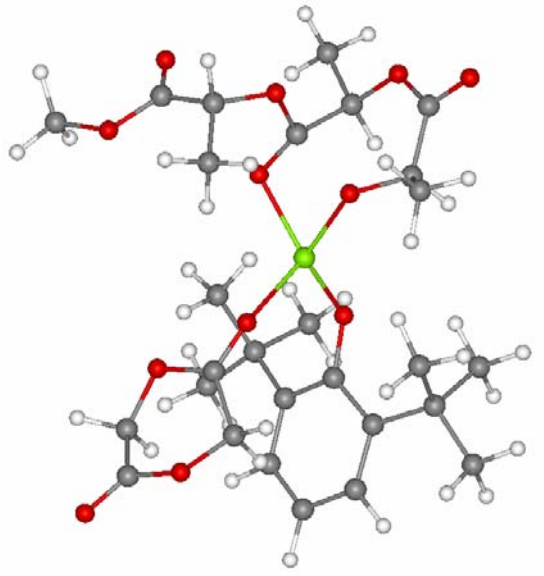
8	0.70545447	-1.46233344	-0.40172213
6	2.00485444	-1.25373340	-0.21262214
6	2.80265450	-0.68693352	-1.26262212
6	4.11705494	-0.30613348	-0.96162212
1	4.73885489	0.14436653	-1.72902215
6	4.68475485	-0.53303349	0.29097787
6	3.95105433	-1.23433340	1.24607790
1	4.43655491	-1.48363340	2.18367791
6	2.62705445	-1.62823343	1.02337790
6	2.29585457	-0.63983345	-2.72052193
6	1.89155459	-2.49123359	2.06587791
6	1.01345444	0.19626653	-2.91332197
1	0.11535451	-0.35523346	-2.63042212
1	0.87885451	0.44226652	-3.97292185
1	1.04825449	1.14686656	-2.37122202
6	2.01685452	-2.08823347	-3.17612195
1	1.27395451	-2.56453347	-2.53272200
1	2.93285441	-2.68733358	-3.14812207
1	1.63775444	-2.09533358	-4.20522213
6	3.35435438	-0.05653346	-3.67382193
1	4.28935480	-0.62463343	-3.65622211
1	3.58325458	0.99346650	-3.45522213
1	2.97405457	-0.09593347	-4.69972181
6	2.82195449	-2.94123363	3.20617795
1	3.18735456	-2.10253358	3.80917788
1	3.68585443	-3.50243354	2.83537793
1	2.26785445	-3.60273361	3.88047791
6	1.35465443	-3.77203369	1.39287782
1	0.66525447	-3.54003358	0.58017784
1	0.83145452	-4.39323378	2.12947798
1	2.18105459	-4.36283350	0.98327786
6	0.73225451	-1.71683347	2.71697807
1	1.09695446	-0.82713342	3.24297786
1	0.21565452	-2.34593344	3.45087790
1	-0.00444548	-1.40383339	1.97657788
8	-2.67034554	-0.52393341	0.40117788
6	-3.21724558	-0.06903347	-0.92952216
6	-4.03424549	-1.26333344	-1.44322217
8	-5.02844524	-1.69273341	-0.48392209
6	-4.85894537	-1.57573342	0.84617788
6	-3.66734552	-0.79693341	1.40067780
8	-2.14444542	0.23456654	-1.63572216
1	-4.06994534	0.16626653	1.72947788
6	-3.02764559	-1.51523340	2.57347798
6	2.93845439	3.24786639	-0.47512212
8	1.59605443	2.71166635	-0.45282212
6	1.27715445	1.94316661	0.57557786
6	2.24105453	1.92216659	1.72977781
8	2.87775445	3.18716645	1.94447780
6	3.36985445	3.82456636	0.85817784
8	0.22545451	1.31316662	0.57397783

1	3.62495446	2.45096636	-0.78102213
1	2.93365455	4.03656673	-1.22312212
6	-3.18214560	-2.45083356	-1.85042214
1	-4.61944532	-0.91113341	-2.29572201
1	1.70215452	1.68406653	2.64417791
1	2.98635459	1.13466656	1.54517782
8	4.08895493	4.78346634	0.95737785
8	-4.14304543	0.97236657	-0.70132214
6	-3.69974542	2.30946636	-0.84392214
6	-3.27564549	2.90206647	0.49847788
8	-2.72174549	4.11906672	0.31497785
6	-2.35044551	4.81396627	1.51567781
6	-4.85214520	3.11436653	-1.44412220
1	-2.83484554	2.34216642	-1.51362216
8	-3.41684556	2.39066648	1.58877790
1	-3.22554541	4.97926664	2.14767790
1	-1.93224549	5.76436663	1.18677783
1	-1.60904551	4.24166679	2.07727790
1	5.70995474	-0.23313347	0.49407786
8	-5.69074535	-2.03543353	1.59677780
1	-4.56584549	4.16006660	-1.57402217
1	-5.11044550	2.69366646	-2.41852212
1	-5.73424530	3.06206656	-0.80042213
1	-3.83054543	-3.26773357	-2.17732215
1	-2.52224541	-2.17513347	-2.67522192
1	-2.57514548	-2.81383348	-1.01522219
1	-3.79404545	-1.73393345	3.31857800
1	-2.56564546	-2.45603347	2.26197791
1	-2.26734543	-0.87653339	3.02877808

TS-34o__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1741695.1 (Joules/Mol)
	416.27512 (Kcal/Mol)
Zero-point correction =	0.663377 (Hartree/Particle)
Thermal correction to Energy =	0.708067
Thermal correction to Enthalpy =	0.709011
Thermal correction to Gibbs Free Energy =	0.582407
Sum of electronic and zero-point Energies =	-2192.728220
Sum of electronic and thermal Energies =	-2192.683530
Sum of electronic and thermal Enthalpies =	-2192.682586
Sum of electronic and thermal Free Energies =	-2192.809190



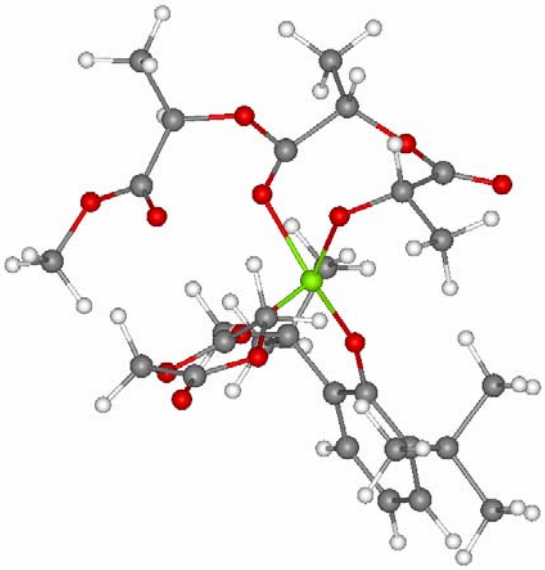
cartesian

8	0.60619527	-1.10572839	-0.84448153
6	1.92919517	-1.00932837	-0.78298157
6	2.61379528	-0.02242832	-1.56888151
6	3.98109508	0.17437167	-1.33768153
1	4.52189541	0.92807162	-1.90168142
6	4.69739532	-0.60462832	-0.43018156
6	4.05269527	-1.66492832	0.20501846
1	4.64429522	-2.31532812	0.84091842
6	2.68529510	-1.91062844	0.03741845
6	1.91079521	0.70067167	-2.73768139
6	2.04079509	-3.16022825	0.66951847
6	0.70899522	1.56367159	-2.30438161
1	-0.16050476	0.95817173	-2.04688144
1	0.39449525	2.20817184	-3.13358140
1	0.95209521	2.21737170	-1.46078146
6	1.42459536	-0.36742833	-3.74088144
1	0.73399526	-1.06652832	-3.26468158
1	2.27029514	-0.93622839	-4.14098167
1	0.90789527	0.10947167	-4.58248138
6	2.87399507	1.63297164	-3.49428153
1	3.74239516	1.10057163	-3.89448166
1	3.23429513	2.46057177	-2.87108159
1	2.34829521	2.07827163	-4.34538126
6	3.08369517	-4.06732845	1.34641850
1	3.56659508	-3.58862829	2.20571852
1	3.86289525	-4.39042807	0.64861846
1	2.58619523	-4.96882820	1.71921849
6	1.35909534	-4.00042820	-0.43018156
1	0.59599525	-3.42592835	-0.95738155
1	0.88769525	-4.88752842	0.00961846
1	2.09739518	-4.34232807	-1.16308153
6	1.01089525	-2.79152822	1.75351846
1	1.45819521	-2.16652822	2.53451848
1	0.62669522	-3.69732833	2.23691845
1	0.15249524	-2.26282835	1.33651853
6	3.06099510	3.15937185	0.90291846
8	1.71489525	2.63407183	0.93651843
6	1.55109525	1.45337164	1.51021850
6	2.71239519	0.91757166	2.30121851

8	3.46139526	1.94637167	2.95871854
6	3.77989507	3.04027176	2.23171854
8	0.48169523	0.86197162	1.41221845
1	2.34039521	0.25607169	3.08051848
1	3.35729527	0.33647168	1.62571847
12	-0.74060476	-0.20002833	0.14111847
1	5.75979519	-0.43362835	-0.27518153
8	-2.28510475	0.89367163	-0.51308155
1	3.61999512	2.63077188	0.12321846
1	2.96659517	4.20957184	0.63891846
8	4.57029533	3.85677171	2.62571859
8	-2.33790493	-1.03652835	0.92081845
6	-3.28300476	0.17647168	-0.16908155
6	-3.82080483	-0.89582837	-1.10648155
8	-4.68580437	-1.81302834	-0.42198157
6	-4.29180479	-2.50862813	0.67171848
6	-2.88530493	-2.29092813	1.24931848
1	-2.28080487	-3.09252834	0.79151845
6	-2.90260482	-2.50582814	2.75991845
6	-4.63200474	-0.28882831	-2.23818159
1	-2.95710492	-1.43492830	-1.51068151
8	-5.05360460	-3.32072830	1.14441848
1	-4.96680450	-1.08332837	-2.90958142
1	-4.01810455	0.41957167	-2.79828143
1	-5.50190449	0.23797168	-1.84318161
1	-3.29590487	-3.49302816	3.00881839
1	-3.52900481	-1.75022840	3.24131846
1	-1.88470483	-2.41542816	3.14791846
8	-4.26230478	0.67547166	0.60521847
6	-4.06350470	1.94057167	1.25071847
6	-3.91280484	3.04307175	0.19681846
8	-3.17890477	4.07047176	0.66121846
6	-3.06800485	5.18917179	-0.23458154
6	-3.02060485	1.91977167	2.35751843
1	-5.04440451	2.12267160	1.70271850
8	-4.46340466	3.03217173	-0.88048154
1	-2.57860470	4.88317156	-1.16118145
1	-2.46560478	5.92697191	0.29371846
1	-4.05580473	5.59337187	-0.46518153
1	-3.12120485	2.82147169	2.96631861
1	-3.18610477	1.04777169	2.99321842
1	-2.00470471	1.88767159	1.96531856

TS-34o__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1741752.8 (Joules/Mol)
	416.28892 (Kcal/Mol)
Zero-point correction =	0.663399 (Hartree/Particle)
Thermal correction to Energy =	0.708230
Thermal correction to Enthalpy =	0.709174
Thermal correction to Gibbs Free Energy =	0.583302
Sum of electronic and zero-point Energies =	-2192.726889
Sum of electronic and thermal Energies =	-2192.682058
Sum of electronic and thermal Enthalpies =	-2192.681114
Sum of electronic and thermal Free Energies =	-2192.806986



cartesian

12	0.09566702	-0.19788152	-0.25082716
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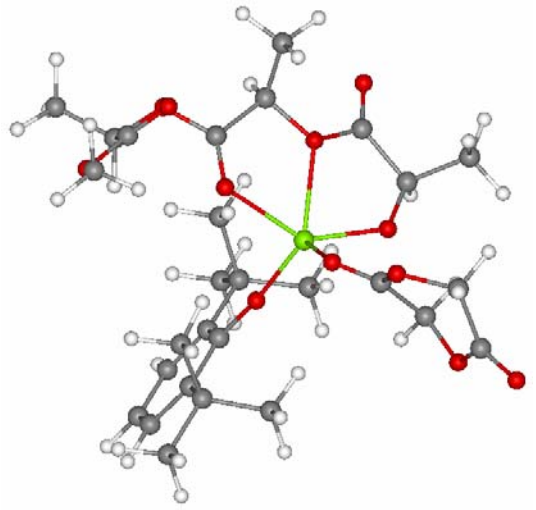
6	-3.36993313	-0.52688158	1.60077274
6	-4.61933279	-0.24278152	2.16067266
1	-4.98993301	-0.84168148	2.98577285
6	-5.41943312	0.79251850	1.69177282
6	-4.97083282	1.56351852	0.62497282
1	-5.61283302	2.36001849	0.26417282
6	-3.73453283	1.33651853	0.01317283
6	-2.52933311	-1.68948150	2.15997267
6	-3.30353308	2.19761848	-1.18832719
6	-1.23003304	-1.14768147	2.79017282
1	-0.68043303	-0.48858151	2.11537266
1	-0.56473303	-1.96638155	3.08897281
1	-1.46233296	-0.55298150	3.68037271
6	-2.23363304	-2.72518158	1.05567276
1	-1.73993301	-2.28558159	0.18937284
1	-3.16863298	-3.17378139	0.70327282
1	-1.59863305	-3.52998137	1.44627273
6	-3.25463295	-2.45898151	3.27907276
1	-4.19113302	-2.90598154	2.92987275
1	-3.47563291	-1.82818151	4.14657307
1	-2.61293292	-3.27678156	3.62727284
6	-4.35683298	3.25541854	-1.56262720
1	-4.53953314	3.96841860	-0.75122714
1	-5.31303310	2.80391860	-1.84642720

1	-4.00023317	3.82861853	-2.42602730
6	-3.11253309	1.30531847	-2.43052721
1	-2.38823295	0.50961852	-2.25402713
1	-2.77853298	1.90241849	-3.28832722
1	-4.06003284	0.83021843	-2.70632720
6	-2.00863290	2.97061849	-0.86632717
1	-2.16773295	3.65491843	-0.02552717
1	-1.69073296	3.56601858	-1.73172724
1	-1.20023298	2.29141855	-0.59052718
8	1.35576701	-0.28488153	-1.78952718
6	1.90536702	-2.03048158	-0.85412717
6	1.47276700	-2.91338158	-2.02382708
8	0.19306701	-2.58348155	-2.55902719
6	0.10586701	-1.50858152	-3.40982723
6	1.16236699	-0.42598149	-3.17302728
8	3.25956702	-2.02008152	-0.79732716
6	3.85936689	-2.10538149	0.50337285
6	3.82796693	-0.79288149	1.27637279
8	3.71566701	-1.04708147	2.58277273
6	3.75626707	0.08591848	3.46927285
6	5.30596685	-2.53028154	0.28557283
1	3.31866693	-2.84868145	1.09357274
8	3.96826696	0.31531847	0.79437286
1	4.69886684	0.62511849	3.35117269
1	3.68046689	-0.33008152	4.47227287
1	2.91526699	0.75031853	3.26817274
1	-6.38653278	0.99151850	2.14717269
8	-0.79953301	-1.45648146	-4.20222712
6	1.38546693	-4.35928154	-1.54702723
6	0.77456701	0.87381852	-3.86562729
8	1.22386706	-1.84358144	0.18337283
6	3.58876705	3.61451840	1.38697278
8	2.38686705	2.85361862	1.61837280
6	1.88886702	2.19061852	0.58557284
6	2.39866710	2.55691862	-0.78352714
8	2.83416700	3.91621852	-0.89602715
6	3.56056690	4.43581867	0.11467283
8	1.03636706	1.33631849	0.78187281
1	4.43676710	2.92291856	1.36287272
1	3.68936706	4.28611851	2.23617268
1	1.59706700	2.42781854	-1.50562727
1	3.20396709	1.86121845	-1.04002714
8	4.14136696	5.48431873	0.00647283
1	5.81116676	-2.64858150	1.24727273
1	5.33356714	-3.48648143	-0.24162719
1	5.83856678	-1.78408146	-0.30832717
1	2.23996711	-2.82988143	-2.79962730
1	2.10096693	-0.77828157	-3.63632727
1	0.59276700	0.70101845	-4.92922688
1	-0.13993299	1.28931856	-3.43492723
1	1.58636701	1.59981847	-3.76802731
1	1.11536705	-4.99758148	-2.39092731
1	2.34676695	-4.69458151	-1.14932728
1	0.62136698	-4.45538139	-0.77322716

I-4c12__RR_DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1740865.2 (Joules/Mol)
	416.07678 (Kcal/Mol)
Zero-point correction =	0.663061 (Hartree/Particle)
Thermal correction to Energy =	0.709208
Thermal correction to Enthalpy =	0.710152
Thermal correction to Gibbs Free Energy =	0.577787
Sum of electronic and zero-point Energies =	-2192.753897
Sum of electronic and thermal Energies =	-2192.707750
Sum of electronic and thermal Enthalpies =	-2192.706805
Sum of electronic and thermal Free Energies =	-2192.839171 -2192.839171 -2192.839171 -2192.839171 -2192.839171 -2192.839171 -2192.839171



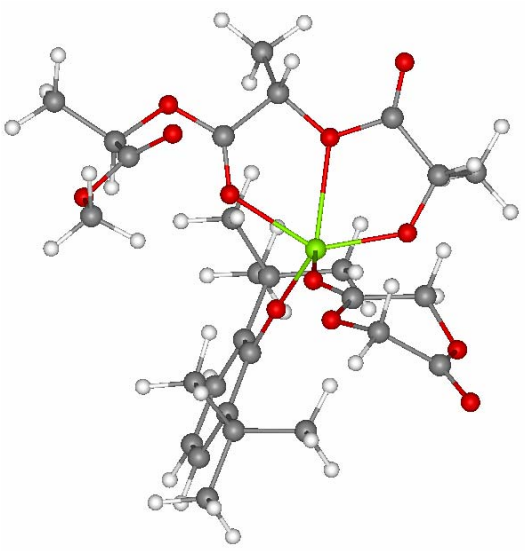
cartesian

12	0.82084346	-0.26931342	-0.62510860
8	-0.00255653	1.30888653	-0.03430860
6	-0.71825647	2.37448668	0.29949141
6	-0.71065652	2.85338664	1.65109146
6	-1.49445653	3.96478653	1.97409141
1	-1.50595653	4.33888674	2.99249148
6	-2.26985645	4.62388659	1.02639151
6	-2.25655651	4.17018652	-0.28780860
1	-2.85475636	4.70508671	-1.01800859
6	-1.49895656	3.06438661	-0.68530864
6	0.14594346	2.18168664	2.74009156
6	-1.51145649	2.62298656	-2.16050863
6	1.63444352	2.23048663	2.34139156
1	1.79024351	1.76648653	1.36689150

1	2.25224352	1.71348655	3.08689141
1	1.97854352	3.26838660	2.27819157
6	-0.31135654	0.72678655	2.96339154
1	-0.28315651	0.14928657	2.04019141
1	-1.33995652	0.70968658	3.34189153
1	0.32824346	0.23008659	3.70429134
6	0.03664346	2.89028668	4.10179138
1	-0.98405659	2.87198663	4.49889135
1	0.37004346	3.93228674	4.05639124
1	0.67614347	2.37428665	4.82729101
6	-2.38905668	3.52918649	-3.04250860
1	-2.03465652	4.56508636	-3.04940844
1	-3.43885660	3.52598667	-2.73030853
1	-2.35555649	3.16678667	-4.07640886
6	-2.09835672	1.20258653	-2.28520846
1	-1.57085657	0.50238657	-1.63460851
1	-2.03875637	0.84408653	-3.32060862
1	-3.15245676	1.19898653	-1.98530853
6	-0.08915654	2.68498659	-2.75410843
1	0.28784347	3.71288657	-2.71680856
1	-0.10115653	2.37338662	-3.80640864
1	0.61834347	2.05468655	-2.21340847
8	2.17734337	-0.19801342	-2.00580859
6	-1.45405650	-2.24411345	-0.69470859
6	-0.98225653	-2.55801344	-2.10260844
8	0.20154347	-1.76161337	-2.21430850
6	0.72624350	-1.48351347	-3.46580863
6	1.95694351	-0.58071339	-3.30620861
8	-2.63105631	-2.77341342	-0.41130862
6	-3.12175655	-2.59811354	0.93659139
6	-2.34315634	-3.53701353	1.85789144
8	-2.67885637	-3.30481339	3.13199139
6	-2.00785637	-4.12341309	4.10989141
6	-4.61035633	-2.90191340	0.91339141
1	-2.93345642	-1.56891346	1.25189149
8	-1.55215657	-4.37321329	1.48369145
1	-2.23185635	-5.17771339	3.93789148
1	-2.39615631	-3.79871345	5.07339144
1	-0.92975652	-3.96431351	4.05499125
1	-2.86905670	5.48688650	1.30649149
8	0.22384347	-1.91201341	-4.47540855
1	-1.72465646	-2.21171331	-2.82850862
6	-0.70015651	-4.04511356	-2.28550863
6	3.16274357	-1.30671346	-3.92620850
1	1.72324347	0.27818659	-3.96430850
8	-0.79695654	-1.56491339	0.08549140
6	5.57904339	-1.82071340	1.22319150
8	4.15174341	-1.83601344	1.41229141
6	3.43704367	-0.93061340	0.75059140
6	4.20534325	0.16338658	0.05159140
8	5.39874363	0.54648656	0.74999142
6	6.18684340	-0.43181342	1.23429143
8	2.22004342	-1.03051341	0.74599141
1	5.82054377	-2.32191348	0.27959138
1	5.99884367	-2.39671350	2.04429150
1	3.58924341	1.05608654	-0.02270860
1	4.42094374	-0.16081342	-0.97200859
8	7.29594374	-0.21391343	1.64939141
1	-5.02485657	-2.76981354	1.91409147
1	-5.11685658	-2.21521330	0.23169139
1	-4.79465628	-3.92731333	0.58399141
1	2.97184324	-1.60791337	-4.96020889
1	4.01894331	-0.62671340	-3.91040850
1	3.41544342	-2.19501352	-3.33710861
1	-0.34625655	-4.22071362	-3.30210853
1	0.05164346	-4.38471365	-1.56960857
1	-1.61655653	-4.61651325	-2.12470865

I-4c12__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1740681.7 (Joules/Mol)
	416.03290 (Kcal/Mol)
Zero-point correction =	0.662991 (Hartree/Particle)
Thermal correction to Energy =	0.708200
Thermal correction to Enthalpy =	0.709144
Thermal correction to Gibbs Free Energy =	0.580829
Sum of electronic and zero-point Energies =	-2192.753812
Sum of electronic and thermal Energies =	-2192.708602
Sum of electronic and thermal Enthalpies =	-2192.707658
Sum of electronic and thermal Free Energies =	-2192.835974



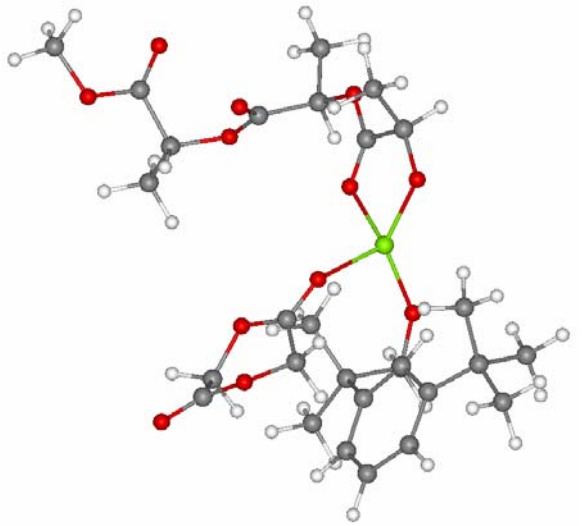
cartesian

12	0.40012082	-0.05823710	0.96147412
8	-0.96627927	-0.97753710	0.07277411
6	-1.92757916	-1.66273701	-0.53372586
6	-1.61147928	-2.57573700	-1.59272599
6	-2.65397930	-3.25853705	-2.22562575
1	-2.43317914	-3.94913697	-3.03262591
6	-3.98327923	-3.08683705	-1.85592592
6	-4.28417921	-2.21493697	-0.81582588
1	-5.32467937	-2.09953713	-0.53112590
6	-3.29457927	-1.49763703	-0.13722590
6	-0.15937921	-2.82073712	-2.03872585
6	-3.69037914	-0.55833709	1.01537406
6	0.66362083	-3.38173699	-0.86082590
1	0.60152084	-2.73893714	0.01817411
1	1.71722078	-3.49783707	-1.14672589
1	0.28562081	-4.36803722	-0.57112586
6	0.45642081	-1.51713705	-2.58492589
1	0.40372083	-0.70613712	-1.85942590
1	-0.08317921	-1.19853711	-3.48412585
1	1.50822079	-1.66983700	-2.85832572
6	-0.05217919	-3.85863709	-3.17052579
1	-0.57337916	-3.53773713	-4.07872581
1	-0.44347921	-4.83813715	-2.87612581
1	1.00352085	-3.99533701	-3.43292594
6	-5.20677900	-0.54843712	1.27897406
1	-5.58317900	-1.53623700	1.56477404
1	-5.77857924	-0.19953710	0.41227412
1	-5.42377901	0.13386290	2.10907412
6	-3.30027914	0.89326286	0.67437410
1	-2.23427916	0.97446287	0.45587412
1	-3.54857922	1.56216300	1.50867403
1	-3.84917927	1.23716295	-0.20962587
6	-3.02207923	-1.01163709	2.32857418
1	-3.37707925	-2.00953698	2.60817409
1	-3.27877927	-0.32513708	3.14587426
1	-1.93577933	-1.06293702	2.24447417
8	1.01452076	-0.49333709	2.73067427
6	0.25262082	2.86216283	0.14467411
6	0.16552082	3.19246292	1.62267411
8	0.21232082	1.90736294	2.24967408
6	0.87552083	1.80146289	3.46207428
6	1.04572082	0.32676291	3.83327413
8	0.12972081	3.92136288	-0.63652587
6	0.28792083	3.70596290	-2.05662584
6	1.76652074	3.44906282	-2.34862590
8	1.91632080	3.08146286	-3.62622571
6	3.26692080	2.79196286	-4.03602600
6	-0.23717919	4.94726276	-2.75822592
1	-0.27947918	2.81826305	-2.34632587
8	2.66272068	3.57596302	-1.54532599
1	3.89932084	3.67186284	-3.90472603
1	3.19752073	2.52026296	-5.08762598
1	3.66432071	1.96226299	-3.44932580
1	-4.77387905	-3.63123703	-2.36682582
8	1.25852084	2.77726293	4.06087399
6	-1.07317924	3.98316288	2.01717401
6	-0.00307918	-0.03843710	4.89787436
8	0.42032081	1.72246289	-0.27312589
6	5.57112074	-1.67983711	-0.01912589
8	4.31282091	-1.15993702	-0.48542589
6	3.33812070	-1.02113700	0.41247413
6	3.59952068	-1.59533703	1.78317404
8	4.35282087	-2.81443715	1.74037409
6	5.43862057	-2.84613705	0.94247413
8	2.31612086	-0.44173712	0.08637411
1	6.14112091	-0.87353712	0.45587412
1	6.10782099	-2.01283717	-0.90412587
1	2.64942074	-1.78343701	2.28707409
1	4.13632107	-0.84313715	2.37617421
8	6.24442101	-3.73893714	0.99297410
1	-0.14617917	4.82096291	-3.83832574
1	-1.29097927	5.09466314	-2.51132584
1	0.32452083	5.83396292	-2.45482588
1	-1.04317927	4.17286301	3.09147429
1	-1.08617926	4.94136286	1.49347401
1	-1.98247910	3.43026304	1.77457404
1	0.07252082	0.60376287	5.78147411
1	-1.01217926	0.03206290	4.48377419
1	0.16572082	-1.07593703	5.19747400
1	2.03252077	0.30886292	4.33357430
1	1.06762087	3.75236297	1.89497411

I-5c__RR__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1741985.0 (Joules/Mol)
	416.34442 (Kcal/Mol)
Zero-point correction =	0.663487 (Hartree/Particle)
Thermal correction to Energy =	0.709509
Thermal correction to Enthalpy =	0.710453

Thermal correction to Gibbs Free Energy =	0.578018
Sum of electronic and zero-point Energies =	-2192.756953
Sum of electronic and thermal Energies =	-2192.710932
Sum of electronic and thermal Enthalpies =	-2192.709988
Sum of electronic and thermal Free Energies =	-2192.842422

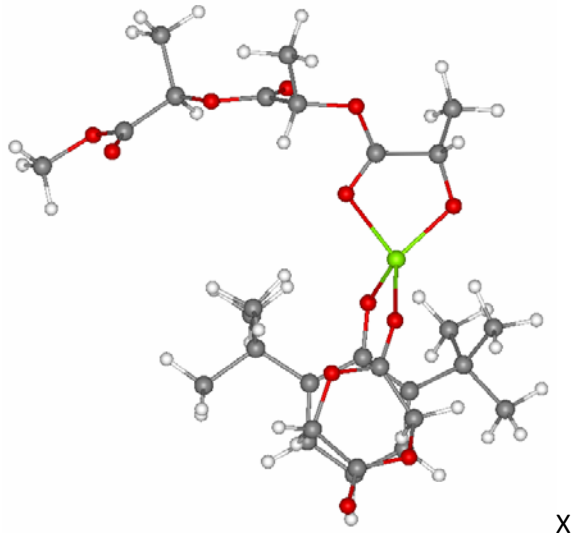


cartesian

8	1.96517396	-1.20024204	-0.69189376
6	2.92127395	-0.28494197	-0.75099373
6	2.73567390	0.89975798	-1.54149377
6	3.67947388	1.92735803	-1.42439377
1	3.55327392	2.84395814	-1.99249375
6	4.81687403	1.79965794	-0.62769377
6	5.06677389	0.58015800	0.00050627
1	5.99817371	0.46785802	0.54560626
6	4.16217375	-0.48604199	-0.06029372
6	1.60677385	0.99345803	-2.58959365
6	4.54177380	-1.86184204	0.52630627
6	0.20017380	0.99715805	-1.96399367
1	-0.02052622	0.05835802	-1.45789373
1	-0.55502617	1.12905800	-2.74869370
1	0.07817379	1.81545794	-1.24699378
6	1.72927380	-0.20644197	-3.55309367
1	1.63577390	-1.15294206	-3.01789355
1	2.69737387	-0.19324198	-4.06509399
1	0.94287378	-0.15874198	-4.31619406
6	1.71997380	2.27055812	-3.44109368
1	2.68167377	2.33995819	-3.95969367
1	1.58117390	3.18435812	-2.85109353
1	0.93667382	2.26185822	-4.20659399
6	5.95977402	-1.84954202	1.12550628
1	6.04297400	-1.18314207	1.99200630
1	6.71777391	-1.55774200	0.39160627
1	6.21277380	-2.85814190	1.46850622
6	4.53437376	-2.90794182	-0.60819376
1	3.55437374	-2.96424198	-1.08599377
1	4.78057384	-3.89944196	-0.20949374
1	5.27817392	-2.65594196	-1.37169373
6	3.59027386	-2.33084178	1.64840627
1	3.35417390	-1.52634203	2.35350633
1	4.05847406	-3.13534188	2.22690630
1	2.66237378	-2.75794196	1.26350629
12	0.67187381	-1.54354203	0.66630626
8	0.16457379	-3.06244183	1.68340623
6	-1.14842629	-3.44844198	1.62010622
6	-1.89822626	-2.56904197	0.62170625
8	-3.15762615	-2.90024185	0.37350628
6	-3.88992620	-2.08154178	-0.55689377
6	-4.18732643	-0.72644198	0.07580628
8	-4.55522633	0.14725801	-0.88349378
6	-4.99362612	1.43195796	-0.42329377
8	-4.13152647	-0.47464201	1.25590622
6	-6.36842632	1.29465795	0.22890627
1	-4.29392624	1.80555797	0.32860628
6	-5.03962612	2.35415816	-1.63259375
8	-1.34762621	-1.61264205	0.05620627
1	5.53497362	2.61305809	-0.55709374
6	1.32227373	3.61335802	1.12760627
8	0.65077376	2.34425807	1.27510631
6	1.36927390	1.34875798	1.77590621
6	2.69107389	1.71695805	2.39490628
8	2.67107391	2.99815822	3.03820634
6	2.10427380	4.01945782	2.36040640
8	0.94007379	0.20435801	1.75110626
1	1.99107385	3.55635810	0.26160628
1	0.54257381	4.34745789	0.94090623
1	2.94157386	0.98845804	3.16300631
1	3.46557379	1.68585801	1.61490631
8	2.21337390	5.16165781	2.72390628
6	-5.17512608	-2.82384181	-0.89019370
6	-1.85652614	-3.39514184	2.98570633
1	-5.35602617	3.35325813	-1.32589376
1	-4.04582644	2.42235804	-2.08099365
1	-5.73752594	1.97485805	-2.38309360
8	-6.65682602	2.40435815	0.92730623
8	-7.10462618	0.34165803	0.10860626
6	-7.94352627	2.41015816	1.57210624
1	-8.00742626	3.36875820	2.08430624
1	-8.74062634	2.31495810	0.83210623
1	-8.01022625	1.58715796	2.28580642
1	-2.89282608	-3.74094200	2.93160629
1	-1.29892612	-4.03594208	3.67260647
1	-1.84212613	-2.37524199	3.38070631
1	-1.26312613	-4.47944212	1.22910631
1	-3.28202605	-1.92104208	-1.45069373
1	-5.77032614	-2.23604178	-1.59089375
1	-4.93472624	-3.78754187	-1.34519374
1	-5.76562595	-2.99304199	0.01250628

I-5c__SS__DBP_Mg_MeL_LA_GL

Zero-point vibrational energy	1741170.5 (Joules/Mol)
	416.14973 (Kcal/Mol)
Zero-point correction =	0.663177 (Hartree/Particle)
Thermal correction to Energy =	0.709346
Thermal correction to Enthalpy =	0.710290
Thermal correction to Gibbs Free Energy =	0.577218
Sum of electronic and zero-point Energies =	-2192.754081
Sum of electronic and thermal Energies =	-2192.707912
Sum of electronic and thermal Enthalpies =	-2192.706968
Sum of electronic and thermal Free Energies =	-2192.840040



X

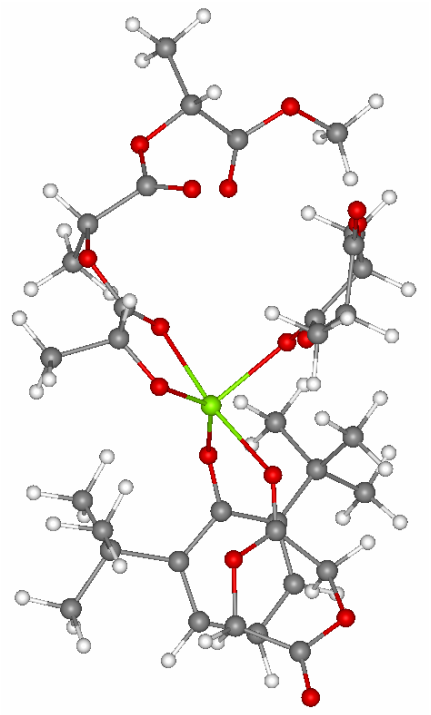
cartesian

8	1.28213692	0.56941724	1.00190234
6	2.32093716	-0.24818274	1.08800244
6	2.14603710	-1.65698266	0.86840242
6	3.29023719	-2.45868278	0.77840251
1	3.19153714	-3.52388287	0.59140247
6	4.57173681	-1.94158268	0.96560246
6	4.71283674	-0.60568279	1.34040236
1	5.71003675	-0.24208274	1.56500244
6	3.61663699	0.25861725	1.43730235
6	0.74173695	-2.29638290	0.86200243
6	3.79823709	1.68681729	1.99140263
6	-0.13636303	-1.82198274	-0.31039757
1	-0.38706303	-0.76558274	-0.22519755
1	-1.08076298	-2.37948275	-0.31979755
1	0.35073698	-1.98798263	-1.27619755
6	0.03973698	-1.94828260	2.19240260
1	-0.06186302	-0.86838275	2.31350255
1	0.60663700	-2.34028292	3.04360247
1	-0.96126300	-2.39618278	2.21850252
6	0.81173700	-3.83118272	0.77380246
1	1.38723695	-4.26938248	1.59570241
1	1.24323702	-4.17938280	-0.17219755
1	-0.20246303	-4.24068260	0.83150250
6	5.25753689	1.95351732	2.40290260
1	5.94453669	1.93751729	1.54870248
1	5.61583662	1.23541725	3.14750242
1	5.32633686	2.94901729	2.85380244
6	2.93153715	1.84661734	3.25830245
1	1.87783694	1.66151726	3.04140258
1	3.02833700	2.86351728	3.65730262
1	3.25323701	1.14621735	4.03650236
6	3.41593719	2.78461719	0.97580248
1	3.81573701	2.57801723	-0.02319756
1	3.82773709	3.75021720	1.29070234
1	2.33793712	2.94101715	0.90720242
12	0.72913700	1.71141732	-0.41839755
8	0.39093697	3.56771708	-0.62199759
6	-0.87226301	3.93581724	-1.00319755
6	-1.71046305	2.69031715	-1.28339756
8	-2.92546296	2.89631724	-1.77639747
6	-3.74836302	1.74401724	-2.02709746
6	-4.25956297	1.19221735	-0.69749755
8	-4.89146328	0.02551726	-0.91489756
6	-5.43386316	-0.63578278	0.24010247
8	-4.12836313	1.72971725	0.37750244
6	-5.39826298	-2.12878275	-0.06299755
1	-4.78856325	-0.43508273	1.09940243
6	-6.84926319	-0.14588273	0.52690244
6	-1.58456302	4.81271744	0.04220244
8	-1.26546299	1.55031729	-1.08909750
6	-4.88296318	2.19241714	-2.93559742
1	5.44333696	-2.58738279	0.89150244
6	3.02203703	-2.18408275	-3.11209750
8	2.13853717	-1.06028271	-2.91299748
6	2.64983702	-0.00938274	-2.28569746
6	4.14513683	0.00741727	-2.11359763
8	4.83893681	-0.59298277	-3.21599746
6	4.37713671	-1.78258276	-3.65869761
8	1.92003703	0.89711726	-1.91079760
1	3.14303708	-2.70698285	-2.15709758
1	2.52523708	-2.83578277	-3.82639742
1	4.48773670	1.03831732	-2.05669761
1	4.40113688	-0.49998274	-1.17199755
8	5.00143671	-2.45768285	-4.43529749
1	-2.57506299	5.13651752	-0.29069754
1	-1.68656301	4.27081728	0.98680240
1	-0.95946300	5.69131756	0.21760243
1	-5.52356291	1.34171724	-3.17439747
1	-5.48246336	2.96911716	-2.45449758
1	-4.47166300	2.59411716	-3.86439753
1	-3.14856291	0.96601725	-2.50629759
1	-0.87306303	4.49661732	-1.95969748
1	-7.26036310	-0.67788279	1.38740253
1	-6.82856321	0.92131722	0.75750250
1	-7.49736309	-0.31408274	-0.33719754
8	-5.69076300	-2.81618285	1.05730247

8	-5.16166306	-2.63248277	-1.13599753
6	-5.72626305	-4.24668264	0.91050249
1	-5.98266315	-4.63318253	1.89560246
1	-6.48006296	-4.53538275	0.17540246
1	-4.75086308	-4.62018251	0.59340245

I-5cm_RR__DBP_Mg_MeL_LA-2_GL

Zero-point vibrational energy	2114247.0 (Joules/Mol)
	505.31717 (Kcal/Mol)
Zero-point correction =	0.805274 (Hartree/Particle)
Thermal correction to Energy =	0.862760
Thermal correction to Enthalpy =	0.863704
Thermal correction to Gibbs Free Energy =	0.703565
Sum of electronic and zero-point Energies =	-2726.844939
Sum of electronic and thermal Energies =	-2726.787453
Sum of electronic and thermal Enthalpies =	-2726.786509
Sum of electronic and thermal Free Energies =	-2726.946648



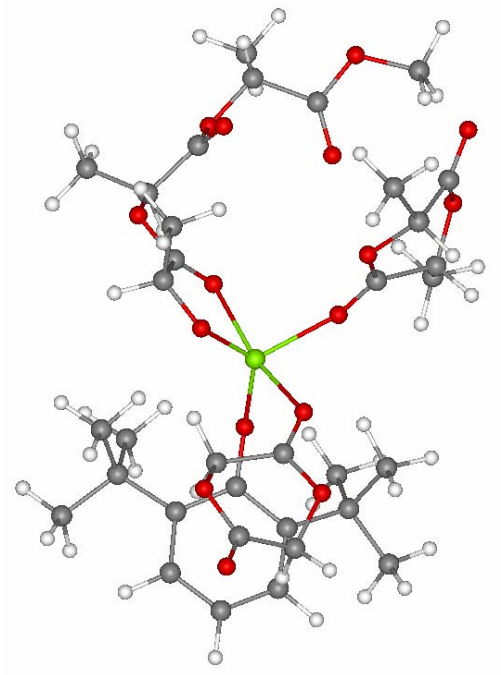
cartesian

12	0.57434064	0.53712320	-0.73691821
8	0.39834064	1.39282322	-2.44411826
6	-4.42955923	-0.51497680	-1.47721827
6	-3.65485954	-1.15707684	-2.62421823
8	-2.70185947	-0.23117679	-3.16931820
6	-1.58945930	0.09602323	-2.50321817
6	-0.68505937	1.10012317	-3.22261834
8	-5.49495935	-1.29187679	-1.18131816
6	-6.33745956	-0.85677677	-0.10851820
6	-7.70505953	-1.49227667	-0.31791818
8	-1.29755926	-0.36397678	-1.40111828
8	-4.18275928	0.54332322	-0.94791824
1	-6.40885925	0.23392323	-0.11961820
6	-5.71775961	-1.28337669	1.22098184
6	-0.30005938	0.55962324	-4.61251831
6	-3.09025955	-2.53527689	-2.28831816
8	-6.37735939	-0.70217675	2.24008179
8	-4.79115963	-2.04877687	1.34758174
1	-8.38535976	-1.18277669	0.47788182
1	-8.11705971	-1.16967678	-1.27701819
1	-7.63005924	-2.58247685	-0.31811818
6	-5.92335939	-1.07217669	3.55428171
1	-6.55005932	-0.51277679	4.24708176
1	-6.04315948	-2.14627671	3.70908189
1	-4.87275934	-0.80547673	3.68208170
1	-1.33775938	1.98322320	-3.39011812
1	-1.17225933	0.37842321	-5.24851799
1	0.34244066	1.30202317	-5.09231806
1	0.27364063	-0.36707675	-4.51421833
1	-4.37325954	-1.26937675	-3.44171834
1	-2.52705956	-2.90897679	-3.14731812
1	-2.44025946	-2.51037693	-1.41601825
1	-3.92015934	-3.21807694	-2.09511828
8	1.33534074	-1.07077670	0.00518180
6	2.45334053	-1.54707670	0.51258177
6	2.61814046	-1.67557693	1.93678176
6	3.89134049	-1.96597672	2.43678188
1	4.04874039	-2.02597690	3.50908184
6	4.98304033	-2.19567680	1.60058177
6	4.76764059	-2.26037693	0.22438180
1	5.59644079	-2.56367683	-0.40821820
6	3.51804066	-1.99557686	-0.34851819
6	1.42694068	-1.54507685	2.90668178
6	3.27964067	-2.29897690	-1.84461820
6	0.24794064	-2.41227674	2.41888189
1	-0.09345936	-2.11057687	1.42888176
1	-0.59295940	-2.33197689	3.11858177
1	0.54484063	-3.46577692	2.37258172
6	0.97834057	-0.07947677	3.04398179
1	0.69654059	0.34672323	2.08268189
1	1.78174067	0.53312325	3.47078180
1	0.11364064	-0.00687677	3.71638179
6	1.78014064	-2.03947687	4.32168198
1	2.53054047	-1.41227674	4.81568193
1	2.14514065	-3.07197690	4.31618166
1	0.88064063	-2.01147676	4.94698191
6	4.45054054	-3.09347677	-2.45411825
1	4.65244055	-4.01927662	-1.90511823
1	5.37824059	-2.51167679	-2.50001812

1	4.19864035	-3.36807680	-3.48421812
6	3.12254047	-1.03067684	-2.70061827
1	2.27374053	-0.40847677	-2.41491818
1	2.97304058	-1.30587673	-3.75201821
1	4.02164078	-0.40757680	-2.65491819
6	2.02524066	-3.18607688	-1.99221826
1	2.15664053	-4.12967682	-1.45101821
1	1.85934067	-3.42587686	-3.04981828
1	1.13534069	-2.69117689	-1.60171819
8	-2.76315951	4.48702335	0.94238180
6	-2.08285952	5.45982313	0.29588181
6	-0.58435941	5.21762323	0.14908180
8	-0.30455935	3.81432319	-0.09131820
6	-0.93925935	2.90922308	0.63818181
6	-2.01605940	3.42872310	1.57528174
8	-2.64445949	6.44282293	-0.11451820
1	-1.50285935	3.84622312	2.45458174
6	-2.99435949	2.35702324	2.00338173
6	5.60864067	1.42502332	-0.88091820
8	4.19694042	1.68772316	-0.98871821
6	3.49034047	1.58762312	0.13568181
6	4.29374075	1.47522330	1.40688181
8	5.48784065	2.27342319	1.37698174
6	6.25644064	2.16852331	0.27018180
8	2.27184057	1.61412334	0.11568180
1	5.76294041	0.34602323	-0.76251823
1	6.05194044	1.75562334	-1.81691825
6	0.03354064	6.00282335	-0.98631823
1	-0.10815936	5.48922300	1.10138178
8	-0.65445936	1.72632313	0.55958176
1	3.69944048	1.83622313	2.24268174
1	4.54124069	0.41902322	1.58388174
8	7.36244059	2.64322329	0.21968180
1	5.96454048	-2.40757680	2.01758170
1	1.10344064	5.79332304	-1.03781819
1	-0.12105937	7.06922340	-0.81781822
1	-0.42825937	5.72792339	-1.93601823
1	-2.46295953	1.56822324	2.53778172
1	-3.48695946	1.91792321	1.13478172
1	-3.74275947	2.79962325	2.66438174

I-5cm_SS__DBP_Mg_MeL_LA-2_GL

Zero-point vibrational energy	2116073.0 (Joules/Mol)
	505.75359 (Kcal/Mol)
Zero-point correction =	0.805970 (Hartree/Particle)
Thermal correction to Energy =	0.863145
Thermal correction to Enthalpy =	0.864089
Thermal correction to Gibbs Free Energy =	0.706251
Sum of electronic and zero-point Energies =	-2726.855610
Sum of electronic and thermal Energies =	-2726.798434
Sum of electronic and thermal Enthalpies =	-2726.797490
Sum of electronic and thermal Free Energies =	-2726.955328



cartesian

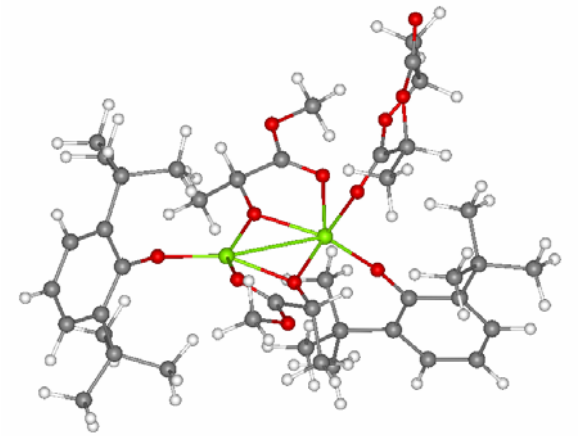
8	1.73062742	0.60133940	-0.87168878
6	3.01282740	0.70193940	-1.18618870
6	3.63012743	-0.25596055	-2.06288886
6	5.02812719	-0.29846057	-2.11468887
1	5.52132750	-1.04996049	-2.72358894
6	5.82392740	0.62263942	-1.43578875
6	5.20322752	1.69193947	-0.79348880
1	5.83092737	2.47433949	-0.37858880
6	3.81052732	1.79363942	-0.69458878
6	2.80052733	-1.15136051	-3.00888896
6	3.17612743	3.08253956	-0.12818877
6	2.08892751	-2.30006051	-2.27478886
1	1.35012734	-1.92556047	-1.56838870
1	1.57222736	-2.94266057	-3.00078893
1	2.80122733	-2.92266059	-1.72338879
6	1.75382733	-0.28526056	-3.74078894
1	1.07702744	0.20083944	-3.03618884
1	2.24492741	0.49253941	-4.33568907
1	1.16332734	-0.90696061	-4.42588902
6	3.68192744	-1.79506052	-4.09568882
1	4.25572729	-1.04836059	-4.65448904
1	4.38192749	-2.53306055	-3.68878889
1	3.04172730	-2.32376051	-4.81128883
6	4.19122744	4.24133968	-0.09058876
1	4.99492741	4.07793951	0.63511121
1	4.64482737	4.42003965	-1.07118869

1	3.67602730	5.16043949	0.21091123
6	2.02022743	3.54633951	-1.03828871
1	1.23312736	2.79513955	-1.10748875
1	1.58892739	4.47653961	-0.64748877
1	2.38842750	3.74833941	-2.05028892
6	2.66662741	2.89103937	1.31051123
1	3.49642730	2.66833949	1.99171126
1	2.18822742	3.81093931	1.67071128
1	1.94202733	2.07913947	1.39411128
1	6.90852737	0.56293941	-1.48808873
6	-2.27267265	-4.06726074	1.58091128
8	-1.57157266	-2.82526040	1.30451131
6	-1.43257260	-2.45156050	0.04011123
6	-2.18477273	-3.26186061	-0.99998873
8	-3.47457266	-3.66356063	-0.49238878
6	-3.55697250	-4.15246058	0.76391119
8	-0.71827269	-1.51126051	-0.25688875
1	-1.61617255	-4.88936043	1.26521122
6	-2.51407266	-4.13336086	3.07181120
6	-2.40407252	-2.50946045	-2.29488873
1	-1.58917260	-4.16826057	-1.18458879
8	-4.58687258	-4.62076044	1.17861128
12	0.65292734	-0.12506056	0.55031121
8	0.65332735	0.28933942	2.43981123
6	-4.14597273	2.06823945	0.96781123
6	-2.95967269	3.02523947	1.05951118
8	-2.07637262	2.57273960	2.09541130
6	-1.17117262	1.64543951	1.77851129
6	-0.27187264	1.17873943	2.92161107
8	-4.96517277	2.45413947	-0.03288879
6	-6.16967249	1.69343948	-0.19458877
6	-7.07927275	2.49003959	-1.11938870
8	-1.04407263	1.21313953	0.63171124
6	-3.38777256	4.44183969	1.41691124
6	-1.12567258	0.59353942	4.05961132
8	-4.34837246	1.12343943	1.69371128
1	-6.63747263	1.54613948	0.78241122
6	-5.85877275	0.31733942	-0.77998883
6	5.36062717	-2.49526048	1.42201126
8	3.96622753	-2.75766063	1.16591120
6	3.13702750	-1.73286057	1.36221123
6	3.67342734	-0.56386054	2.14571118
8	4.64582729	-0.94516057	3.13171124
6	5.60022736	-1.81886053	2.75681114
8	1.99912739	-1.78576052	0.92481118
1	5.76102734	-1.87706053	0.61021119
1	5.85752726	-3.46216059	1.41891122
1	2.83692741	-0.09406056	2.67031121
1	4.10592747	0.15963943	1.44201124
8	6.56322718	-2.04546046	3.44571114
1	-2.91367269	-3.16296053	-3.00628877
1	-3.01207256	-1.61996055	-2.12228894
1	-1.44237256	-2.20936060	-2.71268892
1	-2.99517250	-5.08036041	3.31991124
1	-1.56217265	-4.06116056	3.60101104
1	-3.16617250	-3.31866050	3.39131117
1	-2.50527263	5.08233929	1.48201132
1	-4.05237293	4.83713961	0.64691120
1	-3.90427256	4.46163940	2.37981105
1	-1.84067261	1.31783950	4.46021128
1	-1.67027259	-0.28666055	3.70671105
1	-0.44827265	0.27983946	4.85771132
1	0.19482735	2.10843945	3.30641127
1	-2.43847251	3.00433946	0.09891123
8	-6.92217255	-0.48456055	-0.62488878
8	-4.82967281	0.00903943	-1.33798873
1	-8.02347279	1.96003938	-1.25938869
1	-7.28847265	3.46793938	-0.67938882
1	-6.60547256	2.63793945	-2.09288883
6	-6.79787254	-1.80706048	-1.18248868
1	-7.74957275	-2.29606056	-0.98158878
1	-6.61547279	-1.74756050	-2.25748897
1	-5.98247242	-2.34806061	-0.70158881

S5.5. ROP of LA. Binuclear mechanism

DI-1__DBP-2_Mg-2_MeL-2_ssLA-1

Zero-point vibrational energy	2659987.6 (Joules/Mol)
	635.75230 (Kcal/Mol)
Zero-point correction =	1.013136 (Hartree/Particle)
Thermal correction to Energy =	1.078693
Thermal correction to Enthalpy =	1.079637
Thermal correction to Gibbs Free Energy =	0.907692
Sum of electronic and zero-point Energies =	-2940.381015
Sum of electronic and thermal Energies =	-2940.315458
Sum of electronic and thermal Enthalpies =	-2940.314514
Sum of electronic and thermal Free Energies =	-2940.486459



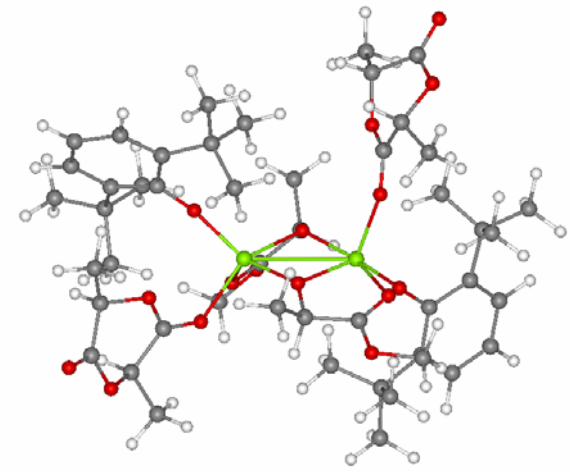
cartesian

12	-1.24222255	0.05696015	0.32584810
12	1.82027745	-0.14263985	-0.06435189
8	-2.70192266	1.22416019	0.00594811
8	3.53187752	-0.01223986	0.73084813
8	0.19107740	0.46246016	-1.05235195
8	2.31167746	-0.63233984	-2.08715200
8	1.65327740	-0.29043984	-4.20235205
6	0.21437739	0.50776017	-2.43745184
6	0.13167739	1.93346024	-2.99385190
1	-0.61432260	-0.07493985	-2.87415195
6	1.49037743	-0.18903986	-2.89445186
6	2.87497735	-0.92143983	-4.64945173
1	2.84587741	-0.86253983	-5.73565197
1	3.73997736	-0.38973987	-4.25175190
6	-3.58002257	2.19686007	-0.18675189
6	-4.74692297	1.96076012	-0.98855186
6	-5.65102291	3.00596023	-1.19795191
1	-6.53542280	2.84356022	-1.80545199
6	-5.45952272	4.26766014	-0.64735186
6	-4.33942270	4.48996019	0.14614812
1	-4.20902300	5.47726011	0.57634813
6	-3.39322257	3.49326015	0.40154809
6	-5.02222300	0.58286017	-1.61625195
6	-2.19272256	3.80606031	1.31344807
6	-6.34112263	0.54066014	-2.40685201
1	-6.34252262	1.23746014	-3.25135183
1	-7.20872259	0.76276016	-1.77685189
1	-6.48522282	-0.46613985	-2.81735182
6	-5.14042282	-0.48353988	-0.50935191
1	-5.30312300	-1.47713983	-0.95555186
1	-6.00242281	-0.26873985	0.13164811
1	-4.25212288	-0.50843984	0.12234811
6	-3.90152264	0.22026016	-2.61005187
1	-3.87032247	0.94706011	-3.42905188
1	-4.08112288	-0.76963985	-3.05395198
1	-2.92662263	0.21936016	-2.12165189
6	-2.21312261	5.24866009	1.84994805
1	-3.10362267	5.45546007	2.45284796
1	-2.15912247	5.99206018	1.04764807
1	-1.34022260	5.40346003	2.49444795
6	-2.22182250	2.88476014	2.54914808
1	-2.26692247	1.83216023	2.26934814
1	-3.10742259	3.09996009	3.15784812
1	-1.33572257	3.05166006	3.17504811
6	-0.86802262	3.65296006	0.54014814
1	-0.76252264	2.67116022	0.07744811
1	-0.01062261	3.81786013	1.20494807
1	-0.81292260	4.39556026	-0.26385191
6	4.76627731	-0.19813985	0.25894809
6	5.54057741	0.91676021	-0.19115189
6	6.79097700	0.66796017	-0.76585186
1	7.39127731	1.49326015	-1.13425195
6	7.30807734	-0.61883986	-0.87805188
6	6.58457708	-1.68753982	-0.35835192
1	7.02497721	-2.67733979	-0.41815192
6	5.32967710	-1.51273990	0.23354812
6	5.04437733	2.36646008	-0.01985189
6	4.61537743	-2.70823979	0.89754814
6	4.46687698	-2.43413973	2.40814805
1	5.45067739	-2.35103989	2.88174796
1	3.92467761	-3.25363994	2.89814806
1	3.92547727	-1.50183988	2.58084798
6	5.41757727	-4.01363993	0.74854815
1	6.41617727	-3.93753982	1.18984807
1	5.52657700	-4.31703997	-0.29885191
1	4.89487696	-4.82173967	1.27214801
6	3.22117734	-2.98503995	0.29084811
1	3.23217750	-2.90243983	-0.80035186

1	2.46657753	-2.30673981	0.70074815
1	2.88607740	-3.99743986	0.54804814
6	6.09697723	3.39496017	-0.47155190
1	6.31817722	3.32506013	-1.54235196
1	7.03587723	3.29026008	0.08154811
1	5.71827698	4.40585995	-0.28375190
6	4.74937725	2.64976025	1.46744812
1	4.00307703	1.95776010	1.86064804
1	4.38047743	3.67516017	1.59544802
1	5.66227722	2.54406023	2.06364799
6	3.78267741	2.64046025	-0.86185187
1	3.94407725	2.37346005	-1.91175199
1	3.51497746	3.70306015	-0.81935185
1	2.91977739	2.08366013	-0.48955190
1	-6.17602301	5.06506014	-0.82845187
1	8.27947807	-0.78383982	-1.33805192
1	2.90237737	-1.96083987	-4.31855202
1	0.15237738	1.93956017	-4.08725214
1	-0.80372262	2.38186026	-2.65355182
1	0.95957738	2.53926015	-2.61525202
8	-3.02912259	-3.18633986	0.56424814
6	-2.45922256	-2.81243992	-0.57445186
6	-2.72392249	-3.70483994	-1.77635193
8	-2.72272253	-5.09033966	-1.37905192
6	-3.43952250	-5.44013977	-0.28565189
6	-4.00052261	-4.26773977	0.51094812
8	-1.76852262	-1.81063986	-0.63365185
1	-4.88482285	-3.88553977	-0.01565189
6	-4.36152267	-4.63664007	1.93104804
6	-1.70772254	-3.53933978	-2.88485193
1	-3.72592258	-3.44553995	-2.14775205
8	-3.60292268	-6.59543991	0.00854811
1	-1.95732260	-4.21503973	-3.70515203
1	-1.72532260	-2.51263976	-3.25155187
1	-0.70382261	-3.77213979	-2.52485204
1	-5.11172295	-5.42833996	1.91894805
1	-3.48512268	-5.00203991	2.46954799
1	-4.76992273	-3.76403975	2.44394803
8	0.45627737	-0.43393987	1.32234812
8	-1.94192255	-0.64153987	2.29234815
8	-1.22952259	-1.28053987	4.32514811
6	0.43557739	-0.78023982	2.66654801
6	1.17347741	0.22706015	3.55464816
1	0.88177735	-1.77503979	2.83224797
6	-1.02572262	-0.89583981	3.07274818
6	-2.60182261	-1.34473979	4.76114798
1	-3.14892268	-2.08383989	4.17414808
1	-3.07742262	-0.36873984	4.65414810
1	-2.55782247	-1.64073980	5.80774784
1	1.16857743	-0.08333986	4.60304785
1	2.20717740	0.29686016	3.20874810
1	0.71467739	1.21666014	3.47314811

DI-1__DBP-2_Mg-2_MeL-2_rrLA-2

Zero-point vibrational energy	3034907.3 (Joules/Mol)
	725.36026 (Kcal/Mol)
Zero-point correction =	1.155935 (Hartree/Particle)
Thermal correction to Energy =	1.232425
Thermal correction to Enthalpy =	1.233369
Thermal correction to Gibbs Free Energy =	1.039407
Sum of electronic and zero-point Energies =	-3474.478799
Sum of electronic and thermal Energies =	-3474.402309
Sum of electronic and thermal Enthalpies =	-3474.401365
Sum of electronic and thermal Free Energies =	-3474.595327



cartesian

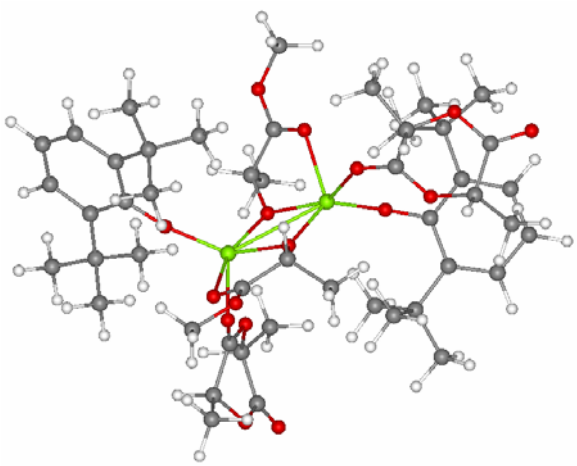
12	-1.16715229	-0.38802907	0.20652893
12	1.78204775	-0.24292907	-0.74167109
8	-2.50715208	0.90237093	0.72782892
8	3.24254799	-1.31062913	-0.13787109
8	0.67944777	0.15537094	0.89302897
8	-0.96545225	-1.59212911	1.97602892
8	0.26784778	-1.79882908	3.83902884
8	-0.08055223	-0.65432906	-1.46667111
8	2.14124799	-0.70632905	-2.84907103
8	1.22264779	-1.83342910	-4.55997086
6	1.01134777	-0.21702906	2.18922901
6	1.04384780	0.97187096	3.15762901
1	1.99294770	-0.71722907	2.22382903
6	0.00914777	-1.26262915	2.65682888
6	-0.64395225	-2.81272888	4.30182886
1	-0.64985222	-3.65542889	3.60842896
1	-1.65045226	-2.40182900	4.39172888
6	-0.19625223	-1.28942907	-2.69437099

1	-0.42725223	-2.36152887	-2.56967115
6	1.16794777	-1.24302912	-3.37287116
6	2.51384783	-1.85222912	-5.20307112
1	2.36514783	-2.40292907	-6.13017130
1	2.84654784	-0.83352906	-5.40977097
6	-3.59545207	1.64967096	0.76702893
6	-4.64135218	1.38257086	1.72122896
6	-5.85225201	2.07337093	1.60552895
1	-6.66335201	1.85577095	2.29272890
6	-6.05575228	3.06347108	0.64962894
6	-4.98725224	3.43157101	-0.16127108
1	-5.13085222	4.26177120	-0.84487110
6	-3.75105214	2.77957106	-0.10937108
6	-4.44215202	0.41707093	2.90692902
6	-2.58135223	3.32367110	-0.95037109
6	-5.60415220	0.47607094	3.91492891
1	-6.54975224	0.12117094	3.49012899
1	-5.76115227	1.48677087	4.30512905
1	-5.37295198	-0.17282908	4.76742887
6	-3.16815209	0.81027097	3.68062901
1	-2.99845219	0.11967093	4.51652908
1	-3.27245212	1.81837094	4.09622908
1	-2.29485202	0.79827094	3.02862883
6	-4.34205198	-1.04332912	2.43642902
1	-5.26425219	-1.33202910	1.91472888
1	-4.22615194	-1.72052908	3.29232883
1	-3.48895216	-1.18972909	1.77712893
6	-2.92615223	4.65727091	-1.63827109
1	-3.22475219	5.42837095	-0.92037106
1	-3.72245216	4.55337095	-2.38267112
1	-2.04125214	5.02707100	-2.17007113
6	-1.37105227	3.60217094	-0.03687108
1	-1.02045226	2.70127106	0.46832895
1	-1.63065219	4.34687090	0.72402894
1	-0.54645222	4.01007080	-0.63917106
6	-2.18425202	2.34097099	-2.06257105
1	-1.84685218	1.38767087	-1.65997112
1	-1.36805224	2.75467110	-2.66987109
1	-3.03095222	2.14567113	-2.72937107
6	4.25494766	-2.03122902	0.31992891
6	4.13134766	-3.45472908	0.47212893
6	5.19704771	-4.17032909	1.02532887
1	5.11184788	-5.24332905	1.16192889
6	6.38374805	-3.55582905	1.40822887
6	6.52274799	-2.18682909	1.20922887
1	7.46374798	-1.72432911	1.48782897
6	5.49944782	-1.40452909	0.66642892
6	2.87484789	-4.21392918	0.00662892
6	5.73534775	0.09997094	0.44362891
6	7.15734768	0.54187095	0.83322895
1	7.36314774	0.39267093	1.89852881
1	7.26984787	1.61287093	0.62852895
1	7.92704773	0.01807094	0.25672892
6	4.77054787	0.92927098	1.31142890
1	4.93394804	0.71217096	2.37302899
1	3.72774792	0.70977098	1.08162892
1	4.94144773	2.00267100	1.15842891
6	5.56644773	0.44617093	-1.04997110
1	4.59214783	0.14077093	-1.43237102
1	6.33234787	-0.06452906	-1.64407110
1	5.68724775	1.52617085	-1.20897102
6	2.96924782	-5.73032904	0.25052893
1	3.05994797	-5.97482920	1.31442893
1	3.81154799	-6.18602896	-0.28007108
1	2.05514789	-6.21052885	-0.11827108
6	2.69564795	-4.01932907	-1.51177108
1	2.68074799	-2.95962906	-1.76707113
1	1.76464772	-4.48752880	-1.85817111
1	3.52784777	-4.48382902	-2.05277109
6	1.62334776	-3.72872901	0.75952893
1	1.74194777	-3.89332891	1.83672893
1	0.73274773	-4.27682877	0.42722893
1	1.45184779	-2.66552901	0.59482890
1	-7.01025200	3.57917094	0.57842892
1	7.19434786	-4.13752890	1.84042895
1	3.24364781	-2.35352898	-4.56607103
1	-0.26395223	-3.11942887	5.27482891
1	1.29424775	0.65777093	4.17482901
1	1.80524778	1.67177093	2.80772901
1	0.07844777	1.48517084	3.16422892
8	-4.31445217	-0.94542903	-1.34457111
6	-3.71085215	-2.00692892	-0.83487105
6	-4.55275202	-3.26532888	-0.71507108
8	-5.44455194	-3.38472891	-1.83947110
6	-6.15705204	-2.29222894	-2.21097112
6	-5.75965214	-0.99552900	-1.51507103
8	-2.54135203	-1.95772910	-0.48767108
1	-6.20205212	-0.98732907	-0.51077110
6	-6.17775202	0.24447092	-2.26887107
6	-3.72645211	-4.53092909	-0.63467109
1	-5.15225220	-3.15352893	0.19972894
8	-7.03065205	-2.37802887	-3.03467107
1	-4.39005232	-5.39072895	-0.52517110
1	-3.05665207	-4.47992897	0.22452894
1	-3.12795210	-4.65812922	-1.53887105
1	-7.26335192	0.24737093	-2.37857103
1	-5.73075199	0.25817093	-3.26517105
1	-5.86885214	1.12997091	-1.71027112
6	-1.25705218	-0.68602902	-3.62267113
1	-1.33755219	-1.25912905	-4.55057096
1	-2.22475219	-0.69612902	-3.11817098
1	-1.01735222	0.35197094	-3.86737108
8	3.53484797	4.98927116	-1.55977106
6	3.44174790	5.44537115	-0.28857109
6	2.40224791	4.73737097	0.57332891
8	2.38694787	3.31147099	0.28512892
6	2.37834787	2.93347096	-0.98347110
6	2.55114794	4.03937101	-2.01317120
8	4.13634777	6.34847116	0.09912891
1	1.58254778	4.55327082	-2.09897113
6	2.98734784	3.52847099	-3.36887097
6	2.64774799	4.90647125	2.05492902
1	1.41344774	5.13347101	0.30742893
8	2.24304795	1.76427090	-1.29787111
1	1.85794771	4.40707111	2.61832881
1	2.64754796	5.96937084	2.30062890
1	3.61514783	4.48627090	2.33552885
1	2.24074793	2.83727098	-3.76177096

1	3.94134784	3.00427103	-3.29267097		1	3.09384799	4.37147093	-4.05437136

DI-1__DBP-2_Mg-2_MeL-2_ssLA-2

Zero-point vibrational energy	3032932.8 (Joules/Mol)
	724.88834 (Kcal/Mol)
Zero-point correction =	1.155183 (Hartree/Particle)
Thermal correction to Energy =	1.231991
Thermal correction to Enthalpy =	1.232935
Thermal correction to Gibbs Free Energy =	1.036645
Sum of electronic and zero-point Energies =	-3474.475434
Sum of electronic and thermal Energies =	-3474.398627
Sum of electronic and thermal Enthalpies =	-3474.397683
Sum of electronic and thermal Free Energies =	-3474.593972



cartesian

12	-1.18456721	-0.39087242	0.09582474
12	1.79613280	-0.16157241	-0.75377530
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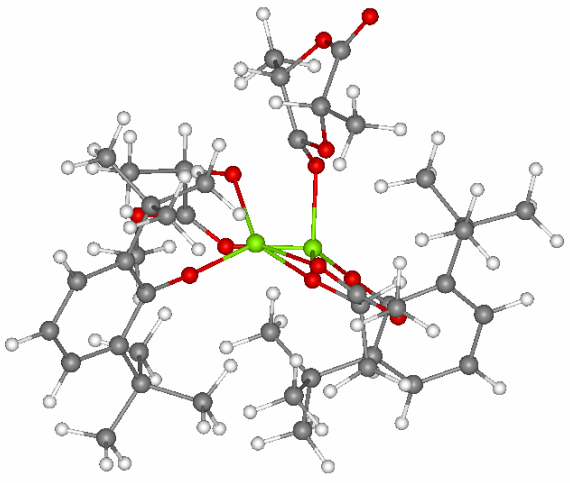
8	3.29753280	-1.21637237	-0.20257527
8	0.65233278	0.07282758	0.87332469
8	-1.01606715	-1.76347244	1.74482477
8	0.14823282	-2.11997247	3.62962461
8	-0.04026719	-0.51457244	-1.56897533
8	2.22233272	-0.45547241	-2.88317537
8	1.35573280	-1.43517244	-4.70887518
6	0.93983281	-0.40267241	2.14582467
6	0.92183280	0.70392758	3.20822477
1	1.92443287	-0.89757246	2.17802477
6	-0.07066719	-1.48847234	2.48702478
6	-0.78526723	-3.15947247	3.98092461
1	-0.77386713	-3.94547248	3.22392464
1	-1.79146719	-2.74727249	4.06812477
6	-0.11596718	-1.05147243	-2.84347534
6	-1.15386713	-0.38327241	-3.75407529
1	-0.34056720	-2.13247252	-2.80967522
6	1.26613283	-0.94657242	-3.47767520
6	2.66173267	-1.39147234	-5.31897545
1	2.54113269	-1.86547244	-6.29157543
1	2.98853278	-0.35657242	-5.43447542
6	-3.63206720	1.58842766	0.74492472
6	-4.69396687	1.24162757	1.65292466
6	-5.89526701	1.95572758	1.58972466
1	-6.71856689	1.68112767	2.24062467
6	-6.07706690	3.03112745	0.72662473
6	-4.99896717	3.45382738	-0.04327526
1	-5.12696695	4.34032774	-0.65537530
6	-3.77006721	2.78692746	-0.03737526
6	-4.52726698	0.15772758	2.73612475
6	-2.59046721	3.38482738	-0.82657528
6	-5.71826696	0.11022758	3.71042466
1	-6.64916706	-0.19717242	3.22182465
1	-5.88806725	1.07342756	4.20252466
1	-5.50976706	-0.62637246	4.49502468
6	-3.27896738	0.47342759	3.58352470
1	-3.12056732	-0.30437243	4.34202480
1	-3.40596724	1.42782760	4.10632467
1	-2.38886738	0.54482758	2.95812464
6	-4.40886688	-1.24587238	2.11842465
1	-5.30106688	-1.47807240	1.52522469
1	-4.32986689	-2.00777245	2.90502477
1	-3.52676725	-1.32547235	1.48672473
6	-2.92246723	4.76322794	-1.42737532
1	-3.22076726	5.48702765	-0.66177529
1	-3.71596718	4.71392775	-2.18107533
1	-2.03126717	5.16182756	-1.92587531
6	-1.38626719	3.59722757	0.11252474
1	-1.04716718	2.66412759	0.56372470
1	-1.65466714	4.28962755	0.91852474
1	-0.55116719	4.03862762	-0.44667524
6	-2.18906736	2.47822738	-2.00007534
1	-1.88296711	1.49052763	-1.65927529
1	-1.35096717	2.91762757	-2.55647540
1	-3.02616739	2.35242748	-2.69607520
6	4.20223284	-1.99047244	0.37582475
6	4.04623318	-3.41907239	0.39362475
6	4.97773314	-4.19137239	1.09302473
1	4.86103296	-5.26927233	1.13382471
6	6.07063293	-3.62847257	1.74242473
6	6.26373291	-2.25447249	1.65752470
1	7.14173317	-1.83357239	2.13612461
6	5.37283278	-1.41777241	0.97902477
6	2.90953279	-4.11927223	-0.37377524
6	5.67883301	0.08772758	0.87582469

6	7.03653288	0.45992759	1.49782467
1	7.07253313	0.26122758	2.57412481
1	7.21423292	1.53362763	1.36172473
1	7.86803293	-0.07037243	1.02202475
6	4.61363316	0.90702754	1.62662470
1	4.60373306	0.63982755	2.68902469
1	3.61433268	0.73322755	1.22792470
1	4.83743286	1.98152757	1.55892467
6	5.74643278	0.50962758	-0.60597527
1	4.82193279	0.27592757	-1.13477528
1	6.56613302	-0.01277242	-1.11127532
1	5.94483280	1.58812761	-0.68737531
6	2.98193264	-5.65367222	-0.27557525
1	2.86133265	-6.01137209	0.75272471
1	3.92243266	-6.05187225	-0.67007530
1	2.16923261	-6.08977222	-0.86837530
6	3.01433277	-3.76707244	-1.87097526
1	3.03633261	-2.68707252	-2.01777530
1	2.16913271	-4.19117212	-2.42977524
1	3.93693280	-4.18257236	-2.29177523
6	1.53283286	-3.71577239	0.18302473
1	1.44903278	-4.01237249	1.23462474
1	0.72683287	-4.21287251	-0.37157527
1	1.36983287	-2.63977242	0.12422474
1	-7.02546692	3.56202745	0.69392473
1	6.77523279	-4.25407219	2.28482461
1	3.38123274	-1.93787241	-4.70787525
1	-0.44046718	-3.54437256	4.93902493
1	-1.20206714	-0.88227242	-4.72627544
1	-2.13536739	-0.43467242	-3.27917528
1	-0.91626716	0.67212754	-3.90887523
1	1.14463282	0.31112757	4.20432472
1	1.68123281	1.44162762	2.94132471
1	-0.05036719	1.20332766	3.22382474
8	2.97053266	5.27792788	-1.37737525
6	2.70203280	5.71372795	-0.12397526
6	2.80053282	4.65132761	0.96562469
8	2.30953264	3.36912751	0.48722473
6	2.69823265	2.95672750	-0.70867527
6	3.50013280	3.94812751	-1.53557527
8	2.41953278	6.86452770	0.08492474
1	4.52713299	3.92972755	-1.14207530
6	3.51223278	3.62102747	-3.01257539
6	2.01763272	5.00792789	2.20872474
1	3.86313272	4.52022791	1.21132469
8	2.43213272	1.83802760	-1.11067533
1	2.14043283	4.22462749	2.95872474
1	2.38773274	5.95252752	2.60972476
1	0.95773280	5.11882782	1.97552466
1	3.93823266	2.62922740	-3.16697526
1	2.49793267	3.63532758	-3.41607523
1	4.11653280	4.36082792	-3.54117537
8	-4.30726719	-0.91157246	-1.55397534
6	-3.63316727	-2.00247240	-1.23047531
6	-4.33946705	-3.32717252	-1.46907532
8	-5.72416687	-3.22937250	-1.09037530
6	-6.43216705	-2.15097260	-1.50607526
6	-5.61546707	-1.04967237	-2.17407537
8	-2.49926734	-1.92997241	-0.78477526
1	-5.44846725	-1.35547245	-3.21667528
6	-6.28686714	0.30412757	-2.12297535
6	-3.72546721	-4.47587204	-0.69927526
1	-4.28816700	-3.52897263	-2.54997540
8	-7.62596703	-2.10657239	-1.36387527
1	-4.27956724	-5.39197206	-0.91327530
1	-2.68366718	-4.60787249	-0.99467528
1	-3.76056719	-4.27677250	0.37292475
1	-7.27086687	0.23512758	-2.58957529
1	-6.40376711	0.64082754	-1.09127533
1	-5.68066692	1.03562760	-2.65977526

DTS-12__DBP-2_Mg-2_MeL-2_ssLA-1

Zero-point vibrational energy	2659906.4 (Joules/Mol)
	635.73290 (Kcal/Mol)
Zero-point correction =	1.013105 (Hartree/Particle)
Thermal correction to Energy =	1.077448
Thermal correction to Enthalpy =	1.078392
Thermal correction to Gibbs Free Energy =	0.911899
Sum of electronic and zero-point Energies =	-2940.353417
Sum of electronic and thermal Energies =	-2940.289074
Sum of electronic and thermal Enthalpies =	-2940.288130
Sum of electronic and thermal Free Energies =	-2940.454622



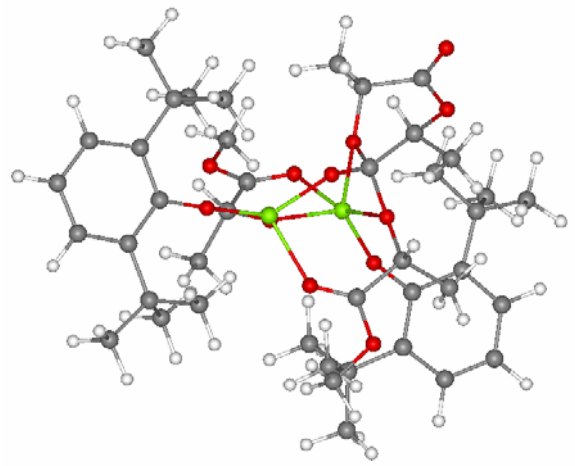
cartesian

12	1.72472477	0.31965083	0.41695487
12	-1.48997521	0.54645085	-0.39404514
8	3.49362469	-0.21334916	0.26305488
8	-2.92337513	-0.63824916	-0.21184513
8	0.37452477	0.14075083	-1.01164520
8	-1.62667525	1.14065075	-2.40974498
8	-0.49857524	1.06065083	-4.34474516
6	0.65172476	0.33775085	-2.37094498
6	1.17662477	-0.92144918	-3.06364512
1	1.39942479	1.13675082	-2.50904512
6	-0.59897524	0.87635082	-3.04344511
6	-1.66447520	1.57435083	-5.02574539
1	-1.38387525	1.61885083	-6.07594538
1	-2.51017523	0.90185082	-4.87804508
6	4.71152496	-0.53314918	-0.16924512
6	5.60312462	0.48245084	-0.64234513
6	6.84552479	0.09305084	-1.15254521
1	7.53142500	0.84275085	-1.53214514
6	7.24602461	-1.23764920	-1.18904519
6	6.40002489	-2.21064925	-0.66944510
1	6.74132490	-3.24024916	-0.67494512
6	5.14352465	-1.89744925	-0.14184514
6	5.24342489	1.97935081	-0.57844514
6	4.28242493	-3.01114917	0.48505485
6	6.39302492	2.88145089	-1.06394517
1	6.64142466	2.71255088	-2.11714506
1	7.30222464	2.74595094	-0.46924514
1	6.09242487	3.93055081	-0.96514511
6	4.94982481	2.39335084	0.87825489
1	4.65722466	3.44935083	0.92515486
1	5.84622478	2.26265073	1.49425483
1	4.15112495	1.79585087	1.31845486
6	4.04062462	2.29585075	-1.48734522
1	4.26972485	2.04475069	-2.52884507
1	3.78522468	3.36095095	-1.43834519
1	3.15522480	1.72925079	-1.19474518
6	4.99322462	-4.37684917	0.47375485
1	5.93862486	-4.35634899	1.02595484
1	5.19512463	-4.73314905	-0.54194510
1	4.34952497	-5.12174940	0.95555490
6	3.99542475	-2.67714906	1.96295488
1	3.47282481	-1.72424912	2.05935502
1	4.93172503	-2.61094928	2.52775502
1	3.38232470	-3.46624923	2.41795492
6	2.96382475	-3.20184922	-0.28734514
1	2.35712481	-2.29584908	-0.29094514
1	2.36812472	-4.00644922	0.16155487
1	3.16582489	-3.47644925	-1.32844520
6	-4.07897520	-1.29144919	-0.19564512
6	-4.06997538	-2.72994924	-0.23484513
6	-5.27917528	-3.41784906	-0.14194512
1	-5.28657532	-4.50214911	-0.15864512
6	-6.49817514	-2.75474906	-0.02664513
6	-6.50367498	-1.36984921	-0.03024513
1	-7.46327543	-0.86384916	0.04195487
6	-5.33067513	-0.60494918	-0.12484512
6	-2.75907516	-3.52344918	-0.39324513
6	-5.55607510	0.92715085	-0.15484512
6	-6.25277519	1.37435079	1.14835489
1	-7.21987534	0.88445085	1.28945482
1	-6.42977524	2.45725083	1.13935483
1	-5.63587523	1.13635087	2.02115488
6	-6.46367502	1.27845085	-1.35634518
1	-7.43727541	0.78535086	-1.30194521
1	-5.99307537	0.97405082	-2.29724503
1	-6.64397526	2.35975075	-1.39794517
6	-4.30207539	1.80235088	-0.30784515
1	-3.77697515	1.58555079	-1.24174511
1	-3.62427521	1.68875086	0.54325491
1	-4.61217499	2.85485077	-0.34404513
6	-2.99147511	-5.04444933	-0.44094515
1	-3.62687516	-5.34204912	-1.28154516
1	-3.43987513	-5.42614937	0.48255485
1	-2.02767515	-5.55014896	-0.56724513
6	-1.81397521	-3.26364923	0.79555488
1	-1.55907524	-2.20654917	0.86655492
1	-0.88517529	-3.83524895	0.67815489
1	-2.28867531	-3.57054925	1.73455489
6	-2.06967521	-3.14224911	-1.71844518
1	-2.71277523	-3.39554906	-2.56844497
1	-1.12597525	-3.69004917	-1.83134520
1	-1.85757518	-2.07314920	-1.76054513
1	8.21562481	-1.51094913	-1.59794521
1	-7.42767525	-3.31274915	0.05295487
1	-1.91007519	2.56875086	-4.65074539
1	1.37812483	-0.73484915	-4.12154531
1	2.10882473	-1.22284913	-2.58244514
1	0.45812476	-1.73924911	-2.97134495
8	-0.35297525	3.07765079	-0.03514513
6	0.15192474	2.67575073	1.19295478
6	-0.13237526	3.68775082	2.32835484
8	-0.02587525	5.03325081	1.81175482
6	-0.74657530	5.34085083	0.71305490
6	-1.33767521	4.13505077	-0.00764513
8	1.27112484	2.09985089	1.17175484
1	-2.21597528	3.79095078	0.55635488
6	-1.72647524	4.46815062	-1.43114519
6	0.87122470	3.61285090	3.46045494
1	-1.15517521	3.55005074	2.69465494
8	-0.87527525	6.48475075	0.35325485
1	0.63312471	4.37825060	4.20285463
1	0.85462475	2.63625073	3.94665504

1	1.87862480	3.78115082	3.07765484
1	-2.44957519	5.28535080	-1.42704523
1	-0.84977525	4.79085064	-1.99734509
1	-2.17257524	3.59785080	-1.91424513
8	-1.09677517	1.38345087	1.44545484
8	0.69042474	-0.67844915	1.90645480
8	-0.28737524	-1.14704919	3.85705495
6	-1.16087520	0.72515082	2.68475485
6	-2.58697510	0.28275084	3.02065492
1	-0.83377528	1.40595078	3.48415494
6	-0.16457525	-0.43254918	2.75665498
6	0.63322473	-2.25074911	4.03095484
1	1.65962481	-1.88364911	4.04325485
1	0.50452471	-2.96764922	3.22035503
1	0.36562476	-2.69334912	4.98805475
1	-2.62327528	-0.20204917	3.99865484
1	-3.22497511	1.16895080	3.04805493
1	-2.97277522	-0.39964914	2.26125503

DI-2__DBP-2_Mg-2_MeL-2_rrLA-1

Zero-point vibrational energy	2665223.0 (Joules/Mol)
	637.00358 (Kcal/Mol)
Zero-point correction =	1.015130 (Hartree/Particle)
Thermal correction to Energy =	1.079260
Thermal correction to Enthalpy =	1.080205
Thermal correction to Gibbs Free Energy =	0.915571
Sum of electronic and zero-point Energies =	-2940.357846
Sum of electronic and thermal Energies =	-2940.293716
Sum of electronic and thermal Enthalpies =	-2940.292772
Sum of electronic and thermal Free Energies =	-2940.457405



cartesian

12	-1.71694827	-0.11208668	0.57231170
12	1.41765177	-0.62828666	-0.56648833
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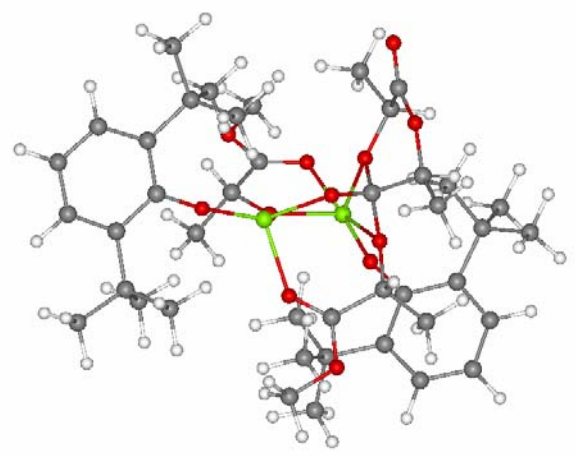
8	2.91745186	0.49801332	-0.68908828
8	-0.45904818	0.04361333	-0.95558828
8	1.20485175	-1.19938672	-2.58888817
8	-0.09064820	-0.85228664	-4.38548803
6	-0.81654817	0.09761332	-2.30708814
6	-0.88584816	1.52951324	-2.85088825
1	-1.79324830	-0.37928668	-2.48208833
6	0.19375181	-0.71338665	-3.10368824
6	0.86385179	-1.57998669	-5.18878841
1	0.46455181	-1.55318677	-6.20058823
1	1.83935177	-1.09428668	-5.14338827
6	-4.83684826	0.13931333	0.02491171
6	-5.55164814	-1.03618670	-0.37218827
6	-6.88244820	-0.90138668	-0.78038830
1	-7.44064808	-1.77468669	-1.10028827
6	-7.53314829	0.32691330	-0.78658831
6	-6.85104799	1.45351326	-0.34138829
1	-7.38384819	2.39821339	-0.32328829
6	-5.51944828	1.39651322	0.08071171
6	-4.90914822	-2.43598676	-0.32348827
6	-4.83544827	2.66731334	0.61961168
6	-5.89124823	-3.54778671	-0.73598832
1	-6.23714828	-3.43838668	-1.76948822
1	-6.76814795	-3.58838677	-0.08178828
1	-5.38674831	-4.51808643	-0.66298831
6	-4.46124792	-2.75928664	1.11641181
1	-3.99074793	-3.75018668	1.15831172
1	-5.32814837	-2.77218676	1.78591180
1	-3.75094819	-2.02758670	1.50131178
6	-3.71854806	-2.53508663	-1.29668820
1	-4.04594803	-2.34838676	-2.32548833
1	-3.27334809	-3.53758669	-1.25928819
1	-2.93984818	-1.80898666	-1.05728829
6	-5.78384829	3.87971330	0.64301169
1	-6.66094828	3.70701337	1.27521181
1	-6.12934828	4.15761375	-0.35838827
1	-5.25134802	4.74521351	1.05381167
6	-4.38104820	2.43941331	2.07571173
1	-3.69404817	1.59581327	2.15591168
1	-5.24524832	2.23201323	2.71581173
1	-3.88424802	3.33821321	2.46431184
6	-3.63854814	3.06671333	-0.26348826
1	-2.88624811	2.27831340	-0.29758829
1	-3.16264820	3.97811341	0.11981171
1	-3.96934795	3.26551318	-1.28878820
6	4.11265182	0.99021333	-0.39098829

6	4.30745173	2.41501331	-0.44648829
6	5.51885176	2.95091319	-0.01008829
1	5.67105198	4.02491331	-0.02038828
6	6.56275177	2.14371324	0.43621174
6	6.40275192	0.76771337	0.39441171
1	7.24395180	0.14641331	0.69181168
6	5.21335173	0.15341334	-0.02598829
6	3.22865176	3.34621334	-1.03178823
6	5.27125168	-1.39098668	-0.12248828
6	5.71295166	-2.00438666	1.22361171
1	6.70535183	-1.66778672	1.53401172
1	5.74505186	-3.09768677	1.15171170
1	5.00955200	-1.74258673	2.02071166
6	6.30515194	-1.76548672	-1.20868826
1	7.29845190	-1.37038672	-0.97858828
1	6.00735188	-1.36088669	-2.18188834
1	6.39045191	-2.85528684	-1.30158830
6	3.96415186	-2.10108662	-0.50658828
1	3.58145189	-1.75848675	-1.47128820
1	3.21325183	-1.97718668	0.28241172
1	4.15225172	-3.17818666	-0.58288831
6	3.68045187	4.81711340	-1.07048821
1	4.58465195	4.95741367	-1.67168820
1	3.86515188	5.22361374	-0.06998829
1	2.88945198	5.42371368	-1.52618825
6	1.93375170	3.30811334	-0.19848827
1	1.49455178	2.31051326	-0.19018829
1	1.19205177	4.00301361	-0.61268830
1	2.14155197	3.61351323	0.83421171
6	2.93825197	2.93211317	-2.48888826
1	3.84055185	3.04051328	-3.10068822
1	2.16005182	3.57241321	-2.92368817
1	2.61405182	1.89151335	-2.54428816
1	-8.56674767	0.40181333	-1.11538827
1	7.49575186	2.58331323	0.77991170
1	0.94625181	-2.60848665	-4.83438826
1	-1.16594827	1.53781331	-3.90778828
1	-1.64044821	2.08161330	-2.28848815
1	0.07535180	2.03331327	-2.72808814
8	-1.03334820	-1.53368676	1.78321171
8	1.16005170	-0.78628665	1.62161171
8	-0.71874821	1.35741329	1.63921177
8	0.53205180	2.39521337	3.16461182
6	1.15445173	0.16491331	2.68701172
6	2.59285188	0.56021333	2.99431181
1	0.70185179	-0.29498667	3.57031178
6	0.23665181	1.35521328	2.40901184
6	-0.33774820	3.54641318	3.05081177
1	-1.35684824	3.27101326	3.32421184
1	-0.31524819	3.92501330	2.02911162
1	0.06965180	4.27731371	3.74601173
1	2.63105178	1.24941325	3.83931184
1	3.15815187	-0.33908668	3.24591184
1	3.06605196	1.02911329	2.12961173
6	0.19145179	-1.92428672	1.66571176
8	0.54745179	-2.41588664	0.30631173
6	0.55035180	-3.05828667	2.66131186
6	0.52535182	-3.84318662	0.14461172
8	1.70085180	-3.82368684	2.25131178
6	0.70845181	-4.21248627	-1.31008828
6	1.62135172	-4.41978645	1.03841174
6	0.78115183	-2.68228674	4.11131191
8	2.38905191	-5.29308653	0.71861172
1	-0.33064818	-3.70878673	2.62601185
1	-0.45034820	-4.21308661	0.48801172
1	0.70545179	-5.30048656	-1.40318823
1	-0.11134820	-3.80248666	-1.90278828
1	1.65925169	-3.84218669	-1.69688821
1	0.87685180	-3.59988666	4.69711161
1	1.70375180	-2.11328673	4.24151182
1	-0.07154820	-2.12138677	4.50031185

DI-2__DBP-2_Mg-2_MeL-2_ssA-1

Zero-point vibrational energy	2663898.2 (Joules/Mol)
	636.68696 (Kcal/Mol)
Zero-point correction =	1.014625 (Hartree/Particle)
Thermal correction to Energy =	1.078962
Thermal correction to Enthalpy =	1.079906
Thermal correction to Gibbs Free Energy =	0.914172
Sum of electronic and zero-point Energies =	-2940.356908
Sum of electronic and thermal Energies =	-2940.292572
Sum of electronic and thermal Enthalpies =	-2940.291628
Sum of electronic and thermal Free Energies =	-2940.457361



cartesian

12	1.71713591	0.07149325	0.54454744
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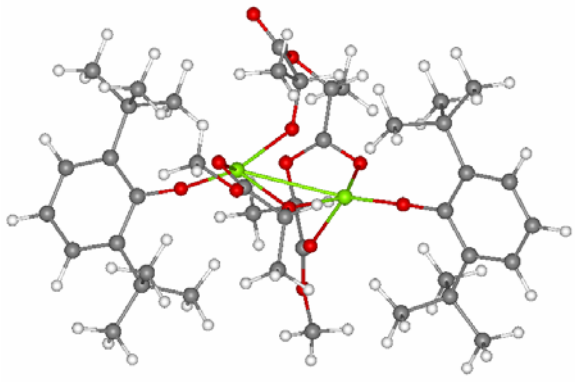
8	-3.02956414	-0.30010676	-0.65635252
8	0.42953593	-0.10700674	-0.96315253
8	-1.20326400	1.13409328	-2.63005257
8	0.07933591	0.69529325	-4.41685247
6	0.77353591	-0.22210674	-2.31485248
6	0.77433592	-1.67420673	-2.80705237
1	1.76853597	0.20509325	-2.51245236
6	-0.20836408	0.60209328	-3.13245249
6	-0.84556413	1.43619335	-5.24185228
1	-0.45426407	1.35399330	-6.25375223
1	-1.84246409	0.99889326	-5.17415237
6	4.80203629	-0.40380675	-0.02105255
6	5.55853605	0.73669326	-0.44175255
6	6.87263584	0.54039323	-0.87765253
1	7.46073627	1.38699329	-1.21515262
6	7.46843624	-0.71560675	-0.88865256
6	6.74873590	-1.80750668	-0.41705257
1	7.24133587	-2.77410674	-0.40125257
6	5.43093586	-1.68860674	0.03484745
6	4.97943592	2.16329312	-0.38915256
6	4.70733595	-2.92130685	0.60964739
6	6.00243616	3.23059320	-0.81935251
1	6.32583618	3.10609317	-1.85845256
1	6.89093590	3.23139310	-0.17965256
1	5.54223585	4.22159338	-0.73785257
6	4.56703615	2.51269317	1.05554748
1	4.12513590	3.51509309	1.09974742
1	5.44663620	2.50219321	1.70844746
1	3.84383583	1.80539334	1.46164739
6	3.78343582	2.31129313	-1.34965253
1	4.09673595	2.12789321	-2.38365245
1	3.36743593	3.32439327	-1.29285264
1	2.98553586	1.60319328	-1.11735260
6	5.60333586	-4.17250681	0.62714744
1	6.50413609	-4.02750683	1.23244739
1	5.90893602	-4.47980690	-0.37865254
1	5.04633617	-5.00830698	1.06614745
6	4.30063629	-2.65120673	2.07274747
1	3.64733577	-1.78100669	2.15304756
1	5.18823624	-2.46500683	2.68704748
1	3.78143573	-3.52400684	2.49074745
6	3.46923590	-3.28040671	-0.23305255
1	2.74753594	-2.46350694	-0.24575254
1	2.97263575	-4.17170668	0.17134744
1	3.75923586	-3.49780679	-1.26715255
6	-4.23546410	-0.73560679	-0.32135254
6	-4.49956369	-2.15000677	-0.35635257
6	-5.72516394	-2.62230682	0.11274745
1	-5.92906380	-3.68770671	0.11674745
6	-6.71906376	-1.76200676	0.57384741
6	-6.49416399	-0.39600676	0.51464748
1	-7.29816389	0.26759326	0.82354748
6	-5.28636408	0.15569326	0.06114745
6	-3.47846413	-3.13950682	-0.94955254
6	-5.27116394	1.70019329	-0.04555255
6	-5.63506413	2.33789325	1.31314743
1	-6.62956381	2.04959321	1.66274738
1	-5.62236404	3.43229318	1.23744738
1	-4.91686392	2.04249334	2.08584762
6	-6.32156372	2.12369323	-1.09715259
1	-7.32416391	1.77409327	-0.83685255
1	-6.07306385	1.70809329	-2.07935238
1	-6.36056376	3.21659327	-1.18745255
6	-3.94346428	2.34019327	-0.47665253
1	-3.60356426	1.97189331	-1.44735253
1	-3.17096424	2.17569327	0.28254744
1	-4.08686399	3.42519307	-0.56175256
6	-4.01026392	-4.58350658	-0.98005259
1	-4.92886400	-4.67330694	-1.56895256
1	-4.20336390	-4.97980690	0.02284745
1	-3.26036406	-5.23250675	-1.44615257
6	-2.17786407	-3.17030692	-0.12445255
1	-1.68216407	-2.19920683	-0.12295255
1	-1.47746408	-3.90560675	-0.54005253
1	-2.39356422	-3.45780683	0.91144741
6	-3.17626405	-2.74910688	-2.41105247
1	-4.08756399	-2.81110692	-3.01595235
1	-2.43856406	-3.43480682	-2.84685254
1	-2.79526424	-1.72860670	-2.47675252
1	8.49033642	-0.83830673	-1.23935258
1	-7.66416407	-2.15320683	0.94184744
1	-0.87606412	2.47999310	-4.92595243
1	1.05003595	-1.73400664	-3.86345243
1	1.50413597	-2.23910689	-2.22525239
1	-0.20916408	-2.12810683	-2.66455245
8	-0.52256411	2.43189311	0.23224744
6	-0.15706408	1.95519328	1.60034740
6	-0.58206409	3.07489324	2.57614756
8	0.20153591	4.24099302	2.24674749
6	0.19993591	4.66289330	0.96764743
6	-0.66556412	3.84909320	0.00884745
8	1.05873597	1.55289328	1.69394743
1	-1.70706403	4.12899351	0.22804745
6	-0.35556406	4.16659307	-1.43845260
6	-0.30706406	2.82059312	4.04574728
1	-1.64386404	3.30169320	2.41914749
8	0.79863590	5.65939331	0.64474750
1	-0.36546406	3.77419329	4.57644749
1	-1.05326402	2.15689325	4.48804760

1	0.69473588	2.40789318	4.18264771
1	-0.45896408	5.24109316	-1.60095263
1	0.66913593	3.87839317	-1.68055260
1	-1.04776406	3.63909316	-2.09715247
8	-1.14746404	0.82489324	1.59904742
8	0.68263590	-1.34860671	1.65704739
8	-0.60456413	-2.34220672	3.18284750
6	-1.13956404	-0.08600675	2.69864750
6	-2.57846427	-0.41190678	3.07454753
1	-0.63336408	0.38799328	3.54594755
6	-0.27166408	-1.31420672	2.42664742
6	0.22443591	-3.52360678	3.06894755
1	1.25633597	-3.28060675	3.32384753
1	0.17383592	-3.91090679	2.05134749
1	-0.19756408	-4.23350668	3.77714753
1	-2.61176419	-1.09090674	3.92794752
1	-3.09076405	0.51449323	3.34284759
1	-3.11046410	-0.86530679	2.23584747

DTS-23__DBP-2_Mg-2_MeL-2_rrLA-1

Zero-point vibrational energy	2661598.8 (Joules/Mol)
	636.13738 (Kcal/Mol)
Zero-point correction =	1.013749 (Hartree/Particle)
Thermal correction to Energy =	1.077781
Thermal correction to Enthalpy =	1.078725
Thermal correction to Gibbs Free Energy =	0.914935
Sum of electronic and zero-point Energies =	-2940.340866
Sum of electronic and thermal Energies =	-2940.276834
Sum of electronic and thermal Enthalpies =	-2940.275890
Sum of electronic and thermal Free Energies =	-2940.439681



cartesian

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8	3.04127312	0.20544995	-0.38771254
8	-0.39572698	0.46424997	-1.14311254
8	1.25907302	-0.59195006	-2.88071251
8	0.11397304	0.16444995	-4.65231276
6	-0.71402699	0.74384993	-2.47121263
6	-0.75512695	2.24565005	-2.77381253
1	-1.69142699	0.31654996	-2.74461246
6	0.31087303	0.04454996	-3.35461259
6	1.08047307	-0.47235006	-5.51851273
1	0.75607300	-0.23555005	-6.52961254
1	2.07617307	-0.07195004	-5.32481241
6	-4.65602684	0.10544996	-0.12861253
6	-5.34852695	-1.00075006	-0.71911252
6	-6.71282721	-0.86905003	-0.99461257
1	-7.25182676	-1.69065011	-1.45421255
6	-7.41902685	0.29014999	-0.69511253
6	-6.75262690	1.34294999	-0.07891254
1	-7.32282686	2.23154998	0.16938747
6	-5.38952684	1.28364992	0.22538747
6	-4.63732719	-2.33054996	-1.02831256
6	-4.71922684	2.46665001	0.94748747
6	-5.58282709	-3.38015008	-1.63911259
1	-6.00142717	-3.05505013	-2.59751248
1	-6.41122675	-3.63125014	-0.96891248
1	-5.02352715	-4.30425024	-1.82471251
6	-4.08342695	-2.94145012	0.27488747
1	-3.55632687	-3.88175011	0.06368747
1	-4.90302706	-3.17015004	0.96468747
1	-3.40452695	-2.25874996	0.78958744
6	-3.50552702	-2.12015009	-2.05201244
1	-3.90542698	-1.71365011	-2.98761249
1	-3.01302695	-3.07305002	-2.28291249
1	-2.75772691	-1.41935003	-1.67621255
6	-5.70782709	3.60395002	1.26228750
1	-6.52562714	3.27504992	1.91168749
1	-6.14102697	4.04015017	0.35608748
1	-5.17822695	4.40735006	1.78758752
6	-4.14922714	1.99724984	2.30148745
1	-3.42952704	1.18514991	2.18618751
1	-4.95572710	1.62934995	2.94478750
1	-3.66362691	2.83095002	2.82578754
6	-3.61482692	3.08174992	0.06728747
1	-2.84462690	2.35104990	-0.18131253
1	-3.13912702	3.93144989	0.57408744
1	-4.04022694	3.45144987	-0.87221253
6	4.32857323	0.53024995	-0.26151255
6	4.74047279	1.89534998	-0.40321255
6	6.08397293	2.21784997	-0.18661253
1	6.41297293	3.24784994	-0.27151254
6	7.03307295	1.25384998	0.13028747
6	6.63897324	-0.07655004	0.20628746
1	7.39637280	-0.82115006	0.42548746
6	5.31297302	-0.47445005	0.00998747
6	3.76267314	3.00125003	-0.84051251

6	4.95437288	-1.96855009	0.09098747
6	4.00657320	-2.22465014	1.27628744
1	4.49477291	-1.93675005	2.21438742
1	3.74857306	-3.28675008	1.34448743
1	3.08447313	-1.64745009	1.20218742
6	6.18567324	-2.86415005	0.31988746
1	6.67477322	-2.66285014	1.27888751
1	6.93037319	-2.76055002	-0.47651255
1	5.86597300	-3.91184998	0.33458745
6	4.32907295	-2.44515014	-1.23621249
1	5.06937313	-2.40195012	-2.04291248
1	3.49177313	-1.81695008	-1.54781258
1	3.97987294	-3.48025012	-1.14911258
6	4.43267298	4.38345003	-0.93681252
1	5.24547291	4.40245008	-1.66981256
1	4.82977295	4.72034979	0.02668747
1	3.68897295	5.12155008	-1.25891256
6	2.60097313	3.15044999	0.15888746
1	2.03877306	2.22254992	0.25738746
1	1.91377306	3.93914986	-0.17401254
1	2.98537302	3.43004990	1.14698744
6	3.22607303	2.67374992	-2.24781251
1	4.04997301	2.64394999	-2.96901250
1	2.51607299	3.44164991	-2.58031249
1	2.73197293	1.70094991	-2.26821256
1	-8.47872734	0.36654997	-0.92571253
1	8.07037258	1.53374994	0.29718748
1	1.07697296	-1.55065000	-5.35371256
1	-1.01182699	2.43214989	-3.82001257
1	-1.51512694	2.70554996	-2.14031243
1	0.20857303	2.70895004	-2.55121255
8	0.20567304	-1.77585006	0.36798745
6	-0.18702696	-1.57985008	2.21418738
6	-0.12592697	-3.04474998	2.65818739
8	0.94387305	-3.80505013	2.09358740
6	0.92237300	-4.02904987	0.75668746
6	-0.01692697	-3.12555003	-0.04591253
8	-1.31762695	-1.03085005	2.22588754
6	0.18647304	-3.32865000	-1.53511250
6	0.02287303	-3.12705016	4.16888762
8	0.94237304	-0.85045004	2.52038741
8	-0.33922699	1.42104995	1.46188748
8	0.28147304	2.61094999	3.25088739
6	0.78957301	0.31194997	3.33178735
6	2.16727304	0.62774992	3.90228748
1	0.08077303	0.10534996	4.14428759
6	0.19017303	1.48694992	2.56688738
6	-0.29972699	3.79204988	2.64938736
1	-1.36802697	3.64104986	2.49528742
1	0.19127303	3.99965000	1.69908750
1	-0.11822696	4.59135008	3.36488748
1	2.11507297	1.48784995	4.57098770
1	2.52487302	-0.23795004	4.46258736
1	2.87747312	0.83664995	3.09978747
1	-1.05332696	-3.40455008	0.19708747
1	-0.03072697	-4.36644983	-1.79961252
1	-0.48882699	-2.67945004	-2.09511256
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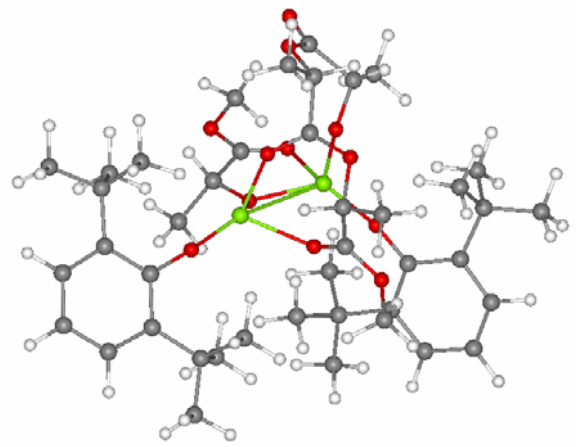
1	-1.08542693	-3.48154998	2.36568737
1	-0.02942697	-4.17315006	4.47888756
1	0.98787302	-2.72084999	4.47898769
1	-0.78452700	-2.57855010	4.66018724
8	1.64107299	-4.87135029	0.27538747

DTS-23__DBP-2_Mg-2_MeL-2_ssLA-1

Zero-point vibrational energy	2661548.1 (Joules/Mol)
	636.12527 (Kcal/Mol)
Zero-point correction =	1.013730 (Hartree/Particle)
Thermal correction to Energy =	1.077827
Thermal correction to Enthalpy =	1.078771
Thermal correction to Gibbs Free Energy =	0.913359
Sum of electronic and zero-point Energies =	-2940.352798
Sum of electronic and thermal Energies =	-2940.288701
Sum of electronic and thermal Enthalpies =	-2940.287757
Sum of electronic and thermal Free Energies =	-2940.453169



cartesian

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8	-3.01421833	-0.16186912	-0.58924991
8	0.31478170	0.73603088	-1.42264998
8	-1.68771839	1.99583089	-2.58844995
8	-0.44171831	2.64153099	-4.33654976
6	0.62738168	1.30993080	-2.66114998
6	1.15588164	0.28823087	-3.67175007
1	1.37908161	2.10843086	-2.55145001
6	-0.61181831	2.01043081	-3.19304991
6	-1.57721841	3.37443089	-4.85125017
1	-1.24011838	3.79123092	-5.79794979
1	-2.42141819	2.70073104	-5.00145006
6	4.40168190	-0.92236912	0.02285009
6	5.51768160	-0.10586913	-0.34404993
6	6.75848198	-0.72186917	-0.53504992
1	7.61828184	-0.12536915	-0.82004988
6	6.93848181	-2.09016895	-0.36814994
6	5.85498190	-2.87196898	0.01505009
1	6.01578188	-3.93556881	0.15465009
6	4.58468199	-2.32656908	0.22305009
6	5.39018154	1.41983080	-0.51214987
6	3.42728186	-3.23776913	0.67165011
6	6.72808170	2.08743095	-0.87944990
1	7.12998199	1.72283089	-1.83074999
1	7.48858166	1.94213080	-0.10524992
1	6.57368183	3.16723108	-0.98464990
6	4.93068171	2.06473088	0.81085008
1	4.82928181	3.15053105	0.69275010
1	5.67148161	1.87853086	1.59615004
1	3.97478175	1.66623080	1.15155005
6	4.41508198	1.75963080	-1.65604997
1	4.26738167	2.84323096	-1.73494995
1	3.44138169	1.28883088	-1.50604999
1	4.80528164	1.39763081	-2.61334991
6	3.86868167	-4.69936895	0.86775011
1	4.64908171	-4.79836893	1.62935007
1	4.23338175	-5.15106916	-0.06064991
1	3.01008177	-5.29346895	1.20125008
6	2.88058186	-2.76286912	2.03345013
1	2.56318188	-1.71956921	1.98845005
1	3.65548182	-2.84246898	2.80355000
1	2.03148174	-3.38416910	2.34704995
6	2.31168175	-3.26016903	-0.39064991
1	1.90738165	-2.26616907	-0.58594990
1	1.48698163	-3.90916920	-0.07094992
1	2.69488168	-3.65196896	-1.33875000
6	-3.76091814	-1.23176920	-0.33094993
6	-3.62941813	-2.42846894	-1.11264992
6	-4.30741835	-3.57926893	-0.69494987
1	-4.19441843	-4.50096893	-1.25534999
6	-5.14041805	-3.58906913	0.41795006
6	-5.36531830	-2.39496899	1.09325004
1	-6.07021809	-2.39806914	1.91795003
6	-4.72711802	-1.20376921	0.73235011
6	-2.78131819	-2.48676896	-2.39734983
6	-5.13551807	0.10733087	1.42825007
6	-3.96731830	0.72913086	2.21495008
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1	-6.57461834	0.67493087	-0.10154992
1	-4.93601847	1.23403084	-0.44174993
1	-5.91891813	2.05073094	0.80005008
6	-2.99361825	-3.79686880	-3.17934990
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1	-2.62931824	-4.67596912	-2.63734984
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1	-0.67581832	-2.49876904	-2.96845007
1	-1.00211835	-3.25486898	-1.40594995
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1	-5.64311838	-4.50286913	0.72515011
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8	0.29138172	4.77463102	1.05185008
6	-0.81851828	4.76523113	0.26435009
6	-1.87891841	3.73423100	0.64925009
8	1.27618170	2.00473094	1.22555006
1	-2.23711824	3.96123099	1.66685009
6	-3.08351827	3.82473087	-0.27084991
6	1.53448164	4.34573078	3.02104998
1	-0.59871829	4.16403103	2.82975006
8	-0.87051827	5.50723076	-0.68864989
1	1.49568164	5.41083097	3.26065016
1	1.57818162	3.78023100	3.95515013
1	2.43348169	4.14433098	2.43604994

1	-3.54971814	4.80983114	-0.17634991
1	-2.80511832	3.69313097	-1.31754994
1	-3.82031822	3.07133102	0.01175009
8	-0.22141831	1.77553082	2.93044996
8	-0.03441831	-0.53906918	1.09335005
8	-0.93261832	-1.51546919	2.89444995
6	0.31368169	0.48763084	3.26425004
6	0.01728169	0.24453086	4.73085022
1	1.39668167	0.49643087	3.08665013
6	-0.24811831	-0.57116914	2.31334996
6	-1.45041835	-2.59356904	2.06255007
1	-0.64301831	-3.00276899	1.45635009
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1	-1.83021832	-3.32896900	2.76754999
1	0.42598170	-0.71696913	5.04764986
1	0.48468170	1.03413093	5.32315016
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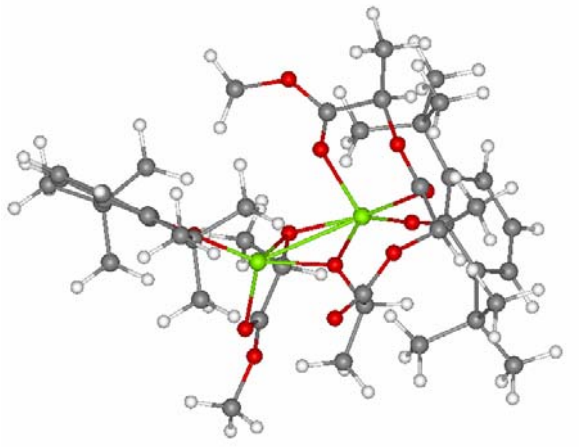
DI-3__DBP-2_Mg-2_MeL-2_rrLA-1

Zero-point vibrational energy	2663404.3 (Joules/Mol)
	636.56890 (Kcal/Mol)
Zero-point correction =	1.014437 (Hartree/Particle)
Thermal correction to Energy =	1.079219
Thermal correction to Enthalpy =	1.080163
Thermal correction to Gibbs Free Energy =	0.914115
Sum of electronic and zero-point Energies =	-2940.358217
Sum of electronic and thermal Energies =	-2940.293435
Sum of electronic and thermal Enthalpies =	-2940.292491
Sum of electronic and thermal Free Energies =	-2940.458539



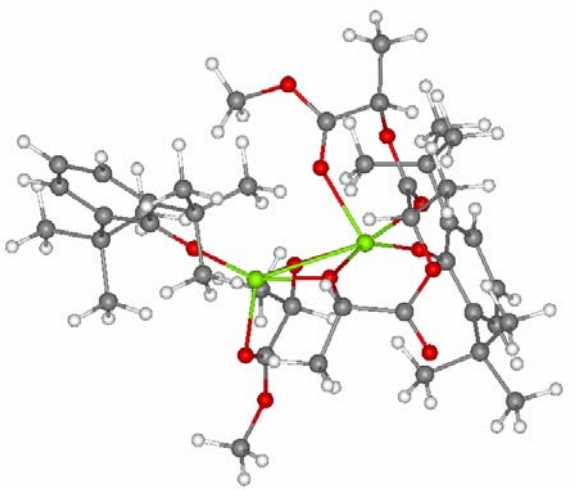
cartesian

12	-1.27068567	0.37295410	-0.15949336
12	1.31891429	-0.51334590	0.94390661
8	-3.08298564	-0.12164590	-0.19739337
8	3.08131433	-0.63204587	0.33410662
8	-0.22888565	-1.35064590	-0.02159336
8	0.82581431	-2.00454593	2.32760668
8	-0.55668569	-3.74404597	2.60740662
6	-0.73868567	-2.51734591	0.54710662
6	-0.50968570	-3.75724578	-0.32739335
1	-1.82088566	-2.43054581	0.72980660
6	-0.08768566	-2.72814584	1.90890670
6	0.06061434	-3.99384570	3.88870668
1	-0.45018566	-4.86884594	4.28550625
1	1.12551427	-4.19094610	3.75920677
6	-4.33978558	-0.52514589	-0.31709337
6	-5.19898558	-0.55624586	0.83030665
6	-6.49538565	-1.05844593	0.68420660
1	-7.15638542	-1.10574591	1.54330671
6	-6.98298550	-1.50304592	-0.53959340
6	-6.16558552	-1.41654587	-1.66089332
1	-6.57118559	-1.74054587	-2.61349320
6	-4.85788536	-0.92714584	-1.59239328
6	-4.73958540	-0.02374589	2.20060658
6	-4.02278566	-0.80734587	-2.88139343
6	-5.83978558	-0.12464589	3.27200675
1	-6.13458538	-1.16104591	3.46850657
1	-6.73578548	0.44275409	3.00010657
1	-5.46488523	0.29125410	4.21410656
6	-4.37278557	1.46995413	2.08340669
1	-3.99528575	1.84855413	3.04300666
1	-5.25788546	2.05845404	1.81740665
1	-3.61948562	1.63745415	1.31180668
6	-3.53948569	-0.82804590	2.73560667
1	-3.79688573	-1.88924599	2.82470679
1	-3.24738574	-0.46664590	3.72990680
1	-2.67858577	-0.74404585	2.07070661
6	-4.80328560	-1.24144590	-4.13469362
1	-5.70618534	-0.64184588	-4.28929377
1	-5.09178543	-2.29704595	-4.09879351
1	-4.16788530	-1.10964584	-5.01809359
6	-3.62178564	0.66515410	-3.10689330
1	-3.09988570	1.07495403	-2.24039340
1	-4.51288557	1.28035414	-3.27399325
1	-2.97928572	0.75625414	-3.99349332
6	-2.77328563	-1.70624590	-2.81449342
1	-2.13888574	-1.46954584	-1.95999336
1	-2.17398572	-1.60434592	-3.72839332
1	-3.06998563	-2.75734591	-2.72619343
6	4.35661459	-0.63784587	-0.05179336

6	4.90871477	-1.78984582	-0.70229340
6	6.22811460	-1.73074591	-1.16369331
1	6.66091442	-2.58834577	-1.66689336
6	7.02201462	-0.60254586	-0.99629337
6	6.49791479	0.49235409	-0.31989336
1	7.13721466	1.35555410	-0.16959336
6	5.18961477	0.50595409	0.17340663
6	4.10191441	-3.08764577	-0.89569336
6	4.69491434	1.72385406	0.97220665
6	3.52301431	2.41585422	0.24920663
1	3.84161425	2.75355411	-0.74439335
1	3.18491435	3.29165411	0.81210661
1	2.66941428	1.74735415	0.11990663
6	5.78291464	2.79955411	1.14650667
1	6.11021471	3.22165418	0.19000664
1	6.66261435	2.41635418	1.67380667
1	5.37701464	3.62275410	1.74420667
6	4.29761457	1.28065407	2.39500666
1	5.17401457	0.88585413	2.92080665
1	3.54801440	0.48615408	2.37860680
1	3.89691424	2.12055397	2.96960664
6	4.93391466	-4.20884609	-1.54479337
1	5.81471443	-4.47174597	-0.94949335
1	5.26591444	-3.95094609	-2.55619335
1	4.31611443	-5.11004591	-1.62829328
6	2.90201426	-2.84154582	-1.82919335
1	2.20261431	-2.11204576	-1.41799331
1	2.35501432	-3.77524590	-2.00939322
1	3.25401425	-2.47824597	-2.80209327
6	3.63281441	-3.63024592	0.46870661
1	4.49651432	-3.88824582	1.09120667
1	3.03331423	-4.53994608	0.33430666
1	3.03911424	-2.89624596	1.01380670
1	-7.99398565	-1.89454579	-0.62189341
1	8.04291439	-0.58504587	-1.37019336
1	-0.07848566	-3.13454580	4.54610634
1	-0.97938573	-4.64214611	0.11070664
1	-0.95248568	-3.57114577	-1.30689335
1	0.55731434	-3.94514585	-0.46259338
8	0.06781434	1.03925407	1.25930667
6	-1.02938569	3.42285419	-0.30769336
6	-0.92988569	4.27725410	0.95050663
8	0.34751433	4.11265421	1.56630671
6	0.64011431	3.07385421	2.42090678
6	-0.22938564	1.80105412	2.41050673
8	-1.82568574	2.50165415	-0.41819334
6	-0.00008566	1.03215408	3.70410657
6	-1.09828568	5.75935411	0.65530664
8	1.61881435	3.20525408	3.11250663
8	-0.18708566	3.79615402	-1.26679337
8	0.16911435	0.89335412	-1.68319333
8	1.55811429	1.74335408	-3.21959329
6	-0.26938567	3.11425424	-2.54829335
6	0.22601435	4.08235407	-3.59989333
1	-1.31358564	2.83505416	-2.71799326
6	0.51111436	1.80305409	-2.43309331
6	2.35111427	0.52365410	-3.17669320
1	1.71231437	-0.33234590	-3.39219332
1	2.80931425	0.41475409	-2.19409323
1	3.10811424	0.65715414	-3.94569325
1	0.17411435	3.61875415	-4.58709335
1	-0.40998566	4.97055387	-3.60029340
1	1.25761437	4.38135386	-3.40909338
1	-1.73168564	3.93245411	1.60730672
1	-1.07808566	6.31295395	1.59650671
1	-0.28838566	6.11785412	0.01790664
1	-2.05598569	5.94605398	0.16100663
1	-0.27398565	1.63645411	4.57460642
1	-0.61488569	0.12965411	3.69920659
1	1.05181432	0.75565410	3.81330657
1	-1.28868568	2.09555411	2.38340664

DI-3__DBP-2_Mg-2_MeL-2_ssLA-1

Zero-point vibrational energy	2662600.9 (Joules/Mol)
	636.37688 (Kcal/Mol)
Zero-point correction =	1.014131 (Hartree/Particle)
Thermal correction to Energy =	1.078927
Thermal correction to Enthalpy =	1.079871
Thermal correction to Gibbs Free Energy =	0.913537
Sum of electronic and zero-point Energies =	-2940.360725
Sum of electronic and thermal Energies =	-2940.295929
Sum of electronic and thermal Enthalpies =	-2940.294984
Sum of electronic and thermal Free Energies =	-2940.461319



cartesian

12	-1.28508651	0.47762078	0.03895428
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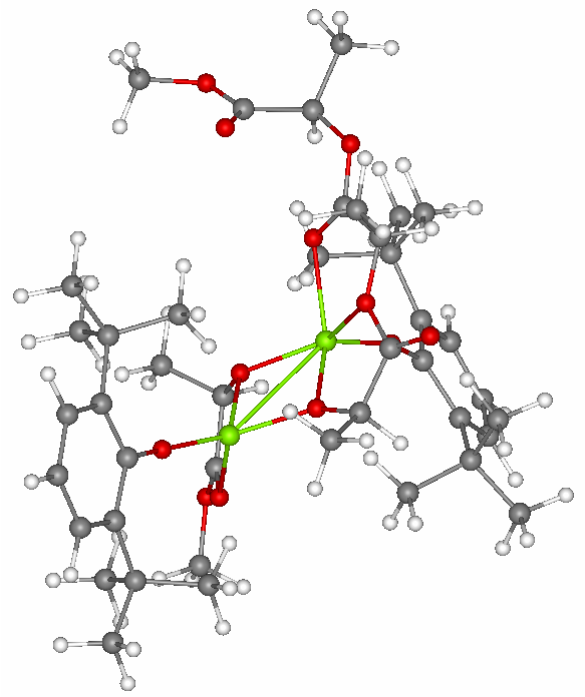
8	-3.10268641	0.15462077	-0.30164570
8	3.05031347	-0.64577925	0.47695428
8	-0.36978653	-1.33347929	-0.08314572
8	0.67241347	-2.38407922	2.11725450
8	-0.88458651	-3.98967910	2.24215436
6	-0.97598654	-2.51507926	0.34525430
6	-0.88098651	-3.64327931	-0.68964571
1	-2.04168653	-2.35867929	0.56915426
6	-0.32318652	-2.95497918	1.64965427
6	-0.29118654	-4.43517923	3.48085427
1	-0.88938653	-5.28877878	3.79285431
1	0.74681348	-4.72737885	3.31645441
6	-4.27088642	-0.43817922	-0.50554574
6	-5.13008642	-0.74757928	0.59955424
6	-6.29688644	-1.47657931	0.35155427
1	-6.94798660	-1.74577928	1.17655432
6	-6.67078638	-1.86427927	-0.93134570
6	-5.88638639	-1.46817923	-2.00914550
1	-6.21938658	-1.73057926	-3.00804567
6	-4.70268631	-0.74407923	-1.83794570
6	-4.83288670	-0.23767921	2.02365422
6	-3.91488647	-0.26317921	-3.07164550
6	-5.95748663	-0.58687925	3.01545429
1	-6.07938671	-1.66767919	3.14815450
1	-6.92098665	-0.16687921	2.70865440
1	-5.71398640	-0.16337922	3.99635434
6	-4.72128630	1.30092072	2.00655437
1	-4.46838665	1.68132079	3.00235438
1	-5.67758656	1.74212074	1.70375431
1	-3.95788646	1.64242077	1.30655432
6	-3.54708648	-0.86007923	2.60005450
1	-3.63038659	-1.95267916	2.63975430
1	-3.36418653	-0.49067923	3.61535430
1	-2.67158651	-0.60797924	1.99865425
6	-4.65088654	-0.55717927	-4.39114571
1	-5.64078665	-0.09037923	-4.42244577
1	-4.77048635	-1.63047922	-4.57214546
1	-4.06908655	-0.15227923	-5.22764540
6	-3.72838664	1.26752079	-3.01094556
1	-3.23468661	1.57232070	-2.08644557
1	-4.70048666	1.77142072	-3.04854560
1	-3.14078641	1.61302078	-3.87324572
6	-2.54998660	-0.97097921	-3.16214561
1	-1.96098650	-0.84857923	-2.25254560
1	-1.96768653	-0.58427924	-4.00974560
1	-2.69218659	-2.04537916	-3.32394552
6	4.30281353	-0.61047924	0.02615428
6	4.87121344	-1.74287927	-0.64474571
6	6.16691351	-1.63487923	-1.16044569
1	6.61081362	-2.47697926	-1.67964578
6	6.92471361	-0.47767922	-1.02834570
6	6.38781357	0.60002077	-0.33514571
1	7.00051355	1.48692071	-0.21604572
6	5.10081339	0.56592077	0.21075428
6	4.10721350	-3.07057929	-0.80464572
6	4.59371328	1.77592075	1.01665425
6	3.36051345	2.40532064	0.34135431
1	3.60411358	2.72302079	-0.67914575
1	3.04371357	3.29922080	0.89495426
1	2.52161336	1.70912075	0.29475427
6	5.64531326	2.89452076	1.12845433
1	5.91381359	3.31492066	0.15345427
1	6.56141329	2.55332065	1.62095428
1	5.23761368	3.71202064	1.73385429
6	4.26311350	1.33952069	2.45715427
1	5.16731358	0.98532075	2.96315432
1	3.53711343	0.52552074	2.46955442
1	3.86271358	2.18082070	3.03745437
6	4.95491362	-4.16097879	-1.48574579
1	5.86831331	-4.38667917	-0.92564571
1	5.23501348	-3.89467931	-2.51054573
1	4.37001371	-5.08597898	-1.54134572
6	2.86661339	-2.87357926	-1.69534576
1	2.16191339	-2.15047932	-1.28134573
1	2.33691359	-3.82417917	-1.83314574
1	3.16841340	-2.52087927	-2.68844557
6	3.71331358	-3.63247919	0.57605428
1	4.61081362	-3.87997913	1.15325427
1	3.12491345	-4.55167913	0.46115428
1	3.13171339	-2.92047930	1.16155422
1	-7.58058643	-2.43777919	-1.09164572
1	7.92801332	-0.42357925	-1.44364572
1	-0.33838654	-3.63847923	4.22445440
1	-1.40018654	-4.54147911	-0.34454572
1	-1.35118651	-3.29917932	-1.61174572
1	0.16171348	-3.88877916	-0.90394574
8	0.14141348	0.83672076	1.47655427
6	-0.67498654	3.44832087	0.07645428
6	-0.21228653	4.09552097	1.37125432
8	-1.01418650	3.64432073	2.44435430
6	-0.86958653	2.41632080	3.04175448
6	0.34261349	1.53182077	2.68775439
8	-1.58628654	2.64322066	-0.00104572
1	1.22291350	2.18752074	2.59055448
6	0.60251349	0.58832079	3.85675430
6	-0.32418653	5.61712122	1.32815433
1	0.83841348	3.81102085	1.49625432
8	-1.69228649	2.11092067	3.86775446
1	0.03361347	6.02522087	2.27545428
1	0.27941349	6.02372122	0.51495427

1	-1.36548650	5.91862106	1.19385421
1	0.78551346	1.14522076	4.78055429
1	-0.25368652	-0.06897923	4.01645422
1	1.49191344	-0.01807923	3.65605450
8	0.05281347	3.85632086	-0.96654570
8	0.15181348	1.00322080	-1.52084577
8	1.39361346	1.80472076	-3.20154572
6	-0.24448654	3.27032065	-2.26524568
6	0.19431347	4.25982094	-3.32104564
1	-1.31928647	3.07492065	-2.31664562
6	0.45031345	1.90772080	-2.29254556
6	2.11111355	0.54132074	-3.25354552
1	1.40421343	-0.27637923	-3.39194560
1	2.67411351	0.40152079	-2.33054566
1	2.78031349	0.63502073	-4.10554552
1	-0.01248653	3.85782075	-4.31494570
1	-0.36698651	5.18902111	-3.19984555
1	1.26171350	4.47372103	-3.24754572

DI-4__DBP-2_Mg-2_MeL-2_rrLA-1

Zero-point vibrational energy	2660985.0 (Joules/Mol)
	635.99069 (Kcal/Mol)
Zero-point correction =	1.013516 (Hartree/Particle)
Thermal correction to Energy =	1.079010
Thermal correction to Enthalpy =	1.079955
Thermal correction to Gibbs Free Energy =	0.908691
Sum of electronic and zero-point Energies =	-2940.384483
Sum of electronic and thermal Energies =	-2940.318988
Sum of electronic and thermal Enthalpies =	-2940.318044
Sum of electronic and thermal Free Energies =	-2940.489307



cartesian

12	1.12330186	-0.08287913	-0.43051589
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8	-3.44989800	-0.15447912	0.39658415
8	-0.00659817	-0.28697914	1.19648409
8	-1.48939812	-2.44967890	1.49098420
8	-0.30699816	-3.18447900	3.24698400
6	0.30440184	-1.05357909	2.31978393
6	0.12220183	-0.26997912	3.62408400
1	1.33920181	-1.42727911	2.27838397
6	-0.58039820	-2.29447913	2.31428409
6	-1.12449813	-4.37607908	3.26668406
1	-0.74789816	-4.96607924	4.09958410
1	-2.17109799	-4.10967922	3.41888404
6	3.65350199	-1.98937905	-0.18181586
6	3.57810187	-3.30557895	-0.74691588
6	4.49430180	-4.27277946	-0.32171589
1	4.43640184	-5.27917910	-0.72141588
6	5.49600172	-3.99337888	0.59988415
6	5.62310171	-2.69377899	1.07428420
1	6.43870163	-2.47687912	1.75568414
6	4.74760151	-1.67287910	0.69138414
6	2.53220201	-3.68587899	-1.81251585
6	5.02180147	-0.23397912	1.16858411
6	2.77090192	-5.08977938	-2.39901590
1	2.64930201	-5.88287926	-1.65361583
1	3.76560187	-5.18657923	-2.84651589
1	2.03520179	-5.27697945	-3.18921590
6	2.60250187	-2.70757890	-3.00201607
1	1.84130180	-2.95607901	-3.75211596
1	3.58170199	-2.77367902	-3.48891592
1	2.46290183	-1.67397916	-2.68241596
6	1.12240183	-3.70547891	-1.19481587
1	1.07860184	-4.43297911	-0.37651587
1	0.37250182	-3.99697900	-1.94131589
1	0.83410180	-2.73117900	-0.80001587
6	6.31820154	-0.12047912	1.99108422
1	7.19650173	-0.45417911	1.42928410
1	6.27040148	-0.68907917	2.92598414
1	6.48210192	0.92932087	2.26078391
6	5.20660162	0.67442089	-0.06351587
1	4.32630157	0.64932084	-0.70731586
1	6.06710148	0.34092087	-0.65381587

1	5.40080166	1.71012092	0.24698414
6	3.89110184	0.28842089	2.07278395
1	2.93290186	0.31002086	1.55568409
1	4.10990191	1.30692089	2.41958404
1	3.78990197	-0.34747910	2.95928407
6	-4.65649843	0.33842087	0.13438413
6	-4.85939837	1.75412083	0.07498413
6	-6.12849808	2.23122096	-0.26771587
1	-6.30359840	3.29982090	-0.33391589
6	-7.19429827	1.37652087	-0.52551585
6	-7.00439835	0.00432088	-0.40301585
1	-7.85509825	-0.64687914	-0.57401586
6	-5.76519823	-0.54577911	-0.06171587
6	-3.73199797	2.75052094	0.40748411
6	-5.63199806	-2.06857896	0.13458413
6	-4.66259813	-2.68257904	-0.89321584
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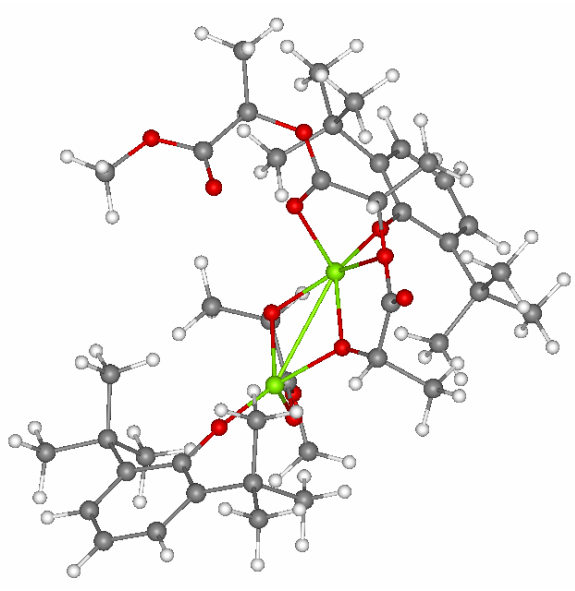
6	-5.15709829	-2.36897898	1.57138419
1	-5.89409828	-2.00537896	2.29588413
1	-4.20309830	-1.88737917	1.78778410
1	-5.04389811	-3.45077896	1.71848416
6	-4.21289825	4.21292067	0.37588412
1	-5.02039814	4.39762068	1.09208417
1	-4.55799818	4.51752090	-0.61791587
1	-3.37889814	4.87132072	0.64458412
6	-2.58619809	2.65312099	-0.61811584
1	-2.15969801	1.64952087	-0.66091585
1	-1.78249812	3.35482097	-0.36311585
1	-2.95099807	2.90132093	-1.62131584
6	-3.20049810	2.49542093	1.83298409
1	-3.99759793	2.65142107	2.56808400
1	-2.38309813	3.18922091	2.06598401
1	-2.83249807	1.47552085	1.94888413
1	6.18740177	-4.76947927	0.91878414
1	-8.16819763	1.77622092	-0.79771584
1	-1.01369822	-4.91847944	2.32688403
1	0.37300181	-0.87757915	4.49758434
1	0.78330183	0.59902084	3.59638405
1	-0.90749818	0.08722088	3.71588397
8	-0.57819819	-0.70997912	-1.36521590
6	2.16590190	2.59812093	-1.28031588
6	1.61860180	2.24652100	-2.65491605
8	0.85230184	1.06682086	-2.37301588
6	0.19140182	0.38982087	-3.37291598
6	-0.69129819	-0.69617915	-2.75621605
8	1.91900182	1.93742085	-0.27771586
6	-2.12639809	-0.51887912	-3.25591588
8	0.32970181	0.64732087	-4.54151583
8	2.91650200	3.68422103	-1.28871584
8	1.09770179	5.03842068	0.17828412
8	2.53350186	5.23282051	1.91888416
6	3.36810184	4.18892097	-0.01281587
6	4.51080179	5.15082073	-0.29091588
1	3.69930196	3.35062099	0.60368413
6	2.18370199	4.86202097	0.68138415
6	1.50030184	5.88322067	2.68688393
1	0.64880180	5.21272087	2.81318402
1	1.17550182	6.79652071	2.18568397
1	1.95650184	6.11212063	3.64808393
1	4.88880157	5.54952097	0.65188414
1	5.32110167	4.62372065	-0.79931587
1	4.17890167	5.98032093	-0.91981584
1	-0.29719818	-1.63427913	-3.17821598
1	-2.15289807	-0.48027915	-4.34791565
1	-2.72939801	-1.36667919	-2.92421603
1	-2.57159805	0.39522088	-2.85521603
1	2.44610190	1.99242091	-3.32591605
6	0.78000182	3.38422108	-3.22651601
1	0.39980182	3.10512090	-4.20851564
1	-0.05249817	3.61932087	-2.56071591
1	1.40460181	4.27372074	-3.32761598

DI-4__DBP-2_Mg-2_MeL-2_ssLA-1

Zero-point vibrational energy	2664380.4 (Joules/Mol)
	636.80219 (Kcal/Mol)
Zero-point correction =	1.014809 (Hartree/Particle)
Thermal correction to Energy =	1.079737
Thermal correction to Enthalpy =	1.080681
Thermal correction to Gibbs Free Energy =	0.912948
Sum of electronic and zero-point Energies =	-2940.385737
Sum of electronic and thermal Energies =	-2940.320809
Sum of electronic and thermal Enthalpies =	-2940.319865
Sum of electronic and thermal Free Energies =	-2940.487599



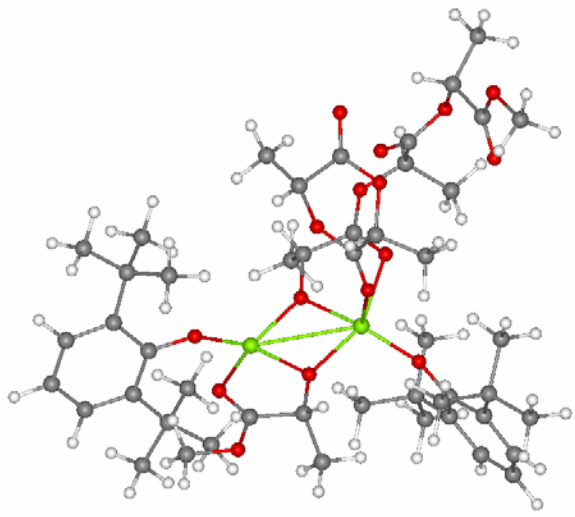
cartesian

12	1.14836144	0.14492238	-0.51415914
12	-1.65723848	-0.91667759	-0.22015914
8	2.94526148	-0.43387759	-0.31355914
8	-3.45353842	-0.46947759	-0.02465914
8	-0.03473852	-0.58907759	0.92834085
8	-1.24843848	-2.87727761	0.40034086
8	-0.01133852	-4.02677774	1.87274086
6	0.34826148	-1.65317762	1.74894083
6	0.04806148	-1.39157760	3.22884083
1	1.42356145	-1.86867762	1.64784086
6	-0.37593853	-2.90917754	1.27734077
6	-0.68673855	-5.23427773	1.45784080
1	-0.25223851	-6.02647781	2.06414104
1	-1.75813854	-5.14617777	1.64224076
6	3.96126151	-1.18457758	0.11284085
6	4.28096151	-2.41967750	-0.54285914
6	5.30726194	-3.21357751	-0.02145914
1	5.55156183	-4.15817785	-0.49485916
6	6.04526186	-2.83397770	1.09264088
6	5.77906179	-1.60557759	1.68444085
1	6.38716173	-1.30727756	2.53154087
6	4.76996183	-0.75617760	1.21954083
6	3.54446149	-2.89027762	-1.81165922
6	4.58636189	0.62012237	1.88824081
6	4.15526152	-4.17357779	-2.40515900
1	4.07216167	-5.03007793	-1.72785914
1	5.20976162	-4.04407787	-2.66955900
1	3.61746144	-4.43537807	-3.32335901
6	3.64316154	-1.81707764	-2.91355896
1	3.13856149	-2.15567756	-3.82705903
1	4.69336176	-1.63197756	-3.16525912
1	3.20296144	-0.87097764	-2.59685898
6	2.07496142	-3.22237754	-1.49365914
1	2.02426147	-4.00257778	-0.72595912
1	1.55416143	-3.59217763	-2.38505912
1	1.52376151	-2.35387754	-1.12985921
6	5.63986158	0.89812237	2.97544098
1	6.66136169	0.86592239	2.58264089
1	5.56956148	0.19632238	3.81304097
1	5.47786188	1.90272236	3.38294101
6	4.74596167	1.72972238	0.83204091
1	4.03086185	1.59352243	0.02144086
1	5.75456190	1.70792234	0.40474084
1	4.59556150	2.71912241	1.28414083
6	3.21426153	0.71892238	2.57874084
1	2.39106154	0.57472235	1.87974083
1	3.08746147	1.70072234	3.05344105
1	3.13226151	-0.04097762	3.36344099
6	-4.77083826	-0.30157763	0.08264086
6	-5.41093826	-0.38587761	1.36124086
6	-6.79993820	-0.23957762	1.42774081
1	-7.30393839	-0.30777761	2.38584089
6	-7.57443810	-0.00637762	0.29774085
6	-6.94513845	0.10632238	-0.93605912
1	-7.56043816	0.30662239	-1.80665922
6	-5.56063843	-0.02347762	-1.07875919
6	-4.61503839	-0.63467759	2.65514088
6	-4.92183828	0.17422238	-2.46465898
6	-3.95753860	1.37652242	-2.41475916
1	-4.50483847	2.28462243	-2.14005899
1	-3.50073862	1.55282235	-3.39685917
1	-3.16783857	1.23612237	-1.67375922
6	-5.95943832	0.49752238	-3.55495906
1	-6.50653839	1.42242241	-3.34535909
1	-6.68613815	-0.31057760	-3.69055915
1	-5.44403839	0.63492239	-4.51235914
6	-4.20333815	-1.10877764	-2.92625904
1	-4.91913843	-1.93247771	-3.02085900
1	-3.43733859	-1.42777765	-2.21665907
1	-3.73343849	-0.96007764	-3.90655899
6	-5.50393820	-0.61057764	3.91184092
1	-6.26553822	-1.39707756	3.89884090
1	-6.00553846	0.35352239	4.04684114
1	-4.87893820	-0.78047764	4.79624081
6	-3.55563855	0.46752238	2.85574102
1	-2.84603858	0.51222235	2.02904105
1	-2.99753857	0.30042237	3.78554106
1	-4.04273844	1.44622242	2.93084097
6	-3.96643853	-2.03157759	2.60764098
1	-4.74123812	-2.80557752	2.57084084
1	-3.35803843	-2.20987773	3.50404096
1	-3.33973861	-2.15627766	1.72424078
1	6.83256149	-3.47577763	1.48014081
1	-8.65383816	0.09642237	0.37914085
1	-0.50723851	-5.41607809	0.39744085
1	0.38276148	-2.22207761	3.85624099
1	0.57676148	-0.48537761	3.52974105
1	-1.02123857	-1.23057759	3.38294101
8	-0.43923852	-0.34997761	-1.67265916
6	1.77746153	3.00982237	-0.93375909
6	1.94056153	2.62832236	-2.39555907
8	1.31906152	1.33792233	-2.48415899
6	0.27256149	1.19212234	-3.37795901
6	-0.57603854	-0.02127763	-3.02465916
8	1.32186151	2.24172235	-0.09145914
1	-1.59853852	0.30522239	-3.24655914
6	-0.23433852	-1.18347764	-3.96155906
6	3.38366151	2.57572246	-2.87355900
1	1.36366153	3.33742237	-2.99705911

8	0.09216148	1.95912242	-4.28855896
1	3.39256144	2.33412242	-3.93835902
1	3.86076140	3.54822230	-2.73205900
1	3.94716144	1.81472242	-2.33125901
1	-0.36193854	-0.89087760	-5.00795889
1	0.79256147	-1.52037764	-3.80595899
1	-0.90823853	-2.01697755	-3.74815917
8	2.16646147	4.24302197	-0.67525911
8	-0.37593853	4.92582226	-0.07365914
8	0.15066147	5.25952196	2.10414100
6	1.93216145	4.73922205	0.66244090
6	2.74376154	6.01422215	0.81464088
1	2.24746156	3.98012233	1.38154078
6	0.42986149	4.97612238	0.82694089
6	-1.24243855	5.50112200	2.39374089
1	-1.83453858	4.61912203	2.14554095
1	-1.60333848	6.35762215	1.82194078
1	-1.28323853	5.70502234	3.46204090
1	2.60166144	6.41862202	1.81834078
1	3.80466151	5.79772234	0.67104089
1	2.43326139	6.76312208	0.08224086

DI-5__DBP-2_Mg-2_MeL-2_rrLA-2

Zero-point vibrational energy	3033923.0 (Joules/Mol)
	725.12499 (Kcal/Mol)
Zero-point correction =	1.155560 (Hartree/Particle)
Thermal correction to Energy =	1.232525
Thermal correction to Enthalpy =	1.233469
Thermal correction to Gibbs Free Energy =	1.034545
Sum of electronic and zero-point Energies =	-3474.478141
Sum of electronic and thermal Energies =	-3474.401177
Sum of electronic and thermal Enthalpies =	-3474.400232
Sum of electronic and thermal Free Energies =	-3474.599157



cartesian

12	-0.48451555	0.86717469	-0.17031091
12	2.28328443	-0.52172530	-0.25931090
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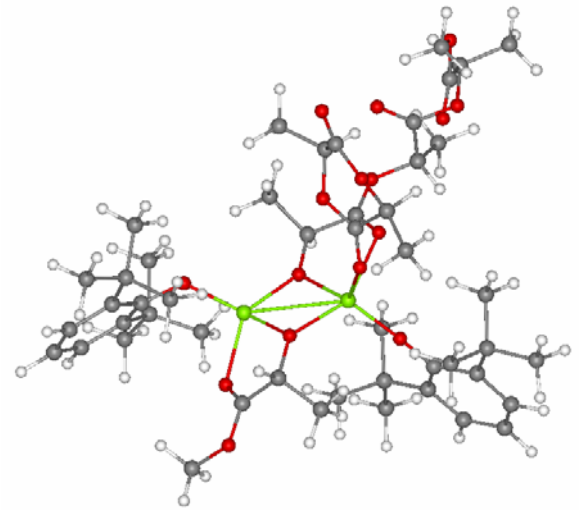
8	3.62718439	-1.42442536	0.72178906
8	1.23698449	0.87037474	-1.23191094
8	3.24168444	-0.45722526	-2.19371080
8	3.35998440	0.76517475	-4.07061052
6	1.72358453	1.40097463	-2.41661096
6	2.23088431	2.84077477	-2.26801085
1	0.95948440	1.38727462	-3.21141100
6	2.84458447	0.48377472	-2.88571095
6	4.45138454	-0.07302528	-4.51071072
1	4.76468468	0.34347475	-5.46601057
1	5.26558447	-0.04372528	-3.78581095
6	-1.07911551	3.98847461	0.07538910
6	-1.78181553	4.75517464	-0.91391093
6	-1.73841548	6.15077448	-0.84331089
1	-2.25221562	6.74477434	-1.59171093
6	-1.05881548	6.82077456	0.16768910
6	-0.42551553	6.07627439	1.15628910
1	0.07648446	6.61197472	1.95518899
6	-0.42261553	4.67837477	1.15028906
6	-2.60351563	4.07867479	-2.02681088
6	0.26578444	3.91927457	2.29888916
6	-3.33751559	5.09617472	-2.91871095
1	-2.64831567	5.75777435	-3.45461082
1	-4.03641558	5.71697474	-2.34821081
1	-3.92211556	4.55747461	-3.67381096
6	-3.68681550	3.17497468	-1.40551090
1	-4.29251528	2.70887470	-2.19321084
1	-4.35981560	3.76687479	-0.77561092
1	-3.24891567	2.39027476	-0.78791094
6	-1.68821549	3.26167488	-2.95841098
1	-0.94781554	3.91407466	-3.43481088
1	-2.27451563	2.78437471	-3.75501084
1	-1.15611553	2.48507476	-2.40861082
6	0.80358440	4.85787439	3.39408898
1	0.00978447	5.46137476	3.84688902
1	1.58088446	5.53377438	3.02238917
1	1.25368452	4.25647449	4.19228935
6	-0.74491554	2.98437476	2.99338913
1	-1.20541549	2.29027486	2.29018903
1	-1.54811549	3.57347488	3.45038915

1	-0.25261554	2.41357470	3.79168916
6	1.48028457	3.13247490	1.76978910
1	1.21718454	2.47107482	0.94328904
1	1.93488443	2.52987480	2.56598902
1	2.24298429	3.82437491	1.39568913
6	4.83088446	-1.91892529	0.43448907
6	6.00808477	-1.13522530	0.65168905
6	7.24038458	-1.66352534	0.25438911
1	8.14638424	-1.08192527	0.38838911
6	7.35428476	-2.93002510	-0.31041092
6	6.21458483	-3.71652532	-0.44261092
1	6.32908440	-4.71662521	-0.84741092
6	4.95068455	-3.25412512	-0.06391090
6	5.94678450	0.24317472	1.33918905
6	3.73128438	-4.19492531	-0.13381091
6	3.17888451	-4.42012548	1.28878903
1	3.92678428	-4.91522551	1.91698909
1	2.28618431	-5.05942535	1.26158905
1	2.91608429	-3.46912527	1.75678909
6	4.10118484	-5.57582521	-0.70421094
1	4.87018442	-6.07602549	-0.10771091
1	4.45398474	-5.51662540	-1.74001098
1	3.21608448	-6.22222567	-0.69471091
6	2.60678434	-3.63692522	-1.03641093
1	3.00948429	-3.16652513	-1.93831086
1	1.98618448	-2.91372514	-0.49801093
1	1.93468463	-4.44582558	-1.35011089
6	7.34678459	0.84707469	1.55278909
1	7.86128426	1.05637467	0.60828906
1	7.98708439	0.19647472	2.15688920
1	7.25148487	1.79837465	2.08778906
6	5.29958487	0.10687472	2.73258901
1	4.29698467	-0.31712526	2.66148901
1	5.23258448	1.08687472	3.22118902
1	5.90378475	-0.54722530	3.37048912
6	5.15978479	1.26657462	0.49678910
1	5.53498459	1.30267465	-0.53131092
1	5.24858475	2.27057481	0.92778909
1	4.09308481	1.03267467	0.47048908
1	-1.03911555	7.90757465	0.19518910
1	8.32508469	-3.31072521	-0.61871094
1	4.10878468	-1.10192525	-4.63121080
1	2.57938433	3.24297476	-3.22361088
1	1.41228449	3.46077490	-1.89711094
1	3.04788446	2.88677478	-1.54211092
8	-1.58871543	-2.35702515	-1.23341095
6	-2.10411549	-1.30292535	-1.84911096
6	-3.19661570	-1.58452535	-2.86771083
8	-4.08961535	-2.60562515	-2.38381100
6	-3.55691552	-3.71432519	-1.82511091
6	-2.04641557	-3.68082523	-1.62221086
8	-1.68961549	-0.17842528	-1.62401092
1	-1.58121550	-3.91042519	-2.59121084
6	-1.57341552	-4.66092539	-0.57311094
6	-4.02411556	-0.36592528	-3.20841098
1	-2.69561553	-1.96422529	-3.77131081
8	-4.24741554	-4.66302538	-1.55281091
1	-4.76351547	-0.63392526	-3.96651101
1	-3.38111567	0.42277473	-3.60021091
1	-4.53361559	0.00997472	-2.32011104
1	-1.85771549	-5.67162561	-0.87011093
1	-2.03611565	-4.43302536	0.38748908
1	-0.48741555	-4.60672522	-0.48041093
8	0.61638445	-0.54732525	0.78898907
8	-1.89891553	-0.04052528	1.24338913
8	-2.02761555	-1.53392529	2.93698907
6	0.09028448	-1.25622535	1.85858905
6	-1.38141549	-0.87842524	1.97418904
6	-3.44161558	-1.35282528	3.14208913
6	-3.88341570	0.08347473	3.40678906
6	-4.21211529	-2.04612517	2.02138901
6	0.83518451	-1.00242531	3.17328906
8	-5.51251554	-2.11462522	2.35218906
8	-3.72241569	-2.52412510	1.02318907
6	-6.39661551	-2.77382517	1.43148911
6	-6.78101540	-1.79502535	0.32308912
1	-5.86801529	-3.60742521	0.95868909
6	-7.59001541	-3.27262521	2.23188901
8	-7.68981552	-2.35752511	-0.48801088
8	-6.32811546	-0.68102527	0.19038908
6	-8.10931587	-1.55162537	-1.60301089
1	-8.85171509	-2.14922523	-2.12941098
1	-8.54591560	-0.61452526	-1.25241089
1	-7.25891542	-1.33862531	-2.25241089
1	-8.28491497	-3.79632521	1.57398903
1	-7.24971533	-3.96412516	3.00628901
1	-8.11381531	-2.44172525	2.71098900
1	-4.90721560	0.06597473	3.78658915
1	-3.23941565	0.52307475	4.17218924
1	-3.84641552	0.69957471	2.51098919
1	-3.62541556	-1.94402528	4.04378939
1	0.40718448	-1.58282530	3.99538922
1	1.87898457	-1.29482532	3.03998899
1	0.80398446	0.05987473	3.42978907
1	0.10008447	-2.34142518	1.66398907

DI-5__DBP-2_Mg-2_MeL-2_ssLA-2

Zero-point vibrational energy	3036616.5 (Joules/Mol)
	725.76877 (Kcal/Mol)
Zero-point correction =	1.156586 (Hartree/Particle)
Thermal correction to Energy =	1.233208
Thermal correction to Enthalpy =	1.234152

Thermal correction to Gibbs Free Energy =	1.037784
Sum of electronic and zero-point Energies =	-3474.486946
Sum of electronic and thermal Energies =	-3474.410324
Sum of electronic and thermal Enthalpies =	-3474.409380
Sum of electronic and thermal Free Energies =	-3474.605748



cartesian

12	-0.32688695	0.92643744	-0.51460576
12	2.39881301	-0.33216253	0.05629426
8	-0.78428692	2.77093744	-0.46500573
8	3.35841298	-1.87596262	0.61479425
8	1.38891304	0.46653748	-1.49130571
8	3.90571284	0.81913745	-0.87440574
8	4.44301319	1.66943741	-2.87480569
6	2.16061306	0.95833749	-2.53780580
6	1.60461307	2.22353745	-3.19180584
1	2.27001286	0.19423747	-3.32860565
6	3.58051300	1.15983737	-2.01560569
6	5.81141329	1.77913737	-2.41860580
1	6.36991310	2.14183736	-3.27930570
1	5.87061310	2.48973751	-1.59300578
6	-0.99938691	4.07243776	-0.32930574
6	-2.03798699	4.71993780	-1.08070576
6	-2.20388699	6.10223770	-0.95420575
1	-2.97578716	6.60613775	-1.52590573
6	-1.40898693	6.87163782	-0.11270574
6	-0.43178695	6.23873758	0.64599425
1	0.16871305	6.84753752	1.31349421
6	-0.20808694	4.86053753	0.57529426
6	-2.97398710	3.93363738	-2.01710558
6	0.85601306	4.22693777	1.48979425
6	-4.03938675	4.82773781	-2.67680573
1	-3.59868693	5.59523773	-3.32190585
1	-4.67968702	5.32373762	-1.93960571
1	-4.68818665	4.20843744	-3.30740571
6	-3.73658705	2.85493731	-1.22260571
1	-4.38788700	2.27463746	-1.88980579
1	-4.37318659	3.32293749	-0.46290573
1	-3.05408716	2.17233753	-0.71650577
6	-2.16678691	3.29423738	-3.16150570
1	-1.61958694	4.06213760	-3.71920586
1	-2.83528709	2.78403735	-3.86740565
1	-1.44458687	2.57303739	-2.78060579
6	1.55811310	5.25563765	2.39479423
1	0.85771310	5.77053785	3.06079435
1	2.10611296	6.01023769	1.82049429
1	2.28651285	4.73593760	3.02799416
6	0.18151306	3.21003747	2.43079424
1	-0.38988695	2.47373748	1.86579430
1	-0.50798696	3.72693753	3.10779428
1	0.93001306	2.68703747	3.03939438
6	1.96541297	3.55833745	0.65769428
1	1.56271303	2.80143738	-0.01530574
1	2.70891285	3.08493733	1.31119430
1	2.48281288	4.30773783	0.04759426
6	4.64821339	-2.17096257	0.43019426
6	5.63531303	-1.66506255	1.33419430
6	6.98401308	-1.87796259	1.03299427
1	7.75511312	-1.47506261	1.68119431
6	7.38271332	-2.60856247	-0.08250574
6	6.41271305	-3.19296265	-0.89090574
1	6.74301338	-3.80606270	-1.72300577
6	5.04551315	-3.01516247	-0.65420574
6	5.23841333	-0.97936255	2.65809417
6	4.00941324	-3.75066257	-1.52860570
6	3.06781292	-4.58626223	-0.63690573
1	3.63411283	-5.35206223	-0.09560575
1	2.31611300	-5.09726238	-1.25240576
1	2.55841303	-3.95636249	0.09399426
6	4.67551327	-4.72666216	-2.51530576
1	5.29471302	-5.46966219	-2.00250578
1	5.29771328	-4.21366215	-3.25690579
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6	3.18231297	-2.76716256	-2.37850571
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1	7.14511299	-1.32356262	3.70239425
1	6.13691330	-0.05806253	4.39759445
6	4.49391317	-2.00556254	3.53649426
1	3.62781286	-2.40976262	3.00809431
1	4.15121317	-1.54186261	4.47059441
1	5.15381336	-2.84046268	3.79489422
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1	0.64111304	1.98983741	-3.64930582
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8	-1.79988694	-2.23366261	-1.12000573

6	-2.18508697	-1.21596253	-1.87500572
6	-3.42988706	-1.41196263	-2.71630573
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6	-3.38198709	-3.76286268	-2.23410583
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1	-3.49918699	-3.00386262	-0.24820574
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1	-3.37378716	0.50323749	-3.67780566
1	-2.61008716	-0.79606253	-4.61390591
1	-2.59808707	-5.33566236	-0.15070574
1	-1.10538697	-4.78976250	-0.93520576
1	-1.55008698	-4.16566229	0.67369425
8	0.69281310	-0.02756254	0.97209430
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6	-4.33918667	-1.34376264	2.45849419
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1	-0.07418694	-2.56056261	1.55859423
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8	-7.23268700	-3.51876259	0.29179427
8	-5.76618671	-1.88856256	-0.26460576
6	-7.26538658	-3.97106266	-1.07850575
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1	-6.29588699	-4.37936258	-1.36700571
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