

Direct arylation of alkyl fluorides using *in situ* mechanochemically generated calcium-based heavy Grignard reagents

Pan Gao,^a Julong Jiang,^b Yamato Fukuzawa,^a Satoshi Maeda,^{b,c} Koji Kubota,^{*a,c} and Hajime Ito^{*a,c}

^aDivision of Applied Chemistry, Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido, Japan.

^bDepartment of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Hokkaido, Japan.

^cInstitute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Hokkaido, Japan.

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1. Chemicals and Instrumentation.

Liquid additives and solvents were purchased from commercial suppliers and further dried over molecular sieve (MS 4Å). Calcium granular (99%) was purchased from Aldrich (215147-100G). All mechanochemical reactions were carried out using grinding vessels in a Retsch MM 400 (Figure S1). The milling jar (1.5 mL) and two balls (7-mm-diameter), which are made of stainless steel (SUC400B and SUS420J2, respectively), are used for standard ball milling reactions (Figure S2a). Other types of milling jars were also investigated under standard conditions (Figure S2b and S2c). The heat gun Takagi HG-1450B with a temperature control function was used for high-temperature ball-milling reactions (Figure S3). NMR spectra were recorded on JEOL JNM-EC X400P and JNM-ECS400 spectrometers (^1H : 396 MHz, ^{13}C : 100 MHz). Tetramethylsilane (^1H), CDCl_3 (^{13}C), and fluorobenzene (^{19}F) were employed as external standards, respectively. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, hept = heptet and m = multiplet. Dibromomethane was used as an internal standard to determine NMR yields. Thermography was recorded with an NEC Avio Thermo GEAR G120. Recycle preparative gel permeation chromatography (GPC) was conducted with a JAI LaboACE LC-5060 using CHCl_3 as eluent with JAIGEL-1HR and JAIGEL-2HR. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

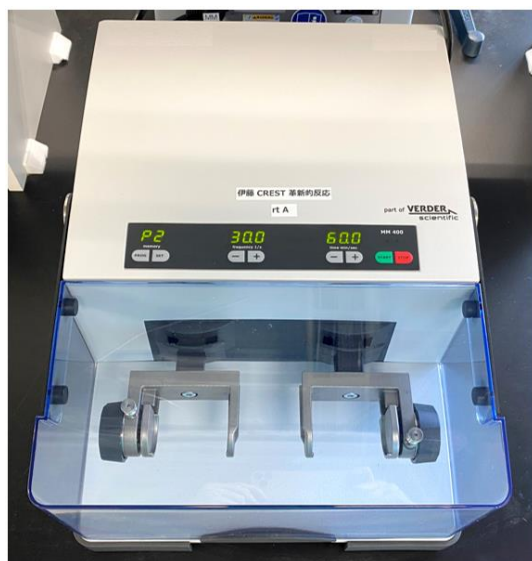


Figure S1. Retsch MM400 used in this study.



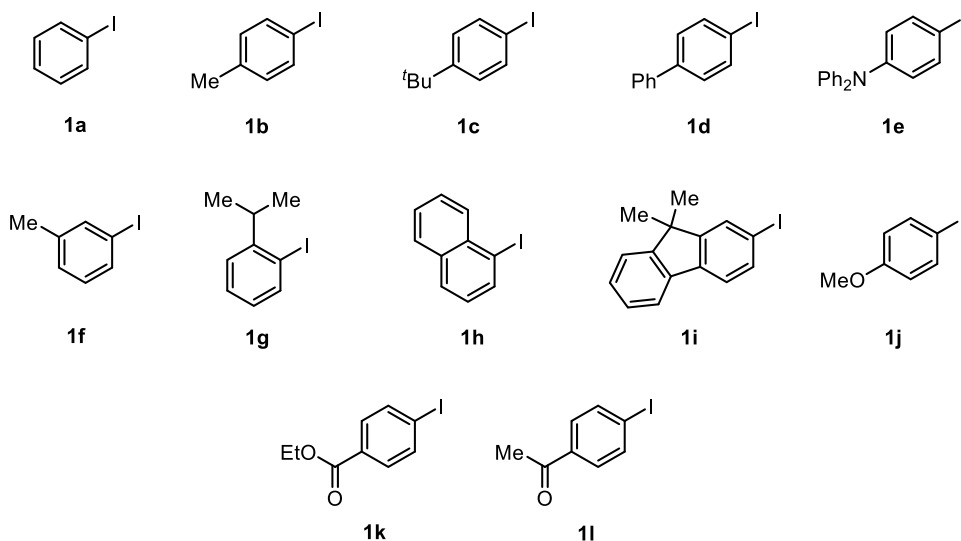
Figure S2. (a) 1.5 mL stainless-steel milling jar with two stainless-steel balls (7 mm); (b) 10 mL stainless-steel milling jar with two stainless-steel balls (10 mm); (c) 10 mL zirconium oxide milling jar with two zirconium oxide balls (10 mm).



Figure S3. The temperature-controllable heat gun Takagi HG-1450B used in this study.

2. List of Substrates.

Aryl iodides



Alkyl fluorides

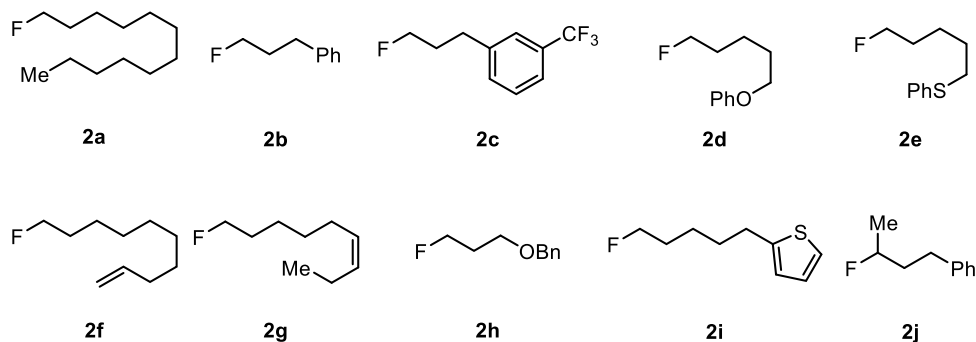
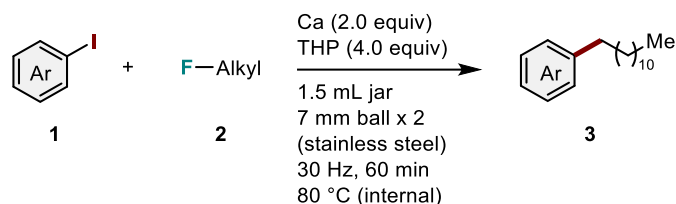


Figure S4. List of substrates.

1a–1l were purchased from commercial suppliers (Tokyo Chemical Industry Co.) (Figure S4). **2a–2c** and **2f–2h** were prepared from the corresponding alcohols via deoxyfluorination with Ishikawa's reagent.¹ **2d** and **2e** were prepared from 1-bromo-5-fluoropentane via nucleophilic substitution with phenol and thiophenol, respectively. **2i** was prepared from 1-bromo-5-fluoropentane via nucleophilic substitution with 2-lithiothiophene. **2j** was prepared from the corresponding alcohol via deoxyfluorination with PyFluor.²

3. General Procedure for Direct Arylation of Alkyl Fluorides.



General procedure: Commercially available Ca metal granular (1.0 mmol, 2.0 equiv) was placed in a stainless milling jar (1.5 mL) with two stainless balls (7 mm, diameter) in air. An aryl halide (1.5 mmol, 3.0 equiv), an alkyl fluoride (0.5 mmol, 1.0 equiv), and THP (2.0 mmol, 4.0 equiv) were added to the jar. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 60 min, 30 Hz). A heat gun was set in a downward direction approximately 1 cm above the jar and was turned on (preset temperature: 150 °C, internal temperature in the jar: ca. 80 °C). After grinding for 60 min, the jar was cooled to room temperature, opened in air, and quenched with 1.0 M aq. HCl and then extracted with CH₂Cl₂ three times. The resultant solution was dried over MgSO₄, filtrated, and evaporated under a vacuum, after removal of the solvents under reduced pressure. NMR yields of the corresponding products were determined by ¹H NMR analysis with dibromomethane as the internal standard. The crude mixtures were purified by recycling gel permeation chromatography (GPC) using CHCl₃ as the eluent to obtain the desired products with isolated yield.

Set-up procedure for high-temperature ball milling

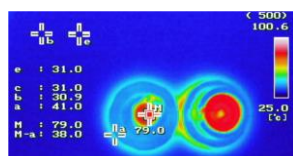
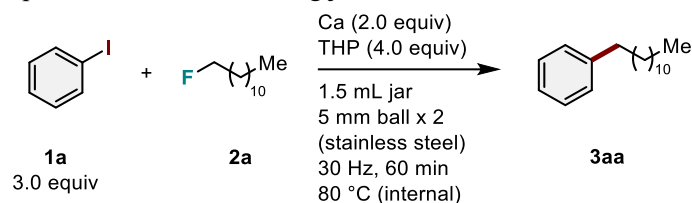
The heat gun was fixed with clamps and placed directly above the ball milling jar (distance between the heat gun and ball milling jar: ca. 1 cm). The set-up procedure for high-temperature ball-milling reactions is shown in Figure S5. After the ball milling jar was closed, the jar was placed in the ball mill (Retsch MM400), and a heat gun was placed directly above the ball milling jar. The mechanochemical generation of organocalcium halide was conducted while applying heated air to the outside of the milling jar (the preset temperature at 120 °C or 80 °C). The temperature inside the milling jar of the mechanochemical reaction was confirmed by thermography immediately after opening the jar.



Figure S5. The set-up procedure for a heat gun on MM400.

Thermography measurements for reaction temperature inside ball milling jars

The temperature inside the milling jar of the mechanochemical reaction was confirmed by thermography immediately after opening the jar. The crude mixtures were prepared under the following conditions: 1.5 mmol of iodobenzene (**1a**); 0.5 mmol of 1-fluorododecane (**2a**); 1.0 mmol of Ca; 2.0 mmol of THP in a stainless-steel ball milling jar (1.5 mL) with two stainless-steel balls (5 mm); the preset temperature of the heat gun: 150 °C; 30 Hz; 1 h. The obtained images revealed that the internal temperature of the ball milling jar was around 80 °C.



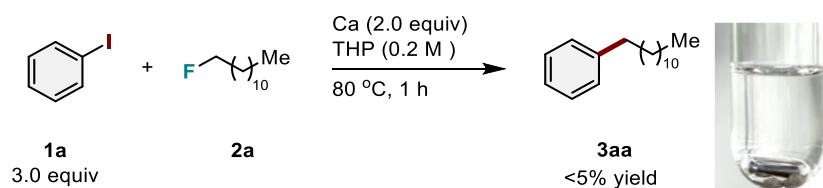
preset Temp.: 150 °C



internal Temp.: 80 °C

Procedure for direct arylation of alkyl fluoride in solution

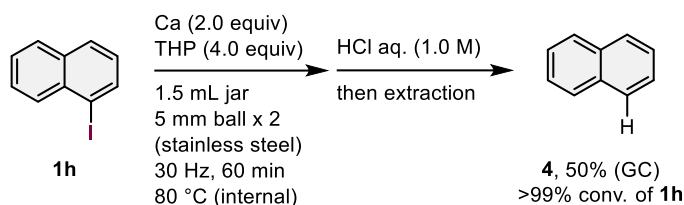
Commercially available Ca metal granular (1.0 mmol, 2.0 equiv) was placed in an oven-dried reaction vial. After being sealed with a screw cap containing a TeflonTM-coated rubber septum, the vial was connected to a nitrogen line through a needle. Iodobenzene (**1a**, 1.5 mmol, 3.0 equiv), 1-fluorododecane (**2a**, 0.5 mmol, 1.0 equiv) and THP (0.25 mL) were added to the vial under a nitrogen atmosphere, and then the reaction mixture was stirred at 80 °C for 60 min. After being cooled to room temperature, the reaction mixture was quenched with 1.0 M aq. HCl and extracted with CH₂Cl₂ (15 mL×3). The organic layer was separated and dried over MgSO₄. The desired product of **3aa** was not detected in ¹H NMR analysis, and a significant quantity of calcium metal remained in the reaction vial.



4. Details of Mechanism Investigations.

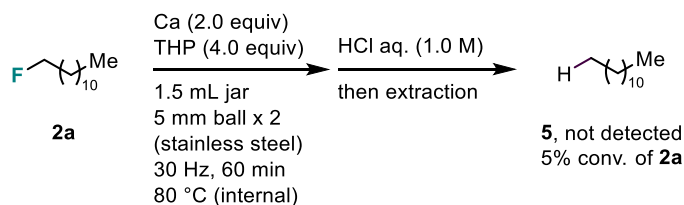
Protonation study of **1h**

Ca metal (1.0 mmol, 2.0 equiv) was placed in a stainless milling jar (1.5 mL) with two stainless balls (5 mm, diameter) in air. 1-Iodonaphthalene (**1h**; 0.5 mmol, 1.0 equiv) and tetrahydropyran (THP) (196 μ L, 2.0 mmol, 4.0 equiv) were added to the jar. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 60 min, 30 Hz). A heat gun was set in a downward direction approximately 1 cm above the jar and was turned on (preset temperature: 150 $^{\circ}$ C, internal temperature: ca. 80 $^{\circ}$ C). After grinding for 60 min, the jar was cooled to room temperature, opened in air, and quenched with 1.0 M aq. HCl and extracted with CH_2Cl_2 three times. The resultant solution was dried over MgSO_4 and filtrated. Biphenyl (0.5 mmol) was added to the solution as the internal standard, followed by GC analysis. The conversion of **1h** was >99%, despite low yield of **4** (50%), indicating inconsistent mass balance and the presence of oligomeric side products that cannot be detected by GC.



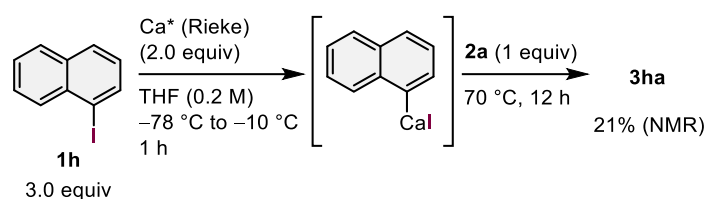
Protonation study of **2a**

Ca metal (1.0 mmol, 2.0 equiv) was placed in a stainless milling jar (1.5 mL) with two stainless balls (5 mm, diameter) in air. 1-Fluorododecane (**2a**; 0.5 mmol, 1.0 equiv) and THP (196 μ L, 2.0 mmol, 4.0 equiv) were added to the jar. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 60 min, 30 Hz). A heat gun was set in a downward direction approximately 1 cm above the jar and was turned on (preset temperature: 150 $^{\circ}$ C, internal temperature: ca. 80 $^{\circ}$ C). After grinding for 60 min, the jar was cooled to room temperature, opened in air, and quenched with 1.0 M aq. HCl and extracted with CH_2Cl_2 three times. The resultant solution was dried over MgSO_4 and filtrated. Biphenyl (0.5 mmol) was added to the solution as the internal standard, followed by GC analysis. The conversion of **2a** was only 5%, and no protonation product **5** could be detected.



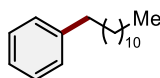
Reaction using Rieke calcium in solution

Lithium (2.0 mmol, 14.0 mg) and biphenyl (2.2 mmol, 339.2 mg) in dry tetrahydrofuran (THF) (3.0 mL) were stirred under N₂ for 3 h. To a well-suspended solution of CaI₂ (1.6 mmol, 470.2 mg) in dry THF (3.0 mL), the preformed lithium biphenylide was transferred via a disposable syringe at room temperature. The reaction mixture was stirred for 1 h at room temperature. Theoretically, 1.0 mmol Rieke calcium should be generated in situ. This suspension was cooled to -78 °C. Then, 1-iodonaphthalene (**1h**, 1.5 mmol, 381.7 mg) was added via syringe at -78 °C under N₂, and the mixture was allowed to warm to -10 °C and stirred for 1 hour. Then, iodoethane (**2a**, 0.5 mmol, 94.4 mg) was added at -10 °C. The resulting mixture was gradually warmed to 75 °C and stirred for 12 hours. Finally, the mixture was quenched with water and extracted with CH₂Cl₂. The organic solvent was removed under reduced pressure. The crude mixture was analyzed by ¹H NMR with CH₂Br₂ as an internal standard (21% NMR yield).



5. Characterization of Defluoroarylation Products.

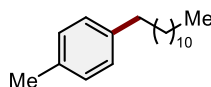
Dodecylbenzene (3aa).



3aa

The reaction was conducted according to the general procedure using iodobenzene (**1a**, 306.1 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.2 mg, 0.5 mmol). The resulting crude mixture was analyzed by ¹H NMR with dibromomethane as an internal standard to determine the NMR yield of **3aa** (86%). The product **3aa** was isolated as a colorless liquid with a yield of 74% (91.2 mg, 0.37 mmol) through GPC separation. The ¹H and ¹³C NMR spectra of product **3aa** were in agreement with the literature.³ ¹H NMR (399 MHz, CDCl₃) δ 0.88 (t, *J* = 6.9 Hz, 3H), 1.19–1.38 (m, 18H), 1.61 (quint, *J* = 7.5 Hz, 2H), 2.59 (t, *J* = 7.8 Hz, 2H), 7.13–7.20 (m, 3H), 7.24–7.30 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) 14.1 (CH₃), 22.7 (CH₂), 29.4 (CH₂), 29.5 (CH₂), 29.60 (CH₂), 29.65 (CH₂), 29.68 (CH₂), 31.5 (CH₂), 31.9 (CH₂), 36.0 (CH₂), 125.5 (CH), 128.2 (CH), 128.4 (CH), 143.0 (C); HRMS-EI (*m/z*): [*M*]⁺ calcd for C₁₈H₃₀, 246.2342; found, 246.2345.

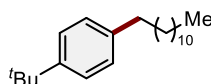
1-Dodecyl-4-methylbenzene (3ba).



3ba

The reaction was conducted according to the general procedure using 4-iodotoluene (**1b**, 327.2 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.2 mg, 0.5 mmol). The resulting crude mixture was analyzed by ¹H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ba** (62%). The product **3ba** was isolated as a colorless liquid with a yield of 43% (55.5 mg, 0.21 mmol) through GPC separation. The ¹H and ¹³C NMR spectra of product **3ba** were in agreement with the literature.⁴ ¹H NMR (399 MHz, CDCl₃) δ 0.89 (t, *J* = 6.9 Hz, 3H), 1.21–1.38 (m, 18H), 1.60 (quint, *J* = 7.5 Hz, 2H), 2.33 (s, 3H), 2.57 (t, *J* = 7.8 Hz, 2H), 7.04–7.13 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) 14.1 (CH₃), 21.0 (CH₃), 22.7 (CH₂), 29.4 (CH₂), 29.5 (CH₂), 29.60 (CH₂), 29.64 (CH₂), 29.7 (CH₂), 31.7 (CH₂), 31.9 (CH₂), 35.5 (CH₂), 128.2 (CH), 128.9 (CH), 134.9 (C), 139.9 (C); HRMS-EI (*m/z*): [*M*]⁺ calcd for C₁₉H₃₂, 260.2499; found, 260.2499.

1-(*tert*-Butyl)-4-dodecylbenzene (3ca).



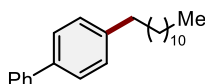
3ca

The reaction was conducted according to the general procedure using 1-(*tert*-butyl)-4-iodobenzene (**1c**, 389.8 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.1 mg, 0.5 mmol). The resulting crude mixture was analyzed by ¹H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ca** (83%). The product **3ca** was isolated as a colorless liquid with a yield of 62% (93.5 mg, 0.31 mmol) through GPC separation. The ¹H and ¹³C NMR spectra of the product **3ca**

were consistent with the literature.⁵

¹H NMR (399 MHz, CDCl₃) δ 0.91 (t, *J* = 6.9 Hz, 3H), 1.20–1.42 (m, 27H), 1.63 (quint, *J* = 7.5 Hz, 2H), 2.60 (t, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 7.30–7.35 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) 14.1 (CH₃), 22.7 (CH₃), 29.4 (CH₂), 29.50 (CH₂), 29.55 (CH₂), 29.62 (CH₂), 29.66 (CH₂), 29.70 (CH₂), 31.4 (CH₂), 31.5 (CH₂), 31.9 (CH₂), 34.3 (C), 35.4 (CH₂), 125.1 (CH), 128.0 (CH), 139.9 (C), 148.2 (C); HRMS-EI (*m/z*): [M]⁺ calcd for C₂₂H₃₈, 302.2968; found, 302.2966.

4-Dodecyl-1,1'-biphenyl (3da).

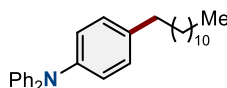


3da

The reaction was conducted according to the general procedure, using 4-iodo-1,1'-biphenyl (**1d**, 420.4 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.9 mg, 0.5 mmol). The resulting crude mixture was analyzed by ¹H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ca** (74%). The product **3da** was isolated as a colorless liquid with a yield of 65% (106.1 mg, 0.33 mmol) through GPC separation. The ¹H and ¹³C NMR spectra of the product **3da** were consistent with the literature.⁶

¹H NMR (399 MHz, CDCl₃) δ 0.88 (t, *J* = 6.9 Hz, 3H), 1.19–1.41 (m, 18H), 1.64 (quint, *J* = 7.5 Hz, 2H), 2.64 (t, *J* = 7.8 Hz, 2H), 7.25 (t, *J* = 4.1 Hz, 2H), 7.32 (tt, *J* = 7.3, 1.5 Hz, 1H), 7.39–7.45 (m, 2H), 7.49–7.53 (m, 2H), 7.56–7.61 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) 14.1 (CH₃), 22.7 (CH₂), 29.36 (CH₂), 29.38 (CH₂), 29.5 (CH₂), 29.60 (CH₂), 29.64 (CH₂), 29.7 (CH₂), 31.5 (CH₂), 31.9 (CH₂), 35.6 (CH₂), 126.9 (CH), 127.0 (CH), 128.7 (CH), 128.8 (CH), 138.5 (C), 141.2 (C), 142.1 (C); HRMS-EI (*m/z*): [M]⁺ calcd for C₂₄H₃₄, 322.2655; found, 322.2659.

4-Dodecyl-*N,N*-diphenylaniline (3ea).

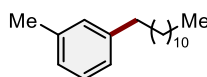


3ea

The reaction was conducted according to the general procedure, using 4-iodo-*N,N*-diphenylaniline (**1e**, 557.2 mg, 1.5 mmol), and 1-fluorododecane (**2a**, 94.3 mg, 0.5 mmol). The resulting crude mixture was analyzed by ¹H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ea** (63%). The product **3ea** was isolated as a colorless liquid with a yield of 55% (113.3 mg, 0.27 mmol) through GPC separation.

¹H NMR (399 MHz, CDCl₃) δ 0.88 (t, *J* = 6.9 Hz, 3H), 1.20–1.39 (m, 18H), 1.60 (quint, *J* = 7.5 Hz, 2H), 2.55 (t, *J* = 7.8 Hz, 2H), 6.92–7.10 (m, 10H), 7.17–7.26 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) 14.1 (CH₃), 22.7 (CH₂), 29.36 (CH₂), 29.4 (CH₂), 29.5 (CH₂), 29.61 (CH₂), 29.65 (CH₂), 29.7 (CH₂), 31.5 (CH₂), 31.9 (CH₂), 35.4 (CH₂), 122.2 (CH), 123.7 (CH), 124.7 (CH), 129.08 (CH), 129.15 (CH), 137.8 (C), 145.3 (C), 148.0 (C); HRMS-EI (*m/z*): [M]⁺ calcd for C₃₀H₃₉N, 413.3077; found, 413.3080.

1-Dodecyl-3-methylbenzene (3fa).

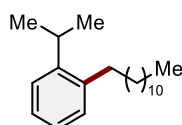


3fa

The reaction was conducted according to the general procedure using 1-iodo-3-methylbenzene (**1f**, 326.7 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.6 mg, 0.5 mmol). The resulting crude mixture was analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3fa** (88%). The product **3fa** was isolated as a colorless liquid with a yield of 73% (95.9 mg, 0.37 mmol) through GPC separation. The ^1H and ^{13}C NMR spectra of product **3fa** were consistent with the literature.⁷

^1H NMR (399 MHz, CDCl_3) δ 0.92 (t, $J = 6.9$ Hz, 3H), 1.24–1.41 (m, 18H), 1.63 (quint, $J = 7.4$ Hz, 2H), 2.36 (s, 3H), 2.60 (t, $J = 7.8$ Hz, 2H), 6.99–7.06 (m, 3H), 7.20 (t, $J = 7.5$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) 14.1 (CH_3), 21.4 (CH_3), 22.7 (CH_2), 29.38 (CH_2), 29.43 (CH_2), 29.55 (CH_2), 29.62 (CH_2), 29.67 (CH_2), 29.70 (CH_2), 31.6 (CH_2), 31.9 (CH_2), 35.9 (CH_2), 125.4 (CH), 126.3 (CH), 128.1 (CH), 129.2 (CH), 137.7 (C), 142.9 (C); HRMS-EI (m/z): $[\text{M}]^+$ calcd for $\text{C}_{19}\text{H}_{32}$, 260.2499; found, 260.2499.

1-Dodecyl-2-isopropylbenzene (3ga).

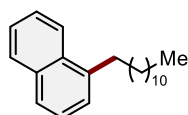


3ga

The reaction was conducted according to the general procedure using 1-iodo-2-isopropylbenzene (**1g**, 369.5 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.3 mg, 0.5 mmol). The resulting crude mixture was analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ga** (80%). Product **3ga** was isolated as a colorless liquid with a yield of 67% (97.5 mg, 0.34 mmol) through GPC separation.

^1H NMR (399 MHz, CDCl_3) δ 0.88 (t, $J = 6.9$ Hz, 3H), 1.18–1.44 (m, 24H), 1.50–1.61 (m, 2H), 2.62 (t, $J = 8.0$ Hz, 2H), 3.17 (sept, $J = 6.8$ Hz, 1H), 7.06–7.20 (m, 3H), 7.23–7.28 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) 14.1 (CH_3), 22.7 (CH_2), 24.1 (CH_3), 28.5 (CH), 29.4 (CH_2), 29.56 (CH_2), 29.63 (CH_2), 29.65 (CH_2), 29.67 (CH_2), 29.8 (CH_2), 31.86 (CH_2), 31.93 (CH_2), 33.0 (CH_2), 125.2 (CH), 125.4 (CH), 126.1 (CH), 129.3 (CH), 139.6 (C), 146.4 (C); HRMS-EI (m/z): $[\text{M}]^+$ calcd for $\text{C}_{21}\text{H}_{36}$, 288.2812; found, 288.2815.

1-Dodecyl-naphthalene (3ha).



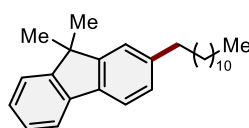
3ha

The reaction was conducted according to the general procedure using 1-iodonaphthalene (**1h**, 381.5 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.4 mg, 0.5 mmol). The resulting crude mixture was

analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ha** (69%). The product **3ha** was isolated as a colorless liquid with a yield of 56% (82.9 mg, 0.36 mmol) through GPC separation. The ^1H and ^{13}C NMR spectra of product **3ha** were consistent with the literature.⁸

^1H NMR (399 MHz, CDCl_3) δ 0.91 (t, $J = 6.9$ Hz, 3H), 1.22–1.51 (m, 18H), 1.77 (quint, $J = 7.6$ Hz, 2H), 3.08 (t, $J = 7.8$ Hz, 2H), 7.34 (d, $J = 5.9$ Hz, 1H), 7.41 (t, $J = 7.5$ Hz, 1H), 7.46–7.55 (m, 2H), 7.72 (d, $J = 8.2$ Hz, 1H), 7.85–7.89 (m, 1H), 8.07 (d, $J = 8.2$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) 14.1 (CH_3), 22.7 (CH_2), 29.4 (CH_2), 29.56 (CH_2), 29.65 (CH_2), 29.69 (CH_2), 29.9 (CH_2), 30.9 (CH_2), 31.9 (CH_2), 33.1 (CH_2), 123.9 (CH), 125.3 (CH), 125.5 (CH), 125.6 (CH), 125.8 (CH), 126.3 (CH), 128.7 (CH), 131.9 (C), 133.8 (C), 139.0 (C); HRMS-EI (m/z): $[\text{M}]^+$ calcd for $\text{C}_{22}\text{H}_{32}$, 296.2499; found, 296.2501.

2-Dodecyl-9,9-dimethyl-9H-fluorene (**3ia**).

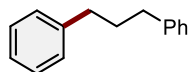


3ia

The reaction was conducted according to the general procedure using 2-iodo-9,9-dimethyl-9H-fluorene (**1i**, 480.5 mg, 1.5 mmol) and 1-fluorododecane (**2a**, 94.4 mg, 0.5 mmol). The resulting crude mixture was analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ia** (85%). Product **3ia** was isolated as a colorless liquid with a yield of 72% (130.9 mg, 0.36 mmol) through GPC separation.

^1H NMR (399 MHz, CDCl_3) δ 0.88 (t, $J = 6.9$ Hz, 3H), 1.20–1.40 (m, 18H), 1.47 (s, 6H), 1.66 (quint, $J = 7.6$ Hz, 2H), 2.67 (t, $J = 8.0$ Hz, 2H), 7.15 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.21–7.34 (m, 3H), 7.39–7.43 (m, 1H), 7.62 (d, $J = 7.8$ Hz, 1H), 7.66–7.70 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) 14.1 (CH_3), 22.7 (CH_2), 27.2 (CH_3), 29.36 (CH_3), 29.45 (CH_2), 29.53 (CH_2), 29.62 (CH_2), 29.65 (CH_2), 29.67 (CH_2), 31.8 (CH_2), 31.9 (CH_2), 36.3 (CH_2), 46.6 (C), 119.6 (CH), 119.7 (CH), 122.5 (CH), 122.6 (CH), 126.7 (CH), 126.8 (CH), 127.1 (CH), 136.7 (C), 139.3 (C), 142.4 (C), 153.5 (C), 153.7 (C); HRMS-EI (m/z): $[\text{M}]^+$ calcd for $\text{C}_{27}\text{H}_{38}$, 362.2968; found, 362.2974.

1,3-Diphenylpropane (**3ab**)



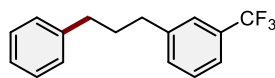
3ab

The reaction was conducted according to the general procedure using iodobenzene (**1a**, 306.8 mg, 1.5 mmol) and (3-fluoropropyl)benzene (**2b**, 69.0 mg, 0.5 mmol). The resulting crude mixture was analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ab** (82%). Product **3ab** was isolated as a colorless liquid with a yield of 78% (76.4 mg, 0.39 mmol) through GPC separation. The ^1H and ^{13}C NMR spectra of the product **3ab** were consistent with the literature.⁹

^1H NMR (399 MHz, CDCl_3) δ 1.91–2.01 (m, 2H), 2.65 (t, $J = 7.8$ Hz, 4H), 7.15–7.22 (m, 6H), 7.24–7.31 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) 32.9 (CH_2), 35.4 (CH_2), 125.7 (CH), 128.3 (CH), 128.4

(CH), 142.2 (C); HRMS-EI (m/z): $[M]^+$ calcd for $C_{15}H_{16}$, 196.1247; found, 196.1249.

1-(3-Phenylpropyl)-3-(trifluoromethyl)benzene (**3ac**)

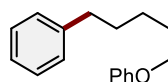


3ac

The reaction was conducted according to the general procedure, using iodobenzene (**1a**, 360.8 mg, 1.8 mmol) and 1-(3-fluoropropyl)-3-(trifluoromethyl)benzene (**2c**, 103.0 mg, 0.5 mmol). The resulting crude mixture was analyzed by 1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ac** (86%). Product **3ac** was isolated as a colorless liquid with a yield of 69% (91.6 mg, 0.35 mmol) through GPC separation.

1H NMR (399 MHz, $CDCl_3$) δ 1.92–2.02 (m, 2H), 2.62–2.73 (m, 4H), 7.15–7.23 (m, 3H), 7.25–7.46 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) 32.7 (CH_2), 35.2 (CH_2), 35.3 (CH_2), 122.6 (q, $J = 3.5$ Hz, CH), 124.3 (q, $J = 264.0$ Hz, C), 125.1 (q, $J = 3.5$ Hz, CH), 125.9 (CH), 128.37 (CH), 128.41 (CH), 128.7 (CH), 130.6 (q, $J = 130.6$ Hz, C), 131.8 (CH), 141.8 (C), 143.1 (C); HRMS-EI (m/z): $[M]^+$ calcd for $C_{16}H_{15}F_3$, 264.1120; found, 264.1126.

(5-Phenoxypropyl)benzene (**3ad**)

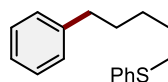


3ad

The reaction was conducted according to the general procedure, using iodobenzene (**1a**, 306.8 mg, 1.5 mmol) and [(5-fluoropentyl)oxy]benzene (**2d**, 91.5 mg, 0.5 mmol). The resulting crude mixture was analyzed by 1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ad** (78%). Product **3ad** was isolated as a colorless liquid with a yield of 66% (79.5 mg, 0.33 mmol) through GPC separation. The 1H and ^{13}C NMR spectra of the product **3ad** were consistent with the literature.¹⁰

1H NMR (401 MHz, $CDCl_3$) δ 1.49–1.59 (m, 2H), 1.72 (quint, $J = 7.6$ Hz, 2H), 1.84 (quint, $J = 7.1$ Hz, 2H), 2.67 (t, $J = 7.8$ Hz, 2H), 3.97 (t, $J = 6.4$ Hz, 2H), 6.88–6.99 (m, 3H), 7.18–7.24 (m, 3H), 7.27–7.34 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) 25.7 (CH_2), 29.1 (CH_2), 31.3 (CH_2), 35.8 (CH_2), 67.7 (CH_2), 114.4 (CH), 120.5 (CH), 125.7 (CH), 128.3 (CH), 128.4 (CH), 129.4 (CH), 142.5 (C), 159.0 (C); HRMS-EI (m/z): $[M]^+$ calcd for $C_{17}H_{20}O$, 240.1509; found, 240.1510.

Phenyl(5-phenylpentyl)sulfane (**3ae**)



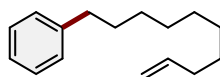
3ae

The reaction was conducted according to the general procedure using iodobenzene (**1a**, 359.0 mg, 1.8 mmol) and (5-fluoropentyl)(phenyl)sulfane (**2e**, 99.4 mg, 0.5 mmol). The resulting crude mixture was analyzed by 1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ae** (70%). Product **3ae** was isolated as a colorless liquid with a yield of 62% (79.1

mg, 0.31 mmol) through GPC separation. The ^1H and ^{13}C NMR spectra of product **3ae** were consistent with the literature.¹¹

^1H NMR (401 MHz, CDCl_3) δ 1.42–1.52 (m, 2H), 1.58–1.73 (m, 4H), 2.60 (t, $J = 7.8$ Hz, 2H), 2.91 (t, $J = 7.6$ Hz, 2H), 7.12–7.21 (m, 4H), 7.24–7.34 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) 28.4 (CH_2), 29.0 (CH_2), 31.0 (CH_2), 33.4 (CH_2), 35.7 (CH_2), 125.7 (CH), 128.2 (CH), 128.4 (CH), 128.8 (CH), 128.9 (CH), 136.8 (C), 142.4 (C); HRMS-EI (m/z): $[\text{M}]^+$ calcd for $\text{C}_{17}\text{H}_{20}\text{S}$, 256.1280; found, 256.1284.

Dec-9-en-1-ylbenzene (**3af**)

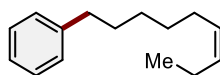


3af

The reaction was conducted according to the general procedure, using iodobenzene (**1a**, 306.6 mg, 1.5 mmol) and 10-fluorodec-1-ene (**2f**, 79.2 mg, 0.5 mmol). The resulting crude mixture was analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3af** (83%). The product **3af** was isolated as a colorless liquid with a yield of 72% (77.6 mg, 0.36 mmol) through GPC separation. The ^1H and ^{13}C NMR spectra of product **3af** were consistent with the literature.¹¹

^1H NMR (399 MHz, CDCl_3) δ 1.25–1.46 (m, 10H), 1.64 (quint, $J = 7.6$ Hz, 2H), 2.02–2.11 (m, 2H), 2.62 (t, $J = 7.8$ Hz, 2H), 4.92–5.07 (m, 2H), 5.78–5.90 (m, 1H), 7.15–7.24 (m, 3H), 7.27–7.34 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) 28.9 (CH_2), 29.1 (CH_2), 29.3 (CH_2), 29.41 (CH_2), 29.44 (CH_2), 31.5 (CH_2), 33.8 (CH_2), 36.0 (CH_2), 114.1 (CH_2), 125.5 (CH), 128.2 (CH), 128.4 (CH), 139.2 (CH), 142.9 (C); HRMS-EI (m/z): $[\text{M}]^+$ calcd for $\text{C}_{16}\text{H}_{24}$, 216.1873; found, 216.1876.

(Z)-Non-6-en-1-ylbenzene (**3ag**)



3ag

The reaction was conducted according to the general procedure, using iodobenzene (**1a**, 306.2 mg, 1.5 mmol) and (Z)-9-fluoronon-3-ene (**2g**, 72.0 mg, 0.5 mmol). The resulting crude mixture was analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of **3ag** (86%). Product **3ag** was isolated as a colorless liquid with a yield of 73% (73.5 mg, 0.36 mmol) through GPC separation.

^1H NMR (399 MHz, CDCl_3) δ 0.95 (t, $J = 7.5$ Hz, 3H), 1.30–1.42 (m, 4H), 1.62 (quint, $J = 7.6$ Hz, 2H), 1.94–2.10 (m, 4H), 2.60 (t, $J = 7.8$ Hz, 2H), 5.27–5.43 (m, 2H), 7.14–7.20 (m, 3H), 7.23–7.30 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) 14.4 (CH_3), 20.5 (CH_2), 27.0 (CH_2), 29.0 (CH_2), 29.6 (CH_2), 31.4 (CH_2), 36.0 (CH_2), 125.5 (CH), 128.2 (CH), 128.4 (CH), 129.1 (CH), 131.6 (CH), 142.8 (C); HRMS-EI (m/z): $[\text{M}]^+$ calcd for $\text{C}_{15}\text{H}_{22}$, 202.1716; found, 202.1720.

6. Computational Details.

The AFIR method¹² was used to suggest the plausible geometry of $\text{PhCa}(\text{THP})_2$ via a comprehensive and unbiased sampling calculation. The preliminary calculations strongly suggested that either monomeric or dimeric $\text{PhCa}(\text{THP})_2$ is highly unstable. Therefore, efforts were made to explore the plausible structures of tetrameric $\text{PhCa}(\text{THP})_2$. The sampling calculation was conducted using the SC-AFIR method at the semi-empirical GFN1-xTB level of theory¹³ as implemented in ORCA 4.0 software package,¹⁴ and a collision energy of $200 \text{ kJ}\cdot\text{mol}^{-1}$ was applied to the entire molecule for any possible bond rearrangements.¹² The AFIR sampling calculation provided in total 1787 possible isomers and conformers for $\text{PhCa}(\text{THP})_2$ tetramer, of which the ones having the lowest energies were further optimized at the DFT level of theory with the B3LYP hybrid functional¹⁵ as implemented in Gaussian 16.¹⁶ It is noteworthy that the energy profile shown in this study was generated with the geometries and energies derived from the following DFT calculations. In order to describe the dispersion properly, an explicit dispersion correction term called GD3,¹⁷ was also employed in the DFT calculations. The polarized triple-zeta 6-311G(d,p) basis set¹⁸ was used for C, H, O, and F atoms during both the geometry optimization and the single-point calculation processes. The Stuttgart/Dresden pseudo-potential basis set SDD,¹⁹ as well as a d-polarization function,²⁰ are used for Ca ($\zeta = 1.245$) and I ($\zeta = 0.289$) atoms. All the minima and transition states were fully optimized without any constraints. Frequency calculations were carried out to characterize all the optimized structures as minima or transition states. Transition states were identified by having one imaginary frequency. An intrinsic reaction coordinate (IRC) calculation²¹ was performed for each transition state to ensure that it connected the correct reactants and products. The free energies were computed at 298.15 K and 1 atm. All the geometries shown in this article is visualized by the CYLview software.²²

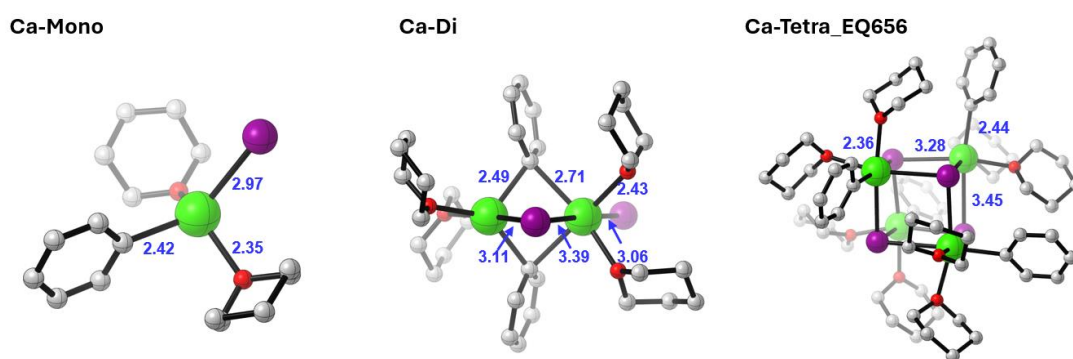


Figure S6. Optimized structures of monomeric, dimeric, and tetrameric organocalcium species.

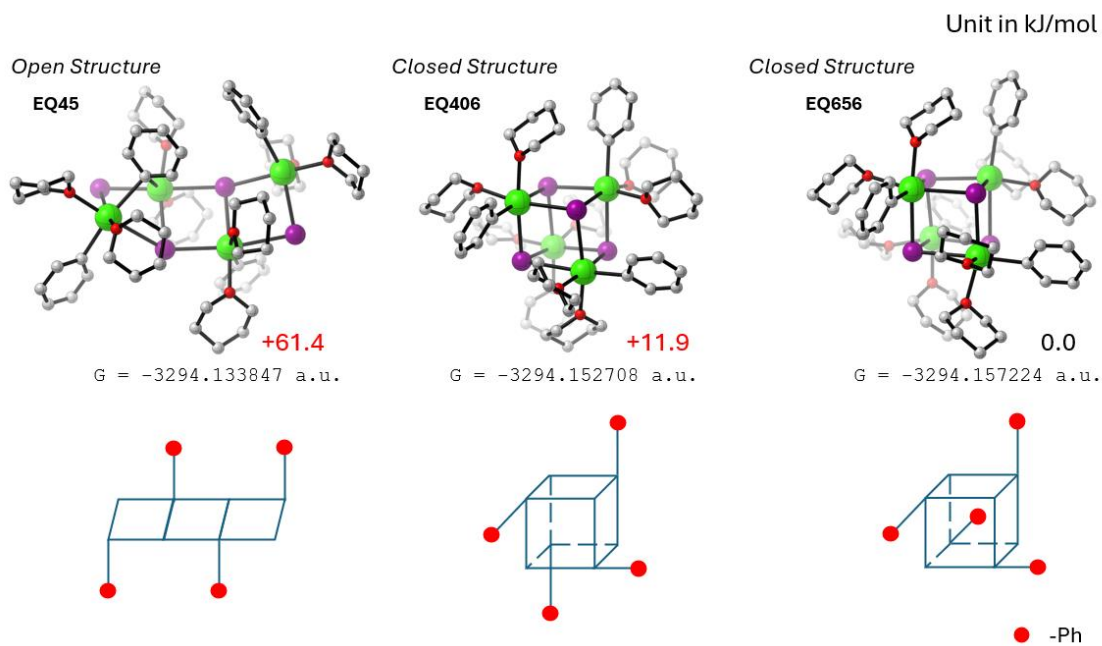


Figure S7. Comparison of the stability of tetrameric organocalcium species.

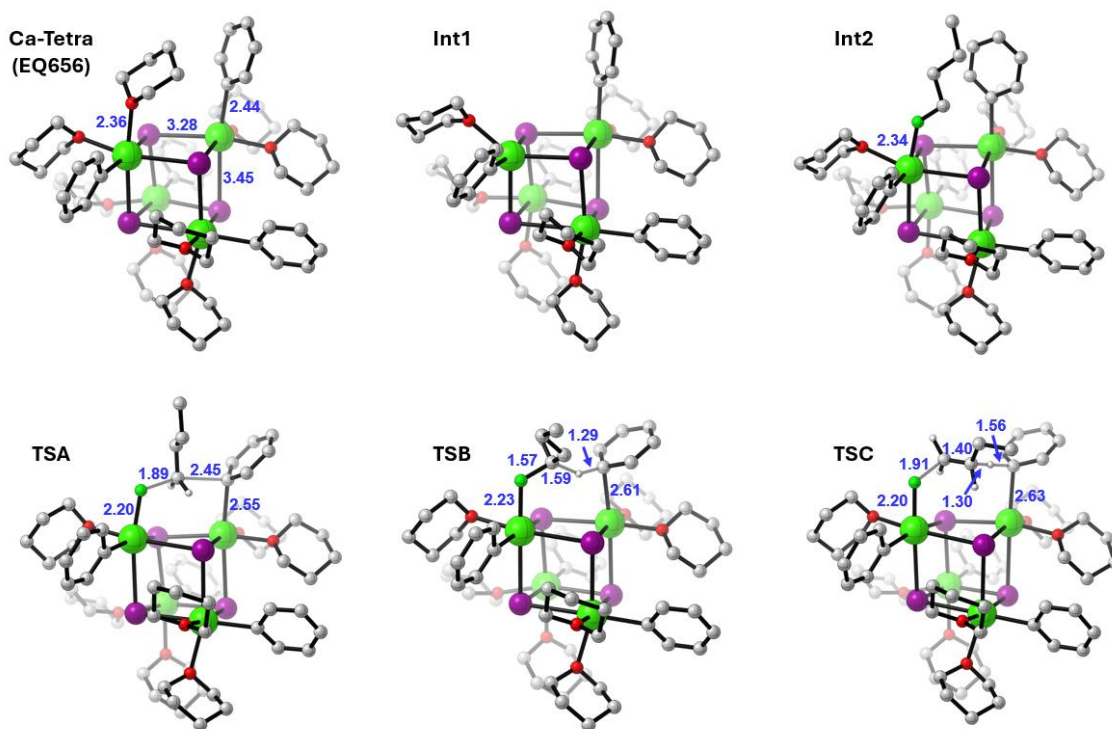


Figure S8. Optimized structures of intermediates and transition states along the reaction pathways.

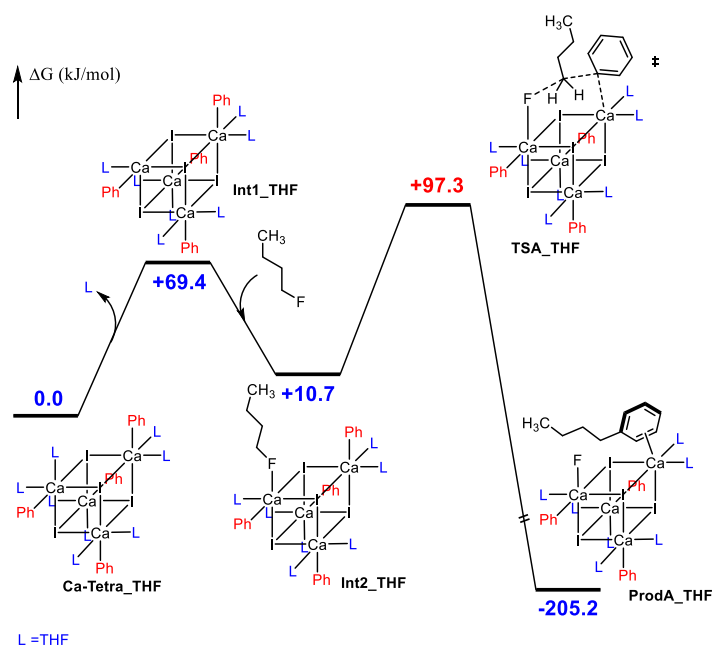


Figure S9. Free energy profile of the defluorinated C-C cross-coupling reaction, in which the ligand is tetrahydrofuran (THF).

Cartesian coordinates of optimized structures

(E_{el} : Electronic Energy; G : Gibbs Free Energy at 298.15 Kelvin and under 1 atm)

Ca-Mono

(E_{el} = -823.837912 a.u.; G = -823.514358 a.u.)

0 1

Ca	0.038417000000	-0.052081000000	-0.385211000000
I	1.066890000000	-2.491396000000	0.954084000000
C	-0.892282000000	2.046554000000	0.392005000000
C	-1.101131000000	2.310264000000	1.763579000000
C	-1.302693000000	3.084999000000	-0.473687000000
C	-1.667652000000	3.497124000000	2.237082000000
H	-0.812839000000	1.562636000000	2.503521000000
C	-1.871320000000	4.280898000000	-0.027546000000
H	-1.179672000000	2.968384000000	-1.554049000000
C	-2.056002000000	4.489629000000	1.338397000000
H	-1.806732000000	3.650100000000	3.303772000000
H	-2.169659000000	5.047236000000	-0.738002000000
H	-2.496677000000	5.413904000000	1.697649000000
C	3.196700000000	-0.049814000000	-1.456878000000
C	2.242833000000	2.171272000000	-1.420752000000
C	4.036256000000	0.234899000000	-0.218872000000
H	2.874478000000	-1.091173000000	-1.488787000000
H	3.738434000000	0.189625000000	-2.380358000000
C	3.033710000000	2.547897000000	-0.175755000000
H	1.268020000000	2.657767000000	-1.435174000000
H	2.788219000000	2.422816000000	-2.338935000000
C	4.333658000000	1.735616000000	-0.092786000000
H	3.484810000000	-0.123577000000	0.656586000000
H	4.959766000000	-0.349149000000	-0.275321000000
H	2.403423000000	2.356091000000	0.699493000000
H	3.236663000000	3.622845000000	-0.194932000000
H	4.853911000000	1.942438000000	0.845797000000
H	5.005887000000	2.044279000000	-0.903626000000
O	1.976516000000	0.741602000000	-1.440303000000
C	-3.044149000000	-0.058400000000	-1.557632000000
C	-2.179345000000	-2.309930000000	-1.422908000000
C	-3.903731000000	-0.254998000000	-0.316873000000
H	-2.686273000000	0.967886000000	-1.633328000000
H	-3.586458000000	-0.322051000000	-2.474233000000
C	-3.005330000000	-2.608448000000	-0.178994000000
H	-1.222704000000	-2.832764000000	-1.402061000000
H	-2.716950000000	-2.574850000000	-2.341792000000
C	-4.267948000000	-1.735766000000	-0.138138000000

H	-3.340412000000	0.112879000000	0.547542000000
H	-4.799661000000	0.367135000000	-0.402689000000
H	-2.378572000000	-2.420846000000	0.699383000000
H	-3.258018000000	-3.672932000000	-0.167825000000
H	-4.803669000000	-1.885962000000	0.802527000000
H	-4.947989000000	-2.041750000000	-0.943477000000
O	-1.855299000000	-0.893621000000	-1.490363000000

Ca-Di

(E_{el} = -1647.748994 a.u.; G = -1647.068063 a.u.)

0 1

Ca	-1.865456000000	0.401504000000	-0.284405000000
I	-0.668322000000	-1.748110000000	-2.186501000000
I	3.206963000000	1.347666000000	1.927030000000
Ca	1.358387000000	-0.161213000000	0.019095000000
C	-0.009822000000	1.951099000000	-0.952215000000
C	0.517114000000	3.086523000000	-0.292420000000
C	-0.389395000000	2.180424000000	-2.296009000000
C	0.661942000000	4.331805000000	-0.908069000000
H	0.861277000000	2.993931000000	0.733752000000
C	-0.280840000000	3.425421000000	-2.925721000000
H	-0.753135000000	1.347094000000	-2.899819000000
C	0.250917000000	4.508952000000	-2.229365000000
H	1.093302000000	5.162632000000	-0.357344000000
H	-0.588697000000	3.543237000000	-3.960904000000
H	0.352645000000	5.475642000000	-2.711782000000
C	-0.743657000000	-0.713632000000	1.638553000000
C	-0.383495000000	-0.178174000000	2.897861000000
C	-1.511175000000	-1.900754000000	1.701670000000
C	-0.739615000000	-0.776456000000	4.109646000000
H	0.221374000000	0.724775000000	2.940263000000
C	-1.896013000000	-2.506494000000	2.901785000000
H	-1.801560000000	-2.398164000000	0.774449000000
C	-1.504137000000	-1.943450000000	4.114986000000
H	-0.417028000000	-0.335857000000	5.048307000000
H	-2.480167000000	-3.422520000000	2.891117000000
H	-1.783279000000	-2.411878000000	5.053027000000
C	2.130288000000	-3.551835000000	-0.218517000000
C	2.895591000000	-2.561902000000	1.820058000000
C	1.083048000000	-4.387944000000	0.505343000000
H	1.789161000000	-3.274302000000	-1.214109000000
H	3.084520000000	-4.089634000000	-0.304405000000
C	1.884360000000	-3.339028000000	2.651577000000
H	3.114797000000	-1.582245000000	2.242036000000

H	3.838807000000	-3.114385000000	1.713489000000
C	1.504824000000	-4.654288000000	1.957139000000
H	0.138515000000	-3.838551000000	0.481077000000
H	0.932419000000	-5.323585000000	-0.042918000000
H	0.995891000000	-2.718585000000	2.791013000000
H	2.309991000000	-3.525278000000	3.642714000000
H	0.698927000000	-5.154046000000	2.501753000000
H	2.366984000000	-5.334005000000	1.966308000000
C	-3.840931000000	3.023698000000	0.183172000000
C	-2.895746000000	2.385943000000	2.304131000000
C	-2.982281000000	4.278722000000	0.104431000000
H	-4.042156000000	2.592817000000	-0.800031000000
H	-4.804664000000	3.223804000000	0.670994000000
C	-2.000540000000	3.616272000000	2.338127000000
H	-2.425775000000	1.521353000000	2.772644000000
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C	-2.611208000000	4.760860000000	1.515327000000
H	-2.076213000000	4.051842000000	-0.463291000000
H	-3.528800000000	5.052835000000	-0.443348000000
H	-1.024691000000	3.345363000000	1.929399000000
H	-1.847375000000	3.917218000000	3.378876000000
H	-1.909631000000	5.596179000000	1.453322000000
H	-3.510804000000	5.134343000000	2.021783000000
O	-3.165609000000	1.988645000000	0.935102000000
O	2.377057000000	-2.314317000000	0.484958000000
C	3.250918000000	-0.840756000000	-2.726066000000
C	3.429830000000	1.457555000000	-2.057339000000
C	4.723138000000	-1.108183000000	-2.439072000000
H	2.621655000000	-1.712389000000	-2.550703000000
H	3.097934000000	-0.523144000000	-3.766052000000
C	4.918605000000	1.314569000000	-1.769116000000
H	2.950272000000	2.162911000000	-1.380100000000
H	3.239768000000	1.780124000000	-3.089049000000
C	5.535300000000	0.184922000000	-2.606959000000
H	4.811568000000	-1.476484000000	-1.411324000000
H	5.087918000000	-1.894871000000	-3.107677000000
H	5.036942000000	1.105848000000	-0.701929000000
H	5.413727000000	2.269566000000	-1.971504000000
H	6.578100000000	0.022985000000	-2.320599000000
H	5.536786000000	0.470954000000	-3.666951000000
C	-5.132567000000	-0.371843000000	0.071512000000
C	-4.449135000000	-0.867754000000	-2.181007000000
C	-5.322007000000	-1.846783000000	0.401591000000
H	-4.796502000000	0.207784000000	0.930066000000

H	-6.064215000000	0.071879000000	-0.304993000000
C	-4.629194000000	-2.364168000000	-1.961968000000
H	-3.623392000000	-0.662810000000	-2.862030000000
H	-5.364427000000	-0.405271000000	-2.573764000000
C	-5.669494000000	-2.637253000000	-0.867322000000
H	-4.394299000000	-2.225794000000	0.842703000000
H	-6.106514000000	-1.945616000000	1.158428000000
H	-3.659713000000	-2.785998000000	-1.681983000000
H	-4.921121000000	-2.827097000000	-2.909573000000
H	-5.722281000000	-3.707164000000	-0.650114000000
H	-6.663937000000	-2.335035000000	-1.220249000000
O	-4.111141000000	-0.197530000000	-0.939367000000
O	2.752644000000	0.192485000000	-1.858192000000

Ca-Tetra_EQ656

($E_{el} = -3295.552147$ a.u.; $G = -3294.157224$ a.u.)

0 1

Ca	1.763270000000	-2.150917000000	0.837352000000
I	0.915250000000	-1.312828000000	-2.117219000000
I	-1.268969000000	-1.646743000000	1.759514000000
Ca	-2.235871000000	-0.845856000000	-1.458219000000
C	1.294346000000	-4.568935000000	0.635739000000
C	0.848112000000	-5.485579000000	1.611875000000
C	1.490224000000	-5.144929000000	-0.641426000000
C	0.646597000000	-6.846796000000	1.364003000000
H	0.632038000000	-5.136069000000	2.620933000000
C	1.289264000000	-6.499153000000	-0.923296000000
H	1.801607000000	-4.507453000000	-1.468867000000
C	0.873346000000	-7.363904000000	0.088914000000
H	0.305158000000	-7.502949000000	2.160528000000
H	1.455946000000	-6.879822000000	-1.927667000000
H	0.718949000000	-8.418666000000	-0.114511000000
C	-3.084527000000	-0.599206000000	-3.736458000000
C	-2.669206000000	-1.550346000000	-4.694832000000
C	-4.087274000000	0.282892000000	-4.193050000000
C	-3.195694000000	-1.626802000000	-5.987555000000
H	-1.891194000000	-2.268626000000	-4.429214000000
C	-4.635093000000	0.229699000000	-5.478337000000
H	-4.462806000000	1.058673000000	-3.525594000000
C	-4.189808000000	-0.732448000000	-6.384947000000
H	-2.832673000000	-2.377743000000	-6.684887000000
H	-5.406242000000	0.936173000000	-5.775208000000
H	-4.608088000000	-0.782308000000	-7.385279000000
C	-3.787329000000	-3.697686000000	-2.270904000000

C	-1.680313000000	-4.159724000000	-1.192133000000
C	-4.485858000000	-4.798714000000	-1.481296000000
H	-4.438284000000	-2.851830000000	-2.490468000000
H	-3.406593000000	-4.076133000000	-3.227240000000
C	-2.288977000000	-5.263701000000	-0.346149000000
H	-0.887720000000	-3.643890000000	-0.658254000000
H	-1.262556000000	-4.552197000000	-2.127101000000
C	-3.488413000000	-5.889993000000	-1.067990000000
H	-4.943617000000	-4.363286000000	-0.587470000000
H	-5.296185000000	-5.209838000000	-2.092274000000
H	-2.602028000000	-4.831797000000	0.610645000000
H	-1.515591000000	-6.002537000000	-0.129931000000
H	-3.976626000000	-6.635291000000	-0.433619000000
H	-3.135421000000	-6.417267000000	-1.963392000000
C	4.815192000000	-1.297807000000	-0.436151000000
C	4.607087000000	-3.692163000000	-0.233074000000
C	5.095893000000	-1.400393000000	-1.927151000000
H	4.259391000000	-0.391758000000	-0.202607000000
H	5.747319000000	-1.294208000000	0.145608000000
C	4.840588000000	-3.889102000000	-1.724008000000
H	3.922775000000	-4.432297000000	0.178411000000
H	5.561521000000	-3.738989000000	0.310198000000
C	5.714420000000	-2.757590000000	-2.278833000000
H	4.153803000000	-1.265404000000	-2.464451000000
H	5.744319000000	-0.571016000000	-2.215400000000
H	3.872036000000	-3.897998000000	-2.232277000000
H	5.300773000000	-4.869981000000	-1.880802000000
H	5.829373000000	-2.853431000000	-3.361904000000
H	6.720885000000	-2.828465000000	-1.845281000000
O	4.001380000000	-2.404772000000	0.036911000000
O	-2.674724000000	-3.155846000000	-1.524549000000
C	-4.910355000000	-1.482378000000	0.512870000000
C	-5.070722000000	0.670145000000	-0.556581000000
C	-6.321491000000	-1.855632000000	0.072989000000
H	-4.244238000000	-2.343907000000	0.541548000000
H	-4.911970000000	-1.008645000000	1.498961000000
C	-6.474170000000	0.377893000000	-1.064383000000
H	-4.505463000000	1.295927000000	-1.246422000000
H	-5.089053000000	1.163544000000	0.417165000000
C	-7.182475000000	-0.599048000000	-0.116238000000
H	-6.268282000000	-2.408904000000	-0.870583000000
H	-6.758839000000	-2.525949000000	0.820401000000
H	-6.406832000000	-0.046510000000	-2.071884000000
H	-7.024706000000	1.321055000000	-1.137348000000

H	-8.170155000000	-0.866706000000	-0.502479000000
H	-7.331346000000	-0.111100000000	0.854004000000
C	-0.036086000000	3.122455000000	-4.362787000000
C	1.278822000000	1.225100000000	-5.057207000000
C	-1.320448000000	2.476060000000	-4.856162000000
H	-0.195538000000	3.733779000000	-3.475222000000
H	0.425815000000	3.745325000000	-5.141868000000
C	0.047923000000	0.509746000000	-5.591203000000
H	2.005336000000	0.525262000000	-4.643320000000
H	1.772360000000	1.821928000000	-5.836470000000
C	-1.036828000000	1.508151000000	-6.010660000000
H	-1.782315000000	1.927230000000	-4.032474000000
H	-2.022514000000	3.259796000000	-5.158644000000
H	-0.348930000000	-0.140536000000	-4.809871000000
H	0.342999000000	-0.131294000000	-6.428119000000
H	-1.948235000000	0.974332000000	-6.283061000000
H	-0.702673000000	2.071349000000	-6.892899000000
O	0.932391000000	2.118321000000	-3.969825000000
O	-4.311654000000	-0.560149000000	-0.425146000000
Ca	1.641180000000	1.796040000000	-1.738154000000
I	-1.470956000000	2.278122000000	-0.795850000000
I	2.053468000000	1.228052000000	1.455857000000
Ca	-1.151166000000	1.465079000000	2.270971000000
C	4.064737000000	1.822557000000	-2.130024000000
C	5.012345000000	2.024546000000	-1.100788000000
C	4.621769000000	1.792654000000	-3.427006000000
C	6.384396000000	2.164294000000	-1.328984000000
H	4.670864000000	2.075864000000	-0.067314000000
C	5.988801000000	1.931657000000	-3.686963000000
H	3.968924000000	1.651536000000	-4.288107000000
C	6.881791000000	2.114450000000	-2.631594000000
H	7.066215000000	2.314387000000	-0.495297000000
H	6.359505000000	1.894970000000	-4.708257000000
H	7.945146000000	2.220695000000	-2.821101000000
C	-3.558496000000	1.752380000000	2.680531000000
C	-4.168273000000	2.905303000000	2.134058000000
C	-4.460673000000	0.871653000000	3.314401000000
C	-5.539140000000	3.169011000000	2.210885000000
H	-3.553837000000	3.622596000000	1.589114000000
C	-5.837388000000	1.104441000000	3.403394000000
H	-4.088291000000	-0.059184000000	3.743842000000
C	-6.384673000000	2.261817000000	2.850055000000
H	-5.950844000000	4.070414000000	1.764045000000
H	-6.484476000000	0.383884000000	3.897457000000

H	-7.451366000000	2.451464000000	2.912504000000
C	0.646891000000	1.450035000000	5.159586000000
C	-1.330950000000	0.093962000000	5.357860000000
C	1.547411000000	0.285623000000	5.547680000000
H	1.125172000000	2.111072000000	4.438187000000
H	0.356419000000	2.038963000000	6.041137000000
C	-0.517570000000	-1.122509000000	5.781005000000
H	-2.200529000000	-0.182154000000	4.764747000000
H	-1.673518000000	0.669551000000	6.228469000000
C	0.787284000000	-0.686279000000	6.460419000000
H	1.854442000000	-0.220781000000	4.628173000000
H	2.447855000000	0.671733000000	6.036065000000
H	-0.298813000000	-1.713430000000	4.886711000000
H	-1.124388000000	-1.743533000000	6.447152000000
H	1.404742000000	-1.554902000000	6.705010000000
H	0.557827000000	-0.189122000000	7.411676000000
C	2.523107000000	4.852818000000	-2.805889000000
C	1.398237000000	5.030352000000	-0.688618000000
C	3.837719000000	5.343831000000	-2.213489000000
H	2.688866000000	4.112499000000	-3.587208000000
H	1.930691000000	5.681793000000	-3.217199000000
C	2.675943000000	5.465337000000	0.018104000000
H	0.740629000000	4.438336000000	-0.053580000000
H	0.828219000000	5.897513000000	-1.049613000000
C	3.594313000000	6.204310000000	-0.966032000000
H	4.444255000000	4.473164000000	-1.957340000000
H	4.378331000000	5.908197000000	-2.979886000000
H	3.178063000000	4.572901000000	0.406369000000
H	2.422755000000	6.101689000000	0.871470000000
H	4.545140000000	6.454535000000	-0.488201000000
H	3.121657000000	7.152926000000	-1.253195000000
O	1.708377000000	4.185925000000	-1.810995000000
O	-0.549616000000	0.971003000000	4.519209000000
C	-1.511576000000	4.079778000000	4.294685000000
C	0.343491000000	4.588646000000	2.856929000000
C	-2.201342000000	5.395923000000	3.961325000000
H	-2.233272000000	3.280648000000	4.458455000000
H	-0.869643000000	4.179591000000	5.181073000000
C	-0.275823000000	5.911352000000	2.423542000000
H	0.939688000000	4.120943000000	2.075261000000
H	0.991020000000	4.729694000000	3.734296000000
C	-1.182045000000	6.460490000000	3.534406000000
H	-2.918704000000	5.213252000000	3.157508000000
H	-2.773335000000	5.725064000000	4.834400000000

H	-0.858384000000	5.741717000000	1.511778000000
H	0.519425000000	6.622121000000	2.179763000000
H	-1.692468000000	7.367741000000	3.200613000000
H	-0.562638000000	6.742590000000	4.395548000000
C	4.020718000000	-1.597713000000	3.350288000000
C	2.290455000000	-3.145260000000	3.974116000000
C	5.074080000000	-2.697531000000	3.343161000000
H	4.214271000000	-0.830740000000	2.601418000000
H	3.966192000000	-1.110054000000	4.332055000000
C	3.254731000000	-4.322754000000	3.964965000000
H	1.284014000000	-3.428402000000	3.666887000000
H	2.233211000000	-2.689601000000	4.969833000000
C	4.677197000000	-3.842837000000	4.285370000000
H	5.168610000000	-3.072865000000	2.322780000000
H	6.039683000000	-2.267292000000	3.627312000000
H	3.216297000000	-4.790527000000	2.977017000000
H	2.916073000000	-5.069401000000	4.689805000000
H	5.388458000000	-4.668814000000	4.202581000000
H	4.718663000000	-3.490451000000	5.324187000000
O	2.712820000000	-2.126796000000	3.040173000000
O	-0.680476000000	3.635575000000	3.194325000000

Ca-Tetra_EQ45

(E_{el} = -3295.520936 a.u.; G = -3294.133847 a.u.)

0 1

Ca	4.482107000000	-1.277329000000	-0.308800000000
I	4.707700000000	1.815308000000	-0.657728000000
I	1.638710000000	-0.851205000000	1.024680000000
Ca	1.473745000000	2.105368000000	-0.120114000000
C	3.563465000000	-3.316103000000	-1.333279000000
C	2.869012000000	-4.175423000000	-0.451592000000
C	3.520431000000	-3.725379000000	-2.683882000000
C	2.197915000000	-5.328929000000	-0.863733000000
H	2.820346000000	-3.929412000000	0.610160000000
C	2.835895000000	-4.860278000000	-3.129710000000
H	4.044485000000	-3.139564000000	-3.439039000000
C	2.169103000000	-5.672302000000	-2.214309000000
H	1.690903000000	-5.957099000000	-0.136740000000
H	2.825807000000	-5.114104000000	-4.186516000000
H	1.637509000000	-6.557966000000	-2.546308000000
C	1.931572000000	3.142769000000	2.052292000000
C	3.130459000000	3.012092000000	2.787033000000
C	0.964785000000	3.967982000000	2.669235000000
C	3.356658000000	3.642003000000	4.014366000000

H	3.934611000000	2.401358000000	2.379859000000
C	1.166890000000	4.621647000000	3.888834000000
H	0.000637000000	4.112008000000	2.180407000000
C	2.372727000000	4.459969000000	4.570587000000
H	4.303350000000	3.508028000000	4.533194000000
H	0.384954000000	5.248117000000	4.311143000000
H	2.541986000000	4.961471000000	5.518373000000
C	2.173585000000	5.265775000000	-0.892049000000
C	-0.067787000000	4.798298000000	-1.652502000000
C	1.676688000000	6.333697000000	0.072434000000
H	3.038457000000	4.735020000000	-0.492204000000
H	2.442264000000	5.694366000000	-1.867712000000
C	-0.668107000000	5.810040000000	-0.688642000000
H	-0.728038000000	3.946377000000	-1.813371000000
H	0.153886000000	5.263202000000	-2.624191000000
C	0.342692000000	6.928863000000	-0.399882000000
H	1.558902000000	5.875741000000	1.056775000000
H	2.444239000000	7.109374000000	0.159664000000
H	-0.936884000000	5.288748000000	0.234603000000
H	-1.592341000000	6.208088000000	-1.118644000000
H	-0.052918000000	7.615188000000	0.353181000000
H	0.501490000000	7.516266000000	-1.314051000000
C	5.190871000000	-2.821000000000	2.563937000000
C	5.541505000000	-0.436598000000	2.775857000000
C	4.095793000000	-2.804299000000	3.623985000000
H	4.998395000000	-3.566249000000	1.788734000000
H	6.172731000000	-3.029128000000	3.008973000000
C	4.470210000000	-0.321048000000	3.850800000000
H	5.573943000000	0.449894000000	2.140879000000
H	6.535980000000	-0.598438000000	3.211852000000
C	4.316163000000	-1.646571000000	4.608743000000
H	3.129639000000	-2.687620000000	3.124926000000
H	4.089780000000	-3.768948000000	4.141431000000
H	3.526632000000	-0.042167000000	3.378313000000
H	4.737214000000	0.495025000000	4.528205000000
H	3.482560000000	-1.584634000000	5.313169000000
H	5.219450000000	-1.840327000000	5.201597000000
O	5.269200000000	-1.548932000000	1.879978000000
O	1.161428000000	4.251340000000	-1.123348000000
C	1.775868000000	-0.049505000000	-2.961612000000
C	1.626138000000	2.250768000000	-3.620169000000
C	3.075194000000	-0.234916000000	-3.737919000000
H	1.759341000000	-0.662266000000	-2.060832000000
H	0.915867000000	-0.335800000000	-3.577284000000

C	2.945621000000	2.179872000000	-4.378714000000
H	1.474971000000	3.228979000000	-3.172405000000
H	0.786219000000	2.032859000000	-4.290554000000
C	3.177037000000	0.757531000000	-4.900700000000
H	3.923244000000	-0.073179000000	-3.065145000000
H	3.117129000000	-1.269089000000	-4.085249000000
H	3.756421000000	2.466634000000	-3.702860000000
H	2.919274000000	2.904272000000	-5.199444000000
H	4.151783000000	0.675924000000	-5.390073000000
H	2.418964000000	0.515945000000	-5.656981000000
C	7.670671000000	-0.533214000000	-1.299172000000
C	6.899905000000	-2.609378000000	-2.232315000000
C	7.759447000000	0.119566000000	-2.672818000000
H	7.397585000000	0.189152000000	-0.530570000000
H	8.618413000000	-1.011440000000	-1.019155000000
C	6.932027000000	-2.051393000000	-3.649340000000
H	6.102549000000	-3.336741000000	-2.090185000000
H	7.859983000000	-3.071200000000	-1.966955000000
C	7.980742000000	-0.935836000000	-3.765707000000
H	6.827250000000	0.664588000000	-2.850326000000
H	8.568085000000	0.856914000000	-2.665836000000
H	5.938304000000	-1.657767000000	-3.889661000000
H	7.136830000000	-2.865258000000	-4.351470000000
H	7.942962000000	-0.473541000000	-4.755738000000
H	8.982282000000	-1.370875000000	-3.656873000000
O	6.636730000000	-1.546544000000	-1.281795000000
O	1.585116000000	1.314300000000	-2.521846000000
Ca	-1.583202000000	-1.109489000000	1.389129000000
I	-1.701365000000	1.868439000000	0.278399000000
I	-4.552968000000	-1.455047000000	2.133773000000
Ca	-4.308013000000	-0.048027000000	-0.787804000000
C	-2.289287000000	-1.828228000000	-0.964238000000
C	-2.995951000000	-3.027773000000	-1.216029000000
C	-1.032973000000	-1.748197000000	-1.608530000000
C	-2.511700000000	-4.041736000000	-2.047752000000
H	-3.958762000000	-3.182707000000	-0.729905000000
C	-0.494078000000	-2.775287000000	-2.389622000000
H	-0.437232000000	-0.847846000000	-1.477323000000
C	-1.244967000000	-3.926496000000	-2.621344000000
H	-3.102717000000	-4.937651000000	-2.219741000000
H	0.509126000000	-2.701394000000	-2.797432000000
H	-0.834270000000	-4.729692000000	-3.223140000000
C	-5.839442000000	1.835797000000	-0.344265000000
C	-5.643977000000	2.724307000000	0.736718000000

C	-7.042699000000	2.047736000000	-1.052992000000
C	-6.551879000000	3.729298000000	1.081110000000
H	-4.743341000000	2.632425000000	1.343026000000
C	-7.970561000000	3.044412000000	-0.732593000000
H	-7.277337000000	1.409419000000	-1.907746000000
C	-7.724867000000	3.894528000000	0.343923000000
H	-6.348259000000	4.384508000000	1.924720000000
H	-8.881243000000	3.157527000000	-1.316619000000
H	-8.435866000000	4.672071000000	0.605909000000
C	-2.959609000000	-0.035489000000	-3.970500000000
C	-4.476525000000	1.781491000000	-3.580882000000
C	-1.753736000000	0.896165000000	-3.984729000000
H	-2.702110000000	-1.012999000000	-3.564860000000
H	-3.371351000000	-0.162903000000	-4.981656000000
C	-3.345828000000	2.800684000000	-3.556356000000
H	-5.278861000000	2.061285000000	-2.902273000000
H	-4.880337000000	1.653890000000	-4.594797000000
C	-2.162637000000	2.315707000000	-4.404241000000
H	-1.316014000000	0.913667000000	-2.982464000000
H	-1.002554000000	0.484109000000	-4.665867000000
H	-3.036570000000	2.936122000000	-2.515121000000
H	-3.723139000000	3.763250000000	-3.915149000000
H	-1.317146000000	3.002777000000	-4.307024000000
H	-2.450114000000	2.314703000000	-5.463622000000
C	-0.303459000000	-4.229958000000	1.370187000000
C	-1.488908000000	-3.746064000000	3.423885000000
C	-1.204725000000	-5.423118000000	1.083996000000
H	0.009571000000	-3.725379000000	0.457165000000
H	0.598029000000	-4.529199000000	1.921328000000
C	-2.439772000000	-4.914582000000	3.209813000000
H	-1.984477000000	-2.903493000000	3.906120000000
H	-0.620879000000	-4.043112000000	4.028934000000
C	-1.758313000000	-6.015228000000	2.385951000000
H	-2.024543000000	-5.085328000000	0.446359000000
H	-0.636912000000	-6.164473000000	0.514643000000
H	-3.325769000000	-4.540308000000	2.688024000000
H	-2.765680000000	-5.290322000000	4.184980000000
H	-2.462594000000	-6.823292000000	2.170144000000
H	-0.938148000000	-6.455042000000	2.968938000000
O	-0.999696000000	-3.237885000000	2.162657000000
O	-4.001903000000	0.490092000000	-3.123944000000
C	-5.999859000000	-2.219796000000	-2.786228000000
C	-7.208256000000	-1.748539000000	-0.753684000000
C	-7.217304000000	-1.909844000000	-3.647916000000

H	-5.068194000000	-1.940613000000	-3.276429000000
H	-5.951323000000	-3.289473000000	-2.540612000000
C	-8.490195000000	-1.458977000000	-1.524457000000
H	-7.113977000000	-1.115974000000	0.127797000000
H	-7.156169000000	-2.798224000000	-0.436188000000
C	-8.506729000000	-2.201490000000	-2.867628000000
H	-7.181964000000	-0.852498000000	-3.931949000000
H	-7.168681000000	-2.501410000000	-4.567986000000
H	-8.559485000000	-0.380521000000	-1.688338000000
H	-9.344829000000	-1.747926000000	-0.904862000000
H	-9.384737000000	-1.915668000000	-3.453363000000
H	-8.581128000000	-3.281931000000	-2.688785000000
C	-2.042331000000	0.604904000000	4.258563000000
C	-0.050253000000	-0.739991000000	4.427631000000
C	-1.260832000000	1.875156000000	4.550813000000
H	-2.870665000000	0.774282000000	3.572128000000
H	-2.446976000000	0.152613000000	5.173465000000
C	0.812827000000	0.479054000000	4.719304000000
H	0.488174000000	-1.499415000000	3.860567000000
H	-0.423196000000	-1.194068000000	5.356785000000
C	-0.019185000000	1.573473000000	5.398531000000
H	-0.954953000000	2.322521000000	3.602548000000
H	-1.920992000000	2.589453000000	5.053088000000
H	1.222245000000	0.862985000000	3.781253000000
H	1.657726000000	0.177566000000	5.347442000000
H	0.582086000000	2.474803000000	5.521860000000
H	-0.327768000000	1.237068000000	6.397885000000
O	-1.192691000000	-0.384807000000	3.617121000000
O	-6.040306000000	-1.468353000000	-1.561529000000

Ca-Tetra_EQ406

(E_{el} = -3295.546275 a.u.; G = -3294.152708 a.u.)

0 1

Ca	0.450127000000	1.523117000000	2.565324000000
I	1.928598000000	1.909403000000	-0.241928000000
I	0.538449000000	-1.629530000000	2.089359000000
Ca	2.351701000000	-1.295020000000	-0.654562000000
C	2.570760000000	1.595250000000	3.796503000000
C	2.948417000000	0.808807000000	4.907121000000
C	3.615031000000	2.392436000000	3.272999000000
C	4.240856000000	0.793857000000	5.441537000000
H	2.213616000000	0.156462000000	5.378081000000
C	4.914822000000	2.402553000000	3.788884000000
H	3.419142000000	3.023517000000	2.406645000000

C	5.235884000000	1.593492000000	4.878889000000
H	4.474173000000	0.161309000000	6.294371000000
H	5.677349000000	3.035386000000	3.341278000000
H	6.242169000000	1.589528000000	5.285661000000
C	3.622648000000	-1.553168000000	-2.757010000000
C	2.981559000000	-2.097616000000	-3.893417000000
C	5.024387000000	-1.440409000000	-2.895969000000
C	3.655224000000	-2.502852000000	-5.048575000000
H	1.899579000000	-2.220390000000	-3.885303000000
C	5.726052000000	-1.828337000000	-4.041883000000
H	5.617188000000	-1.043043000000	-2.074726000000
C	5.040743000000	-2.368609000000	-5.129010000000
H	3.101038000000	-2.916758000000	-5.887402000000
H	6.806260000000	-1.714937000000	-4.085581000000
H	5.575714000000	-2.677520000000	-6.021283000000
C	5.126971000000	0.147467000000	0.388331000000
C	4.355748000000	-1.184997000000	2.217982000000
C	6.571756000000	-0.279660000000	0.608462000000
H	4.911752000000	0.348888000000	-0.660689000000
H	4.883698000000	1.042873000000	0.969075000000
C	5.762976000000	-1.667076000000	2.542422000000
H	3.600193000000	-1.930534000000	2.454615000000
H	4.109177000000	-0.275366000000	2.768186000000
C	6.803643000000	-0.637617000000	2.082778000000
H	6.788386000000	-1.143595000000	-0.029711000000
H	7.232358000000	0.533898000000	0.291974000000
H	5.942656000000	-2.628639000000	2.048996000000
H	5.828901000000	-1.830619000000	3.622251000000
H	7.817260000000	-1.020606000000	2.231930000000
H	6.700389000000	0.264147000000	2.695208000000
C	-0.845460000000	0.165525000000	5.337013000000
C	-2.288898000000	1.916806000000	4.520063000000
C	-1.966046000000	-0.859182000000	5.267166000000
H	0.123847000000	-0.277779000000	5.110224000000
H	-0.787571000000	0.643521000000	6.324076000000
C	-3.472011000000	0.964118000000	4.428957000000
H	-2.304052000000	2.669607000000	3.731216000000
H	-2.255389000000	2.426484000000	5.492988000000
C	-3.334170000000	-0.187028000000	5.433397000000
H	-1.927451000000	-1.360545000000	4.297355000000
H	-1.804011000000	-1.622170000000	6.035295000000
H	-3.515747000000	0.554753000000	3.418082000000
H	-4.397109000000	1.526245000000	4.593329000000
H	-4.129380000000	-0.917363000000	5.274955000000

H	-3.435038000000	0.199467000000	6.456775000000
O	-1.039851000000	1.206578000000	4.349289000000
O	4.217710000000	-0.909149000000	0.795664000000
C	3.008968000000	-4.360363000000	0.689373000000
C	2.339432000000	-4.594877000000	-1.597210000000
C	4.461217000000	-4.676214000000	0.358373000000
H	2.903724000000	-3.668281000000	1.522614000000
H	2.456208000000	-5.275932000000	0.942730000000
C	3.747115000000	-4.984663000000	-2.030704000000
H	1.823312000000	-4.032781000000	-2.373819000000
H	1.741415000000	-5.481234000000	-1.341799000000
C	4.531013000000	-5.600998000000	-0.864505000000
H	4.977827000000	-3.734855000000	0.146778000000
H	4.940811000000	-5.129906000000	1.231523000000
H	4.254270000000	-4.088895000000	-2.394297000000
H	3.674196000000	-5.681364000000	-2.871515000000
H	5.569925000000	-5.774491000000	-1.156505000000
H	4.105854000000	-6.578538000000	-0.601104000000
C	-0.407543000000	4.658744000000	1.701027000000
C	0.349898000000	4.513949000000	3.996518000000
C	0.697777000000	5.634876000000	1.339208000000
H	-0.647593000000	4.001021000000	0.870519000000
H	-1.325506000000	5.181273000000	1.996455000000
C	1.478630000000	5.502425000000	3.730475000000
H	0.646429000000	3.752541000000	4.719208000000
H	-0.550901000000	5.026909000000	4.361024000000
C	1.119692000000	6.444361000000	2.572037000000
H	1.548046000000	5.064745000000	0.950630000000
H	0.340930000000	6.276616000000	0.530565000000
H	2.381359000000	4.933448000000	3.491040000000
H	1.680844000000	6.061323000000	4.650087000000
H	1.966252000000	7.094442000000	2.334354000000
H	0.292301000000	7.099435000000	2.874985000000
O	-0.005257000000	3.794332000000	2.795386000000
O	2.356438000000	-3.731449000000	-0.433675000000
Ca	-0.657526000000	2.176458000000	-2.034667000000
I	-0.524946000000	-1.149871000000	-2.271873000000
I	-2.468628000000	1.414816000000	0.554352000000
Ca	-2.218618000000	-1.774137000000	0.511346000000
C	-1.006884000000	4.593327000000	-1.746162000000
C	-2.108578000000	5.140603000000	-1.049443000000
C	-0.140278000000	5.558861000000	-2.302906000000
C	-2.328022000000	6.513226000000	-0.904657000000
H	-2.825824000000	4.466664000000	-0.579984000000

C	-0.334439000000	6.938556000000	-2.176209000000
H	0.737689000000	5.232863000000	-2.859968000000
C	-1.434433000000	7.423600000000	-1.470105000000
H	-3.191978000000	6.875052000000	-0.352507000000
H	0.371879000000	7.634779000000	-2.621416000000
H	-1.593178000000	8.491869000000	-1.362393000000
C	-3.687409000000	-2.342113000000	2.384945000000
C	-3.601721000000	-3.404424000000	3.308961000000
C	-4.907336000000	-1.630320000000	2.434535000000
C	-4.626542000000	-3.738763000000	4.199667000000
H	-2.690123000000	-4.001855000000	3.355764000000
C	-5.950321000000	-1.939618000000	3.312669000000
H	-5.056240000000	-0.780152000000	1.765362000000
C	-5.812975000000	-3.005035000000	4.202684000000
H	-4.502366000000	-4.566787000000	4.893152000000
H	-6.863656000000	-1.349742000000	3.310854000000
H	-6.613870000000	-3.255202000000	4.891063000000
C	-1.647783000000	-4.573135000000	-1.389431000000
C	-0.912925000000	-4.857149000000	0.884844000000
C	-2.160800000000	-6.006770000000	-1.456380000000
H	-2.254483000000	-3.888389000000	-1.979907000000
H	-0.616043000000	-4.503033000000	-1.751841000000
C	-1.404425000000	-6.297131000000	0.918215000000
H	-1.016354000000	-4.372335000000	1.853512000000
H	0.138087000000	-4.789662000000	0.581263000000
C	-1.382049000000	-6.907186000000	-0.488879000000
H	-3.224258000000	-6.020772000000	-1.196455000000
H	-2.074150000000	-6.364418000000	-2.487277000000
H	-2.423958000000	-6.309230000000	1.317953000000
H	-0.777187000000	-6.870135000000	1.608316000000
H	-1.799752000000	-7.917404000000	-0.480798000000
H	-0.342985000000	-6.994629000000	-0.831110000000
C	-2.544780000000	3.313353000000	-4.533886000000
C	-3.495461000000	1.250642000000	-3.738629000000
C	-3.764144000000	4.109561000000	-4.091132000000
H	-1.629998000000	3.894210000000	-4.422120000000
H	-2.637065000000	2.976277000000	-5.575595000000
C	-4.735693000000	1.959439000000	-3.209197000000
H	-3.208054000000	0.386857000000	-3.139503000000
H	-3.644411000000	0.911724000000	-4.773317000000
C	-5.014616000000	3.222082000000	-4.037250000000
H	-3.553002000000	4.530617000000	-3.105687000000
H	-3.905450000000	4.948668000000	-4.779467000000
H	-4.561968000000	2.223022000000	-2.160359000000

H	-5.588410000000	1.275480000000	-3.241503000000
H	-5.856565000000	3.777298000000	-3.615541000000
H	-5.304969000000	2.926906000000	-5.054197000000
O	-2.360816000000	2.135923000000	-3.706985000000
O	-1.692598000000	-4.063972000000	-0.038936000000
C	-4.897200000000	-3.464747000000	-0.515557000000
C	-4.999069000000	-1.234845000000	-1.380199000000
C	-5.456730000000	-4.054971000000	-1.803676000000
H	-4.193218000000	-4.126046000000	-0.015325000000
H	-5.687896000000	-3.220328000000	0.202015000000
C	-5.558189000000	-1.707411000000	-2.716721000000
H	-4.376082000000	-0.346342000000	-1.471574000000
H	-5.804697000000	-1.008156000000	-0.669975000000
C	-6.327309000000	-3.024405000000	-2.536587000000
H	-4.625737000000	-4.361416000000	-2.448276000000
H	-6.032471000000	-4.954719000000	-1.564905000000
H	-4.724864000000	-1.849210000000	-3.413781000000
H	-6.209069000000	-0.933892000000	-3.134293000000
H	-6.654835000000	-3.413763000000	-3.504360000000
H	-7.232073000000	-2.833408000000	-1.946771000000
C	0.475050000000	1.695894000000	-5.215901000000
C	2.071396000000	2.934347000000	-3.917847000000
C	1.486692000000	0.597338000000	-5.505057000000
H	-0.537637000000	1.304216000000	-5.128466000000
H	0.487100000000	2.471643000000	-5.994356000000
C	3.147310000000	1.879704000000	-4.129171000000
H	2.157764000000	3.416310000000	-2.945236000000
H	2.106344000000	3.708841000000	-4.696012000000
C	2.922997000000	1.132092000000	-5.449151000000
H	1.363620000000	-0.186990000000	-4.756925000000
H	1.266182000000	0.155341000000	-6.482544000000
H	3.119847000000	1.166795000000	-3.300270000000
H	4.129671000000	2.362320000000	-4.110344000000
H	3.631427000000	0.306447000000	-5.537983000000
H	3.096887000000	1.812992000000	-6.293277000000
O	0.751459000000	2.335723000000	-3.948273000000
O	-4.158430000000	-2.252762000000	-0.803823000000

Int1

(E_{el} = -3023.642382 a.u.; G = -3022.395192 a.u.)

0 1

Ca	2.270493000000	-1.392753000000	0.793880000000
I	1.485759000000	-0.719040000000	-2.244835000000
I	-0.808670000000	-1.879829000000	1.484756000000

Ca	-1.681255000000	-1.382489000000	-1.841527000000
C	2.733733000000	-3.778318000000	0.444959000000
C	2.537341000000	-4.852382000000	1.339471000000
C	3.290882000000	-4.158237000000	-0.797929000000
C	2.880189000000	-6.176215000000	1.046701000000
H	2.080725000000	-4.666820000000	2.310977000000
C	3.637355000000	-5.472978000000	-1.122167000000
H	3.445310000000	-3.398781000000	-1.564619000000
C	3.439060000000	-6.492706000000	-0.191106000000
H	2.704332000000	-6.961795000000	1.777184000000
H	4.058859000000	-5.703948000000	-2.097068000000
H	3.707062000000	-7.516969000000	-0.429517000000
C	-2.308541000000	-1.114872000000	-4.163030000000
C	-1.393605000000	-1.537905000000	-5.152934000000
C	-3.530464000000	-0.622787000000	-4.669227000000
C	-1.663907000000	-1.485189000000	-6.523633000000
H	-0.418447000000	-1.922876000000	-4.849364000000
C	-3.827755000000	-0.559476000000	-6.033746000000
H	-4.292379000000	-0.263901000000	-3.976781000000
C	-2.890516000000	-0.994632000000	-6.970141000000
H	-0.921519000000	-1.822572000000	-7.242872000000
H	-4.786409000000	-0.170789000000	-6.368802000000
H	-3.111763000000	-0.949615000000	-8.032053000000
C	-1.881484000000	-4.449182000000	-3.091938000000
C	0.012411000000	-4.282393000000	-1.605223000000
C	-2.227699000000	-5.837601000000	-2.567558000000
H	-2.758379000000	-3.872205000000	-3.385849000000
H	-1.217532000000	-4.505550000000	-3.963121000000
C	-0.254165000000	-5.655661000000	-1.014305000000
H	0.431959000000	-3.607649000000	-0.864315000000
H	0.709838000000	-4.335512000000	-2.448990000000
C	-0.973985000000	-6.546598000000	-2.034788000000
H	-2.965035000000	-5.739725000000	-1.763654000000
H	-2.698493000000	-6.412150000000	-3.371812000000
H	-0.870682000000	-5.533968000000	-0.116537000000
H	0.697727000000	-6.087458000000	-0.698747000000
H	-1.237963000000	-7.510087000000	-1.589595000000
H	-0.294723000000	-6.758077000000	-2.870190000000
C	4.907286000000	0.547024000000	-0.194243000000
C	5.598122000000	-1.676591000000	0.450411000000
C	5.532461000000	0.394089000000	-1.569870000000
H	4.009631000000	1.159464000000	-0.234894000000
H	5.608695000000	1.008097000000	0.514535000000
C	6.247330000000	-1.919128000000	-0.905234000000

H	5.167098000000	-2.591020000000	0.858639000000
H	6.329563000000	-1.265526000000	1.160021000000
C	6.702618000000	-0.594838000000	-1.530199000000
H	4.761351000000	0.042011000000	-2.261224000000
H	5.844964000000	1.380045000000	-1.918622000000
H	5.519955000000	-2.412970000000	-1.554890000000
H	7.084985000000	-2.611484000000	-0.772383000000
H	7.097747000000	-0.760433000000	-2.536067000000
H	7.521145000000	-0.170782000000	-0.933414000000
O	4.501274000000	-0.737304000000	0.351825000000
O	-1.219120000000	-3.670247000000	-2.068904000000
C	-4.062792000000	-3.114265000000	-0.209701000000
C	-4.924579000000	-1.046866000000	-1.103119000000
C	-5.184901000000	-3.915459000000	-0.859346000000
H	-3.127434000000	-3.672101000000	-0.170695000000
H	-4.329490000000	-2.802772000000	0.804996000000
C	-6.071517000000	-1.761964000000	-1.801299000000
H	-4.576526000000	-0.181925000000	-1.667084000000
H	-5.203887000000	-0.714510000000	-0.101751000000
C	-6.435787000000	-3.044354000000	-1.041013000000
H	-4.843942000000	-4.277663000000	-1.835284000000
H	-5.399532000000	-4.793074000000	-0.240584000000
H	-5.770624000000	-2.000051000000	-2.827115000000
H	-6.927542000000	-1.082295000000	-1.855838000000
H	-7.215553000000	-3.599461000000	-1.570135000000
H	-6.836899000000	-2.775818000000	-0.056651000000
O	-3.776450000000	-1.927460000000	-0.981964000000
Ca	1.047114000000	2.302496000000	-1.610146000000
I	-2.087297000000	1.787908000000	-1.092729000000
I	1.467772000000	1.893861000000	1.497615000000
Ca	-1.787547000000	1.081808000000	1.977226000000
C	3.305068000000	3.036566000000	-2.111741000000
C	4.077935000000	3.783689000000	-1.195700000000
C	3.899167000000	2.871258000000	-3.381563000000
C	5.329521000000	4.323459000000	-1.507953000000
H	3.695810000000	3.947342000000	-0.187038000000
C	5.142435000000	3.409437000000	-3.725188000000
H	3.381265000000	2.285934000000	-4.143309000000
C	5.865873000000	4.141048000000	-2.783019000000
H	5.885696000000	4.887284000000	-0.763305000000
H	5.552987000000	3.252064000000	-4.719011000000
H	6.834363000000	4.559408000000	-3.037529000000
C	-4.131696000000	0.422398000000	2.207625000000
C	-5.141056000000	1.267264000000	1.694589000000

C	-4.606845000000	-0.815049000000	2.694387000000
C	-6.498163000000	0.930716000000	1.675991000000
H	-4.858747000000	2.222257000000	1.251649000000
C	-5.956892000000	-1.180713000000	2.688791000000
H	-3.893220000000	-1.548983000000	3.071775000000
C	-6.913491000000	-0.302214000000	2.179533000000
H	-7.229491000000	1.619637000000	1.261183000000
H	-6.264185000000	-2.150508000000	3.072329000000
H	-7.963287000000	-0.576865000000	2.168584000000
C	-0.359300000000	1.865684000000	4.967195000000
C	-1.987287000000	0.113699000000	5.204579000000
C	0.768740000000	0.957863000000	5.438456000000
H	-0.020452000000	2.586941000000	4.224330000000
H	-0.811332000000	2.409139000000	5.808473000000
C	-0.936856000000	-0.875258000000	5.693312000000
H	-2.778991000000	-0.358985000000	4.626394000000
H	-2.448896000000	0.651322000000	6.044016000000
C	0.220718000000	-0.129693000000	6.373480000000
H	1.223606000000	0.503709000000	4.553142000000
H	1.536721000000	1.560269000000	5.933831000000
H	-0.570138000000	-1.439048000000	4.829438000000
H	-1.405120000000	-1.588562000000	6.378352000000
H	1.012616000000	-0.825875000000	6.663853000000
H	-0.139529000000	0.335229000000	7.299903000000
C	0.973955000000	4.895722000000	-3.746174000000
C	-0.595851000000	5.270825000000	-1.970251000000
C	1.846313000000	6.062226000000	-3.304124000000
H	1.576282000000	4.094289000000	-4.170492000000
H	0.218250000000	5.203747000000	-4.479824000000
C	0.214472000000	6.439181000000	-1.421005000000
H	-1.123747000000	4.720203000000	-1.193363000000
H	-1.339745000000	5.610250000000	-2.702250000000
C	1.016297000000	7.108465000000	-2.547124000000
H	2.642094000000	5.668392000000	-2.666631000000
H	2.321809000000	6.501369000000	-4.186340000000
H	0.897103000000	6.061919000000	-0.651012000000
H	-0.461792000000	7.153666000000	-0.940673000000
H	1.664799000000	7.890053000000	-2.142828000000
H	0.319139000000	7.598605000000	-3.238734000000
O	0.273076000000	4.315225000000	-2.613776000000
O	-1.389295000000	1.091364000000	4.323208000000
C	-2.973408000000	3.770606000000	3.581063000000
C	-1.487013000000	4.521389000000	1.840732000000
C	-4.102404000000	4.656723000000	3.069782000000

H	-3.349091000000	2.834216000000	3.991521000000
H	-2.382087000000	4.286812000000	4.350339000000
C	-2.562746000000	5.407368000000	1.228093000000
H	-0.816361000000	4.099468000000	1.093480000000
H	-0.879172000000	5.078477000000	2.566873000000
C	-3.549413000000	5.869049000000	2.309068000000
H	-4.741382000000	4.060199000000	2.414244000000
H	-4.715733000000	4.970764000000	3.920135000000
H	-3.086935000000	4.832177000000	0.457610000000
H	-2.087338000000	6.262780000000	0.738443000000
H	-4.364900000000	6.445396000000	1.864596000000
H	-3.031390000000	6.537458000000	3.008850000000
C	3.913112000000	-0.468550000000	3.640643000000
C	2.397359000000	-2.305696000000	4.023512000000
C	5.101752000000	-1.291562000000	4.124487000000
H	4.184217000000	0.219098000000	2.840511000000
H	3.479007000000	0.112771000000	4.463618000000
C	3.526270000000	-3.210083000000	4.496133000000
H	1.615766000000	-2.851676000000	3.495848000000
H	1.937270000000	-1.781097000000	4.868442000000
C	4.650084000000	-2.370563000000	5.117828000000
H	5.576537000000	-1.767237000000	3.262709000000
H	5.838283000000	-0.618924000000	4.575427000000
H	3.902966000000	-3.776180000000	3.639284000000
H	3.126410000000	-3.931901000000	5.215241000000
H	5.493280000000	-3.005258000000	5.402364000000
H	4.285992000000	-1.892845000000	6.036685000000
O	2.881607000000	-1.314528000000	3.090265000000
O	-2.076694000000	3.391005000000	2.511623000000

Int2

(E_{el} = -3281.457485 a.u.; G = -3280.089275 a.u.)

0 1

Ca	-2.202187000000	-1.869226000000	0.657846000000
I	-1.332893000000	0.864196000000	2.024359000000
I	0.907613000000	-2.565739000000	0.417205000000
Ca	1.859146000000	0.324738000000	1.946350000000
C	-2.316943000000	-3.205706000000	2.738381000000
C	-2.043694000000	-4.570136000000	2.976204000000
C	-2.682041000000	-2.487805000000	3.901787000000
C	-2.152921000000	-5.178101000000	4.230188000000
H	-1.714314000000	-5.207185000000	2.155775000000
C	-2.788513000000	-3.063389000000	5.171340000000
H	-2.882646000000	-1.419475000000	3.826126000000

C	-2.53265000000	-4.42371200000	5.33989600000
H	-1.93272300000	-6.23630200000	4.34547100000
H	-3.07206300000	-2.45422500000	6.02570500000
H	-2.61883100000	-4.88538000000	6.31826500000
C	2.41274200000	2.41304000000	3.10252300000
C	2.25415600000	2.46151200000	4.50584800000
C	3.01100500000	3.56576800000	2.54522500000
C	2.67192800000	3.53889300000	5.29386300000
H	1.78129400000	1.62144200000	5.01613900000
C	3.43887600000	4.65649900000	3.30860200000
H	3.14967800000	3.62171600000	1.46532300000
C	3.27720500000	4.64330500000	4.69417200000
H	2.52844600000	3.52004500000	6.37137100000
H	3.90060400000	5.51513500000	2.82706600000
H	3.60873000000	5.48388900000	5.29534900000
C	2.93975600000	-1.10177300000	4.77411300000
C	0.67912200000	-1.80179400000	4.27926200000
C	3.37803000000	-2.54102900000	5.01952500000
H	3.73126700000	-0.49569300000	4.33308200000
H	2.61912700000	-0.62409200000	5.70885600000
C	1.02633800000	-3.26297700000	4.50235600000
H	-0.07008000000	-1.68826200000	3.50018100000
H	0.29792500000	-1.33206500000	5.19449600000
C	2.19268200000	-3.39542300000	5.48914200000
H	3.77878800000	-2.95180800000	4.08751400000
H	4.19026600000	-2.54427800000	5.75387600000
H	1.29320600000	-3.70421600000	3.53686200000
H	0.13325400000	-3.78069200000	4.85670600000
H	2.49277400000	-4.44182300000	5.59354500000
H	1.87117700000	-3.05645000000	6.48241100000
C	-4.97208800000	0.06553400000	0.19174200000
C	-5.36457800000	-1.61408900000	1.88533600000
C	-5.35994400000	1.18262000000	1.14686300000
H	-4.18855400000	0.38792700000	-0.49206000000
H	-5.83490600000	-0.26963500000	-0.40037300000
C	-5.73283900000	-0.55623200000	2.91545500000
H	-4.85857600000	-2.46584900000	2.33699900000
H	-6.26481500000	-1.96426800000	1.36047300000
C	-6.32537400000	0.67688300000	2.22345500000
H	-4.45055100000	1.57334900000	1.60911300000
H	-5.79255400000	1.99865100000	0.56571400000
H	-4.83176500000	-0.27782800000	3.46938500000
H	-6.43437600000	-0.99522400000	3.63219600000
H	-6.53100700000	1.46692200000	2.95073100000

H	-7.286482000000	0.410454000000	1.763621000000
O	-4.443357000000	-1.091193000000	0.897871000000
O	1.842413000000	-1.051239000000	3.839211000000
C	4.588144000000	-1.667889000000	1.392614000000
C	5.066407000000	0.695631000000	1.265481000000
C	5.887746000000	-1.940479000000	2.138469000000
H	3.784126000000	-2.330846000000	1.710807000000
H	4.716420000000	-1.779457000000	0.313198000000
C	6.381503000000	0.517582000000	2.011499000000
H	4.596687000000	1.648193000000	1.504876000000
H	5.208127000000	0.621033000000	0.183167000000
C	6.946775000000	-0.889996000000	1.780550000000
H	5.698554000000	-1.922634000000	3.217528000000
H	6.230736000000	-2.947397000000	1.881089000000
H	6.206767000000	0.686893000000	3.079999000000
H	7.083877000000	1.285711000000	1.672415000000
H	7.855077000000	-1.043133000000	2.370683000000
H	7.217914000000	-1.004433000000	0.725548000000
O	4.111260000000	-0.323442000000	1.662298000000
Ca	-1.142908000000	2.546049000000	-0.691686000000
I	2.002070000000	1.728078000000	-0.980372000000
I	-1.613971000000	-0.190747000000	-2.339859000000
Ca	1.587705000000	-1.136679000000	-2.323388000000
C	-3.483645000000	3.201893000000	-0.873799000000
C	-4.385844000000	2.759734000000	-1.866361000000
C	-3.997777000000	4.205593000000	-0.024626000000
C	-5.684304000000	3.259786000000	-2.003560000000
H	-4.066333000000	1.987145000000	-2.566204000000
C	-5.290249000000	4.726181000000	-0.138720000000
H	-3.366445000000	4.605177000000	0.771177000000
C	-6.143590000000	4.250480000000	-1.134528000000
H	-6.338367000000	2.882124000000	-2.785797000000
H	-5.635377000000	5.496966000000	0.545777000000
H	-7.149510000000	4.646114000000	-1.232398000000
C	3.985515000000	-1.676340000000	-2.258772000000
C	4.937068000000	-0.630789000000	-2.272420000000
C	4.547665000000	-2.962254000000	-2.098877000000
C	6.313947000000	-0.833859000000	-2.136860000000
H	4.592845000000	0.398649000000	-2.371394000000
C	5.918756000000	-3.196237000000	-1.952814000000
H	3.893844000000	-3.833427000000	-2.065410000000
C	6.812691000000	-2.125637000000	-1.971172000000
H	6.996909000000	0.012060000000	-2.150717000000
H	6.291562000000	-4.209060000000	-1.822775000000

H	7.878697000000	-2.295300000000	-1.858425000000
C	0.029674000000	-3.056474000000	-4.682659000000
C	1.113297000000	-4.413484000000	-3.019023000000
C	-1.325176000000	-3.688602000000	-4.393602000000
H	-0.062138000000	-2.006601000000	-4.956154000000
H	0.553588000000	-3.587640000000	-5.489467000000
C	-0.197655000000	-5.088835000000	-2.643381000000
H	1.765958000000	-4.299020000000	-2.155195000000
H	1.651190000000	-4.973634000000	-3.795360000000
C	-1.152285000000	-5.109944000000	-3.843852000000
H	-1.837120000000	-3.063557000000	-3.658450000000
H	-1.925150000000	-3.684487000000	-5.309329000000
H	-0.642849000000	-4.521387000000	-1.822188000000
H	0.008980000000	-6.099280000000	-2.277433000000
H	-2.121049000000	-5.531695000000	-3.561401000000
H	-0.743293000000	-5.761246000000	-4.626780000000
C	-1.329558000000	5.524114000000	-2.197453000000
C	0.057624000000	4.068517000000	-3.505875000000
C	-2.389736000000	5.590205000000	-3.288954000000
H	-1.773766000000	5.571238000000	-1.205019000000
H	-0.591058000000	6.330872000000	-2.296363000000
C	-0.953287000000	4.024126000000	-4.645666000000
H	0.618072000000	3.142152000000	-3.397409000000
H	0.781029000000	4.882729000000	-3.648332000000
C	-1.775167000000	5.321698000000	-4.670274000000
H	-3.156088000000	4.845056000000	-3.062666000000
H	-2.869383000000	6.573472000000	-3.257647000000
H	-1.613870000000	3.163657000000	-4.492082000000
H	-0.428113000000	3.873048000000	-5.594473000000
H	-2.558859000000	5.264383000000	-5.430405000000
H	-1.118052000000	6.154867000000	-4.951980000000
O	-0.612526000000	4.265808000000	-2.249131000000
O	0.870364000000	-3.077382000000	-3.510916000000
C	2.732475000000	-0.948098000000	-5.436893000000
C	1.182752000000	0.866098000000	-5.110723000000
C	3.878980000000	0.012286000000	-5.720518000000
H	3.079453000000	-1.837140000000	-4.911003000000
H	2.219673000000	-1.246615000000	-6.361942000000
C	2.268091000000	1.909739000000	-5.340978000000
H	0.428352000000	1.187174000000	-4.393048000000
H	0.671294000000	0.614689000000	-6.050477000000
C	3.356160000000	1.347820000000	-6.266660000000
H	4.428784000000	0.169471000000	-4.789414000000
H	4.568249000000	-0.460196000000	-6.427291000000

H	2.699979000000	2.180000000000	-4.371682000000
H	1.817914000000	2.812119000000	-5.765870000000
H	4.175592000000	2.063567000000	-6.372187000000
H	2.934206000000	1.196904000000	-7.268855000000
C	-4.065866000000	-3.275841000000	-1.881255000000
C	-3.026607000000	-4.894233000000	-0.450193000000
C	-5.444055000000	-3.559894000000	-1.298070000000
H	-3.949388000000	-2.235435000000	-2.182737000000
H	-3.868416000000	-3.911802000000	-2.753510000000
C	-4.342298000000	-5.235728000000	0.232942000000
H	-2.177124000000	-4.982460000000	0.224089000000
H	-2.850388000000	-5.541759000000	-1.318184000000
C	-5.516666000000	-4.982114000000	-0.723210000000
H	-5.635450000000	-2.828648000000	-0.511541000000
H	-6.197783000000	-3.410314000000	-2.077595000000
H	-4.428124000000	-4.620500000000	1.133184000000
H	-4.316650000000	-6.279595000000	0.559683000000
H	-6.469570000000	-5.137374000000	-0.210372000000
H	-5.477522000000	-5.708048000000	-1.545597000000
O	-3.026674000000	-3.521355000000	-0.906806000000
O	1.748678000000	-0.340485000000	-4.563685000000
F	-0.585191000000	4.291374000000	0.769927000000
C	-0.481417000000	4.479887000000	2.210809000000
H	-1.491769000000	4.317533000000	2.587399000000
H	0.191639000000	3.698060000000	2.559414000000
C	0.047444000000	5.863496000000	2.475109000000
H	1.055122000000	5.935951000000	2.056692000000
H	-0.584840000000	6.601348000000	1.968969000000
C	0.093126000000	6.143024000000	3.984173000000
H	-0.926749000000	6.138055000000	4.387151000000
H	0.637341000000	5.335100000000	4.480602000000
C	0.771398000000	7.476287000000	4.304336000000
H	1.808355000000	7.471082000000	3.957101000000
H	0.781625000000	7.665309000000	5.381001000000
H	0.256814000000	8.312965000000	3.820766000000

TSA

(E_{el} = -3281.431396 a.u.; G = -3280.063980 a.u.)

0 1

Ca	-1.595700000000	-1.616421000000	-1.753100000000
I	-0.687027000000	-2.257177000000	1.205916000000
I	1.371840000000	-0.416872000000	-2.242007000000
Ca	2.265717000000	-1.032731000000	0.951358000000
C	-0.734673000000	-3.736846000000	-2.709795000000

C	-0.122606000000	-3.937053000000	-3.966326000000
C	-0.826136000000	-4.912155000000	-1.928103000000
C	0.314116000000	-5.181590000000	-4.429478000000
H	0.044055000000	-3.085432000000	-4.625686000000
C	-0.389547000000	-6.169079000000	-2.357547000000
H	-1.246134000000	-4.851072000000	-0.924627000000
C	0.173733000000	-6.312398000000	-3.625219000000
H	0.771561000000	-5.269922000000	-5.411626000000
H	-0.489560000000	-7.034442000000	-1.707347000000
H	0.508490000000	-7.283804000000	-3.974785000000
C	2.942951000000	-1.852431000000	3.272247000000
C	2.740835000000	-3.237329000000	3.440534000000
C	4.189644000000	-1.363550000000	3.712843000000
C	3.704338000000	-4.080831000000	3.998073000000
H	1.794186000000	-3.675976000000	3.126783000000
C	5.174994000000	-2.189033000000	4.258863000000
H	4.405829000000	-0.299221000000	3.636378000000
C	4.930017000000	-3.555444000000	4.406783000000
H	3.502161000000	-5.141463000000	4.118538000000
H	6.125741000000	-1.771832000000	4.578888000000
H	5.684797000000	-4.201863000000	4.842298000000
C	4.319916000000	-3.634850000000	0.474695000000
C	2.266087000000	-3.907231000000	-0.768769000000
C	5.151840000000	-4.146113000000	-0.695849000000
H	4.841732000000	-2.879373000000	1.063395000000
H	4.046444000000	-4.451736000000	1.150834000000
C	3.011756000000	-4.405664000000	-1.992870000000
H	1.379053000000	-3.345174000000	-1.046532000000
H	1.957891000000	-4.733195000000	-0.116867000000
C	4.323244000000	-5.086292000000	-1.582354000000
H	5.501955000000	-3.296652000000	-1.290017000000
H	6.039163000000	-4.650721000000	-0.299666000000
H	3.212875000000	-3.549997000000	-2.646381000000
H	2.357516000000	-5.083671000000	-2.543563000000
H	4.897276000000	-5.385513000000	-2.463782000000
H	4.095253000000	-6.003865000000	-1.025195000000
C	-4.655063000000	-1.876775000000	-0.207007000000
C	-4.100489000000	-3.877987000000	-1.435679000000
C	-4.808850000000	-2.659709000000	1.086898000000
H	-4.259579000000	-0.880665000000	-0.017033000000
H	-5.615431000000	-1.779599000000	-0.732156000000
C	-4.182552000000	-4.732623000000	-0.179047000000
H	-3.350154000000	-4.241664000000	-2.136162000000
H	-5.077037000000	-3.850276000000	-1.939803000000

C	-5.180386000000	-4.120201000000	0.811220000000
H	-3.866298000000	-2.607769000000	1.636012000000
H	-5.556215000000	-2.160291000000	1.706119000000
H	-3.189316000000	-4.783050000000	0.277149000000
H	-4.466022000000	-5.751060000000	-0.463727000000
H	-5.197831000000	-4.688894000000	1.744748000000
H	-6.192306000000	-4.173013000000	0.387595000000
O	-3.719124000000	-2.517564000000	-1.119485000000
O	3.102376000000	-3.006628000000	0.011226000000
C	4.955850000000	-0.349989000000	-0.919826000000
C	4.883006000000	1.084808000000	1.010589000000
C	6.449402000000	-0.592106000000	-0.743940000000
H	4.438907000000	-1.215920000000	-1.329640000000
H	4.764997000000	0.510156000000	-1.567274000000
C	6.368543000000	0.894747000000	1.276671000000
H	4.314224000000	1.214188000000	1.930034000000
H	4.693182000000	1.948374000000	0.368415000000
C	7.109648000000	0.597063000000	-0.033253000000
H	6.599687000000	-1.504578000000	-0.156633000000
H	6.896382000000	-0.760535000000	-1.729168000000
H	6.501417000000	0.067768000000	1.983321000000
H	6.757763000000	1.801902000000	1.749208000000
H	8.166552000000	0.391091000000	0.158568000000
H	7.058323000000	1.479758000000	-0.680010000000
O	4.327739000000	-0.091365000000	0.361774000000
Ca	-1.682338000000	0.575146000000	2.574129000000
I	1.231138000000	1.943102000000	1.693196000000
I	-2.288288000000	1.485793000000	-0.683760000000
Ca	0.762576000000	2.555600000000	-1.365930000000
C	-4.069641000000	0.140773000000	2.838565000000
C	-5.124529000000	0.702959000000	2.087131000000
C	-4.488361000000	-0.639058000000	3.939472000000
C	-6.475521000000	0.505170000000	2.387914000000
H	-4.888210000000	1.322465000000	1.221542000000
C	-5.831491000000	-0.853729000000	4.264506000000
H	-3.736716000000	-1.107140000000	4.576500000000
C	-6.835648000000	-0.280756000000	3.483591000000
H	-7.247913000000	0.961579000000	1.773096000000
H	-6.097914000000	-1.466180000000	5.122331000000
H	-7.881348000000	-0.441041000000	3.726857000000
C	3.111752000000	3.272375000000	-1.602603000000
C	3.638225000000	4.137245000000	-0.615428000000
C	4.062015000000	2.844020000000	-2.554419000000
C	4.974547000000	4.546606000000	-0.573354000000

H	2.985937000000	4.488660000000	0.184396000000
C	5.405489000000	3.234124000000	-2.539036000000
H	3.758146000000	2.150944000000	-3.339793000000
C	5.869391000000	4.093097000000	-1.542871000000
H	5.321162000000	5.209136000000	0.215765000000
H	6.091925000000	2.865996000000	-3.297648000000
H	6.909575000000	4.402031000000	-1.521523000000
C	-1.186320000000	3.556058000000	-3.956134000000
C	0.933753000000	2.714464000000	-4.731199000000
C	-1.950773000000	2.570808000000	-4.829168000000
H	-1.702676000000	3.747666000000	-3.016375000000
H	-1.027202000000	4.511632000000	-4.475496000000
C	0.256554000000	1.705126000000	-5.648985000000
H	1.865208000000	2.332611000000	-4.317970000000
H	1.147751000000	3.653974000000	-5.258354000000
C	-1.126942000000	2.214472000000	-6.073852000000
H	-2.137052000000	1.673196000000	-4.233555000000
H	-2.919149000000	3.003506000000	-5.099911000000
H	0.160690000000	0.759750000000	-5.106075000000
H	0.898295000000	1.524101000000	-6.516726000000
H	-1.643903000000	1.467051000000	-6.681519000000
H	-1.012068000000	3.105325000000	-6.704675000000
C	-2.500512000000	2.765775000000	4.916952000000
C	-2.038127000000	3.933790000000	2.867571000000
C	-3.983615000000	3.110946000000	4.844731000000
H	-2.320469000000	1.784568000000	5.356750000000
H	-1.939570000000	3.514567000000	5.493108000000
C	-3.504119000000	4.302467000000	2.674732000000
H	-1.520545000000	3.763081000000	1.924136000000
H	-1.497656000000	4.718376000000	3.415144000000
C	-4.205699000000	4.399386000000	4.038176000000
H	-4.509214000000	2.279527000000	4.370121000000
H	-4.373721000000	3.215100000000	5.862324000000
H	-3.979218000000	3.526867000000	2.066225000000
H	-3.573695000000	5.247983000000	2.126207000000
H	-5.275301000000	4.580841000000	3.903845000000
H	-3.801545000000	5.257969000000	4.591166000000
O	-1.917929000000	2.703015000000	3.594419000000
O	0.098505000000	3.017346000000	-3.593558000000
C	0.689200000000	5.836532000000	-1.885873000000
C	-1.215434000000	5.329112000000	-0.513945000000
C	1.161415000000	6.917235000000	-0.921509000000
H	1.528386000000	5.326247000000	-2.357809000000
H	0.033858000000	6.254451000000	-2.662805000000

C	-0.814395000000	6.358823000000	0.533728000000
H	-1.724968000000	4.466506000000	-0.088260000000
H	-1.879666000000	5.776391000000	-1.267273000000
C	-0.013700000000	7.493843000000	-0.119688000000
H	1.898967000000	6.476027000000	-0.245865000000
H	1.673620000000	7.699297000000	-1.490436000000
H	-0.206493000000	5.861037000000	1.296191000000
H	-1.713580000000	6.740698000000	1.027263000000
H	0.346818000000	8.195782000000	0.636846000000
H	-0.672852000000	8.059794000000	-0.790402000000
C	-4.077420000000	-0.322469000000	-3.723692000000
C	-2.270890000000	-1.248409000000	-5.004874000000
C	-5.011013000000	-1.459592000000	-4.118156000000
H	-4.275856000000	0.050557000000	-2.719547000000
H	-4.160996000000	0.518552000000	-4.424086000000
C	-3.098661000000	-2.453460000000	-5.425844000000
H	-1.215098000000	-1.490768000000	-4.895919000000
H	-2.367972000000	-0.428846000000	-5.727481000000
C	-4.588277000000	-2.082827000000	-5.456434000000
H	-4.978504000000	-2.213412000000	-3.330502000000
H	-6.035604000000	-1.077374000000	-4.166360000000
H	-2.909632000000	-3.261882000000	-4.713181000000
H	-2.756550000000	-2.800751000000	-6.405459000000
H	-5.198612000000	-2.962852000000	-5.675781000000
H	-4.766972000000	-1.363011000000	-6.265719000000
O	-2.699208000000	-0.759114000000	-3.714235000000
O	-0.052596000000	4.808167000000	-1.185943000000
F	-0.747080000000	-0.053827000000	4.461131000000
C	0.965264000000	-0.825449000000	4.282596000000
H	0.542163000000	-1.528518000000	3.593971000000
H	1.367924000000	0.094102000000	3.900472000000
C	1.203468000000	-1.214831000000	5.703296000000
H	2.275460000000	-1.376229000000	5.848938000000
H	0.930620000000	-0.352040000000	6.320506000000
C	0.410479000000	-2.451940000000	6.129183000000
H	-0.650533000000	-2.259493000000	5.947026000000
H	0.698917000000	-3.291819000000	5.488335000000
C	0.642497000000	-2.818364000000	7.595881000000
H	1.698613000000	-3.037189000000	7.783785000000
H	0.062717000000	-3.699828000000	7.882278000000
H	0.349640000000	-1.997717000000	8.258683000000

ProdA

(E_{el} = -3281.554988 a.u.; G = -3280.180200 a.u.)

0 1

Ca	3.011619000000	-0.356412000000	-0.320620000000
I	0.840406000000	0.689482000000	-2.425172000000
I	0.847092000000	-2.680619000000	0.463376000000
Ca	-1.244402000000	-1.487173000000	-1.616633000000
C	4.013535000000	-2.031684000000	-1.856126000000
C	4.533977000000	-3.316961000000	-1.590498000000
C	4.088294000000	-1.659319000000	-3.219145000000
C	5.112754000000	-4.138592000000	-2.562164000000
H	4.481932000000	-3.721939000000	-0.580049000000
C	4.646978000000	-2.463372000000	-4.217494000000
H	3.679660000000	-0.698004000000	-3.529292000000
C	5.177481000000	-3.710402000000	-3.888048000000
H	5.504022000000	-5.115526000000	-2.289749000000
H	4.673834000000	-2.116944000000	-5.247459000000
H	5.624805000000	-4.339910000000	-4.650590000000
C	-4.334547000000	0.811642000000	-3.019337000000
C	-2.980537000000	0.730043000000	-3.384036000000
C	-5.207358000000	-0.180324000000	-3.479021000000
C	-2.523663000000	-0.323354000000	-4.182272000000
H	-2.308442000000	1.514693000000	-3.047848000000
C	-4.753986000000	-1.234763000000	-4.272731000000
H	-6.257356000000	-0.127621000000	-3.207257000000
C	-3.409174000000	-1.312650000000	-4.626052000000
H	-1.483107000000	-0.344604000000	-4.492448000000
H	-5.451013000000	-1.991637000000	-4.615567000000
H	-3.054451000000	-2.118343000000	-5.257421000000
C	-1.249748000000	-4.027914000000	-3.855406000000
C	0.966521000000	-3.127883000000	-3.469922000000
C	-0.765890000000	-5.448678000000	-3.590770000000
H	-2.274799000000	-3.873446000000	-3.519604000000
H	-1.188363000000	-3.790557000000	-4.925774000000
C	1.527398000000	-4.509081000000	-3.189551000000
H	1.459862000000	-2.371014000000	-2.865973000000
H	1.073412000000	-2.849913000000	-4.525089000000
C	0.723997000000	-5.584402000000	-3.929273000000
H	-0.926214000000	-5.686758000000	-2.534726000000
H	-1.376522000000	-6.142933000000	-4.177399000000
H	1.494383000000	-4.683075000000	-2.109714000000
H	2.578918000000	-4.514977000000	-3.480891000000
H	1.085390000000	-6.582857000000	-3.669339000000
H	0.863681000000	-5.467520000000	-5.011603000000
C	4.099891000000	2.815309000000	-0.820881000000
C	5.531531000000	1.232075000000	-1.959076000000

C	3.83476000000	3.57142800000	-2.11119200000
H	3.22586100000	2.82785700000	-0.17298800000
H	4.94774600000	3.24623200000	-0.27166300000
C	5.29382300000	1.91143300000	-3.30039800000
H	5.65948500000	0.15523200000	-2.06116400000
H	6.42074200000	1.65544100000	-1.47078600000
C	4.99489700000	3.40172900000	-3.09741800000
H	2.90769600000	3.19435700000	-2.55053900000
H	3.66114300000	4.61996600000	-1.86460800000
H	4.44787200000	1.42559200000	-3.79549400000
H	6.17483800000	1.75691600000	-3.93191900000
H	4.75659200000	3.88076400000	-4.05075600000
H	5.88985400000	3.90277100000	-2.70492900000
O	4.40333300000	1.41110900000	-1.07031600000
O	-0.45496400000	-3.06084500000	-3.13578000000
C	-2.62471700000	-4.28539200000	-0.41814700000
C	-4.29558200000	-2.62892500000	-0.94464000000
C	-3.51547100000	-5.41586100000	-0.91273100000
H	-1.56771500000	-4.48472000000	-0.59103800000
H	-2.76666700000	-4.09831300000	0.64836400000
C	-5.25093900000	-3.68682600000	-1.47485500000
H	-4.39884400000	-1.68418600000	-1.47519600000
H	-4.44385700000	-2.45050500000	0.12411300000
C	-4.99605600000	-5.03391500000	-0.78552200000
H	-3.27587400000	-5.63933100000	-1.95842600000
H	-3.29146000000	-6.31176500000	-0.32610300000
H	-5.11144100000	-3.77870200000	-2.55795300000
H	-6.27781400000	-3.34633700000	-1.30808100000
H	-5.63199800000	-5.81351700000	-1.21426200000
H	-5.24937800000	-4.95053500000	0.27637500000
O	-2.91677500000	-3.05071000000	-1.13794500000
Ca	-0.57946200000	2.93743700000	-0.38350000000
I	-2.58377300000	0.34213200000	0.48255900000
I	1.35141900000	1.41833900000	1.93187800000
Ca	-0.74339600000	-0.97065400000	2.67910700000
C	1.08100900000	4.76183600000	-0.41819800000
C	2.03046300000	5.14231800000	0.55483400000
C	1.02753600000	5.61658100000	-1.54365100000
C	2.86406000000	6.25788700000	0.42610100000
H	2.13723000000	4.53815400000	1.45715500000
C	1.84823200000	6.73838700000	-1.69959500000
H	0.31373300000	5.40033200000	-2.33909300000
C	2.77757800000	7.06287800000	-0.71074200000
H	3.57956800000	6.50282000000	1.20810700000

H	1.766595000000	7.358892000000	-2.588724000000
H	3.419940000000	7.931079000000	-0.821541000000
C	-2.351632000000	-2.813369000000	3.014218000000
C	-3.733812000000	-2.564448000000	2.848333000000
C	-2.036600000000	-4.174868000000	3.221501000000
C	-4.712348000000	-3.563401000000	2.881382000000
H	-4.069961000000	-1.545419000000	2.657976000000
C	-2.990892000000	-5.197090000000	3.252913000000
H	-0.995374000000	-4.472369000000	3.344707000000
C	-4.341645000000	-4.893139000000	3.081575000000
H	-5.760925000000	-3.308579000000	2.746589000000
H	-2.684755000000	-6.228405000000	3.409332000000
H	-5.091242000000	-5.677696000000	3.106488000000
C	1.344659000000	-0.651090000000	5.352666000000
C	1.402651000000	-2.873299000000	4.421662000000
C	2.841859000000	-0.468163000000	5.137598000000
H	0.799856000000	0.282144000000	5.212156000000
H	1.130148000000	-1.041711000000	6.356887000000
C	2.892735000000	-2.765654000000	4.130409000000
H	0.885661000000	-3.466584000000	3.668850000000
H	1.213798000000	-3.319286000000	5.407004000000
C	3.563221000000	-1.821864000000	5.136777000000
H	2.985693000000	0.030290000000	4.176690000000
H	3.234831000000	0.192684000000	5.916835000000
H	3.014138000000	-2.373871000000	3.116706000000
H	3.338819000000	-3.764584000000	4.158564000000
H	4.622019000000	-1.689798000000	4.896379000000
H	3.521600000000	-2.265991000000	6.139484000000
C	-3.363418000000	4.168063000000	0.986049000000
C	-1.420549000000	5.108014000000	2.044559000000
C	-3.552849000000	5.394510000000	0.105120000000
H	-3.670498000000	3.253599000000	0.483082000000
H	-3.927034000000	4.258965000000	1.924900000000
C	-1.549940000000	6.401112000000	1.247548000000
H	-0.374330000000	4.860438000000	2.225881000000
H	-1.947364000000	5.176348000000	3.007825000000
C	-3.001765000000	6.640881000000	0.811287000000
H	-3.027821000000	5.206281000000	-0.835696000000
H	-4.617890000000	5.506727000000	-0.124780000000
H	-0.899720000000	6.322440000000	0.372797000000
H	-1.174778000000	7.229657000000	1.856972000000
H	-3.058006000000	7.511886000000	0.152756000000
H	-3.621171000000	6.865504000000	1.690644000000
O	-1.967201000000	3.981588000000	1.319728000000

O	0.78620000000	-1.56802000000	4.38764200000
C	-2.15547300000	-0.05551400000	5.52418200000
C	-1.95045200000	1.89722700000	4.11065200000
C	-3.67024400000	0.08410700000	5.58757000000
H	-1.84998300000	-1.10273700000	5.52950400000
H	-1.67260600000	0.46412000000	6.36362300000
C	-3.45661600000	2.11424200000	4.11661400000
H	-1.50816100000	2.18680900000	3.15917300000
H	-1.46105000000	2.46558600000	4.91297400000
C	-4.08664700000	1.54850200000	5.39603600000
H	-4.10566400000	-0.54231100000	4.80444700000
H	-4.02159300000	-0.30544900000	6.54825600000
H	-3.87858500000	1.62210700000	3.23503100000
H	-3.65642500000	3.18515900000	4.01849200000
H	-5.17586300000	1.63405600000	5.35736700000
H	-3.75173500000	2.13951500000	6.25846800000
C	5.12772100000	0.41212800000	2.26995900000
C	5.31346400000	-1.87442000000	1.57994900000
C	6.46503600000	0.77336500000	1.63657500000
H	4.41649900000	1.23640100000	2.23627800000
H	5.25497700000	0.10892100000	3.31697000000
C	6.64006300000	-1.62683400000	0.87726500000
H	4.72461300000	-2.64438800000	1.08609000000
H	5.46561200000	-2.16909900000	2.62640400000
C	7.38015900000	-0.45633900000	1.54076000000
H	6.26956900000	1.17331700000	0.64040600000
H	6.93352100000	1.56924600000	2.22402600000
H	6.43103600000	-1.41331800000	-0.17522700000
H	7.23944900000	-2.54174100000	0.90622800000
H	8.28912500000	-0.21229800000	0.98455800000
H	7.69593200000	-0.75283100000	2.54933900000
O	4.49696300000	-0.68136600000	1.56387500000
O	-1.63063600000	0.49718500000	4.29566400000
F	-1.99739600000	3.33717200000	-1.84476600000
C	-4.83111600000	1.96623400000	-2.18392300000
H	-3.98941600000	2.37101800000	-1.62166100000
H	-5.57935400000	1.59959800000	-1.47257400000
C	-5.43646000000	3.11263300000	-3.02142400000
H	-6.30283000000	2.74687700000	-3.58882300000
H	-5.81934200000	3.86794500000	-2.32356800000
C	-4.42906900000	3.77390200000	-3.96891000000
H	-3.52322600000	4.01241200000	-3.40405300000
H	-4.12720700000	3.05140500000	-4.73581200000
C	-4.99409400000	5.02610600000	-4.64350600000

H	-5.897072000000	4.798971000000	-5.221294000000
H	-4.265686000000	5.473298000000	-5.325776000000
H	-5.260273000000	5.785713000000	-3.900694000000

TSB

($E_{el} = -3281.406577$ a.u.; $G = -3280.043307$ a.u.)

0 1

Ca	1.468844000000	-1.690414000000	1.724848000000
I	1.396521000000	-1.722213000000	-1.440086000000
I	-1.746915000000	-1.211952000000	1.629837000000
Ca	-1.715791000000	-1.205049000000	-1.654093000000
C	0.974017000000	-4.096948000000	2.047328000000
C	0.207968000000	-4.725461000000	3.052788000000
C	1.527588000000	-4.996765000000	1.106546000000
C	0.038410000000	-6.109831000000	3.149455000000
H	-0.300124000000	-4.118039000000	3.801645000000
C	1.368995000000	-6.384450000000	1.169671000000
H	2.103756000000	-4.601730000000	0.270166000000
C	0.628641000000	-6.951515000000	2.206780000000
H	-0.558965000000	-6.532986000000	3.953012000000
H	1.822340000000	-7.021979000000	0.414976000000
H	0.504609000000	-8.027631000000	2.273016000000
C	-1.279906000000	-1.123402000000	-4.226800000000
C	-1.141697000000	-2.491067000000	-4.545348000000
C	-2.418673000000	-0.470721000000	-4.741914000000
C	-2.090856000000	-3.170556000000	-5.309398000000
H	-0.264765000000	-3.026214000000	-4.188868000000
C	-3.387814000000	-1.144279000000	-5.484694000000
H	-2.531304000000	0.595752000000	-4.561926000000
C	-3.225406000000	-2.501535000000	-5.770554000000
H	-1.950707000000	-4.221188000000	-5.546124000000
H	-4.260304000000	-0.614132000000	-5.854346000000
H	-3.968624000000	-3.028236000000	-6.359485000000
C	-3.110777000000	-4.233718000000	-2.253382000000
C	-1.340216000000	-4.353066000000	-0.611783000000
C	-3.995730000000	-5.167381000000	-1.434536000000
H	-3.686228000000	-3.487541000000	-2.801950000000
H	-2.515912000000	-4.799351000000	-2.979545000000
C	-2.164309000000	-5.259697000000	0.282465000000
H	-0.703981000000	-3.696014000000	-0.026791000000
H	-0.704092000000	-4.925049000000	-1.297275000000
C	-3.144924000000	-6.090573000000	-0.552485000000
H	-4.665023000000	-4.574102000000	-0.804833000000
H	-4.625536000000	-5.740855000000	-2.122671000000

H	-2.705998000000	-4.635846000000	1.001468000000
H	-1.482578000000	-5.890878000000	0.854466000000
H	-3.784744000000	-6.699704000000	0.091885000000
H	-2.581012000000	-6.784907000000	-1.188232000000
C	4.727557000000	-1.010381000000	1.026033000000
C	4.468541000000	-3.298160000000	1.756720000000
C	5.371642000000	-1.452892000000	-0.277613000000
H	4.130050000000	-0.112346000000	0.879784000000
H	5.483256000000	-0.807623000000	1.797344000000
C	5.059771000000	-3.830638000000	0.459319000000
H	3.702553000000	-3.956776000000	2.163344000000
H	5.261270000000	-3.162905000000	2.506166000000
C	6.051365000000	-2.817380000000	-0.124972000000
H	4.597189000000	-1.501200000000	-1.046409000000
H	6.075879000000	-0.681122000000	-0.593074000000
H	4.246805000000	-4.008726000000	-0.250884000000
H	5.536776000000	-4.795344000000	0.660582000000
H	6.431864000000	-3.161233000000	-1.090450000000
H	6.917373000000	-2.728181000000	0.544521000000
O	3.820648000000	-2.020075000000	1.552683000000
O	-2.202108000000	-3.490858000000	-1.411079000000
C	-4.841583000000	-1.612750000000	-0.557197000000
C	-4.735993000000	0.228327000000	-2.100635000000
C	-6.155217000000	-2.102886000000	-1.152142000000
H	-4.220835000000	-2.427375000000	-0.189339000000
H	-5.014066000000	-0.909069000000	0.261657000000
C	-6.037958000000	-0.185950000000	-2.768240000000
H	-4.043994000000	0.683562000000	-2.804876000000
H	-4.903876000000	0.928328000000	-1.279006000000
C	-6.934231000000	-0.936811000000	-1.775221000000
H	-5.945249000000	-2.859371000000	-1.916370000000
H	-6.737811000000	-2.589778000000	-0.363176000000
H	-5.807962000000	-0.822727000000	-3.629839000000
H	-6.537467000000	0.712564000000	-3.143513000000
H	-7.839715000000	-1.300559000000	-2.269253000000
H	-7.245716000000	-0.246107000000	-0.984308000000
O	-4.045647000000	-0.937233000000	-1.565311000000
Ca	1.909085000000	1.452244000000	-1.836353000000
I	-1.327659000000	1.949130000000	-1.685224000000
I	1.550061000000	1.687381000000	1.505489000000
Ca	-1.722496000000	1.957016000000	1.466335000000
C	4.327947000000	1.522286000000	-1.511512000000
C	5.056322000000	2.058994000000	-0.427719000000
C	5.121912000000	1.141915000000	-2.616674000000

C	6.447534000000	2.197498000000	-0.427171000000
H	4.518638000000	2.385389000000	0.463099000000
C	6.514243000000	1.269898000000	-2.644818000000
H	4.638512000000	0.724642000000	-3.500339000000
C	7.186136000000	1.798961000000	-1.542540000000
H	6.957720000000	2.617138000000	0.436894000000
H	7.076075000000	0.958013000000	-3.521727000000
H	8.266605000000	1.902994000000	-1.553816000000
C	-4.168206000000	2.085229000000	1.175089000000
C	-4.659087000000	3.037245000000	0.251597000000
C	-5.168816000000	1.265385000000	1.739500000000
C	-6.010591000000	3.173029000000	-0.079822000000
H	-3.953300000000	3.689343000000	-0.263804000000
C	-6.528283000000	1.375361000000	1.427992000000
H	-4.885274000000	0.481070000000	2.442428000000
C	-6.956964000000	2.336267000000	0.512461000000
H	-6.326162000000	3.921068000000	-0.802656000000
H	-7.252721000000	0.711074000000	1.892895000000
H	-8.009134000000	2.430060000000	0.263555000000
C	-0.736136000000	2.664074000000	4.636343000000
C	-2.695655000000	1.265141000000	4.631046000000
C	0.031564000000	1.668924000000	5.495221000000
H	-0.083854000000	3.172789000000	3.927852000000
H	-1.245071000000	3.417285000000	5.254346000000
C	-2.016875000000	0.220447000000	5.507618000000
H	-3.381941000000	0.817456000000	3.915209000000
H	-3.252668000000	1.993232000000	5.236079000000
C	-0.937974000000	0.874608000000	6.380668000000
H	0.566188000000	0.992558000000	4.822673000000
H	0.773823000000	2.205327000000	6.094852000000
H	-1.567071000000	-0.534632000000	4.855604000000
H	-2.774390000000	-0.279949000000	6.118666000000
H	-0.403420000000	0.120105000000	6.963944000000
H	-1.411320000000	1.551189000000	7.103774000000
C	2.814698000000	4.309429000000	-3.314064000000
C	1.492010000000	4.778163000000	-1.365478000000
C	4.067261000000	4.897874000000	-2.675645000000
H	3.039926000000	3.468432000000	-3.968018000000
H	2.262222000000	5.064366000000	-3.890212000000
C	2.688540000000	5.348060000000	-0.612922000000
H	0.785521000000	4.272105000000	-0.708217000000
H	0.948858000000	5.565840000000	-1.906040000000
C	3.701466000000	5.937789000000	-1.606205000000
H	4.639714000000	4.084522000000	-2.225106000000

H	4.686314000000	5.345584000000	-3.459746000000
H	3.152833000000	4.539671000000	-0.039472000000
H	2.345684000000	6.107417000000	0.097977000000
H	4.600025000000	6.272062000000	-1.080745000000
H	3.261752000000	6.823328000000	-2.084478000000
O	1.915630000000	3.783842000000	-2.307934000000
O	-1.725672000000	1.985099000000	3.841321000000
C	-2.651261000000	4.941870000000	2.575632000000
C	-0.401823000000	5.199665000000	1.778228000000
C	-3.139481000000	6.117918000000	1.739937000000
H	-3.414532000000	4.169741000000	2.666891000000
H	-2.340953000000	5.266451000000	3.578604000000
C	-0.786787000000	6.367169000000	0.879131000000
H	0.409648000000	4.598661000000	1.371587000000
H	-0.092973000000	5.557046000000	2.770998000000
C	-1.999119000000	7.107094000000	1.461905000000
H	-3.539451000000	5.728276000000	0.799857000000
H	-3.967106000000	6.605500000000	2.264223000000
H	-1.027782000000	5.976769000000	-0.114902000000
H	0.071101000000	7.037731000000	0.769966000000
H	-2.332345000000	7.894741000000	0.781079000000
H	-1.704803000000	7.599136000000	2.397777000000
C	3.031119000000	-0.409818000000	4.490970000000
C	1.261382000000	-1.932131000000	5.050356000000
C	4.097516000000	-1.399372000000	4.941500000000
H	3.361185000000	0.207145000000	3.656034000000
H	2.736545000000	0.255938000000	5.312441000000
C	2.239035000000	-3.011736000000	5.490671000000
H	0.356118000000	-2.348700000000	4.611404000000
H	0.976673000000	-1.288622000000	5.891778000000
C	3.540404000000	-2.370138000000	5.992941000000
H	4.436350000000	-1.954587000000	4.065734000000
H	4.956043000000	-0.843863000000	5.331961000000
H	2.429664000000	-3.667704000000	4.636171000000
H	1.773027000000	-3.623502000000	6.269106000000
H	4.280250000000	-3.138836000000	6.231181000000
H	3.340418000000	-1.822939000000	6.923310000000
O	1.846956000000	-1.096904000000	4.027185000000
O	-1.514965000000	4.300488000000	1.945848000000
F	1.976447000000	1.333442000000	-4.057694000000
C	1.041486000000	0.286718000000	-4.754610000000
H	-0.211701000000	-0.413031000000	-4.072579000000
H	0.640542000000	0.912538000000	-5.561849000000
C	2.000337000000	-0.740608000000	-5.295659000000

H	2.483881000000	-1.259202000000	-4.457164000000
H	1.379420000000	-1.497919000000	-5.795769000000
C	3.077157000000	-0.233460000000	-6.268172000000
H	2.587214000000	0.205348000000	-7.146028000000
H	3.626999000000	0.578730000000	-5.782918000000
C	4.052702000000	-1.329783000000	-6.704762000000
H	4.575085000000	-1.751995000000	-5.840021000000
H	4.809698000000	-0.948163000000	-7.396605000000
H	3.526984000000	-2.150594000000	-7.204546000000

TSC

(E_{el} = -3281.409037 a.u.; G = -3280.043231 a.u.)

0 1

Ca	-1.819971000000	-1.901132000000	-1.135088000000
I	-0.800704000000	-1.772674000000	1.857502000000
I	1.205232000000	-1.150704000000	-1.957710000000
Ca	2.325345000000	-1.021015000000	1.295317000000
C	-1.247656000000	-4.288969000000	-1.498514000000
C	-0.850295000000	-4.951104000000	-2.680398000000
C	-1.325942000000	-5.138881000000	-0.369835000000
C	-0.589146000000	-6.322770000000	-2.753902000000
H	-0.723292000000	-4.382154000000	-3.601033000000
C	-1.062579000000	-6.511446000000	-0.407952000000
H	-1.597377000000	-4.714437000000	0.596410000000
C	-0.700116000000	-7.115446000000	-1.611732000000
H	-0.292415000000	-6.773171000000	-3.697691000000
H	-1.142150000000	-7.108921000000	0.496644000000
H	-0.500192000000	-8.181135000000	-1.657410000000
C	3.451045000000	-0.861171000000	3.667786000000
C	4.102450000000	-2.087795000000	3.901395000000
C	4.247105000000	0.291626000000	3.821386000000
C	5.460022000000	-2.171020000000	4.221759000000
H	3.532369000000	-3.012746000000	3.837407000000
C	5.602991000000	0.233385000000	4.139522000000
H	3.784519000000	1.270842000000	3.698726000000
C	6.216616000000	-1.005769000000	4.335012000000
H	5.925124000000	-3.137893000000	4.392327000000
H	6.183426000000	1.146025000000	4.237450000000
H	7.270320000000	-1.059800000000	4.587289000000
C	4.118374000000	-3.929496000000	1.132631000000
C	1.859462000000	-4.200370000000	0.312214000000
C	4.685823000000	-4.723909000000	-0.038785000000
H	4.793238000000	-3.140266000000	1.461410000000
H	3.926390000000	-4.591614000000	1.986790000000

C	2.344655000000	-4.963185000000	-0.905536000000
H	0.984188000000	-3.602810000000	0.077346000000
H	1.605514000000	-4.875905000000	1.137702000000
C	3.646382000000	-5.706911000000	-0.590688000000
H	4.994623000000	-4.034582000000	-0.829416000000
H	5.587143000000	-5.243116000000	0.303628000000
H	2.497050000000	-4.250066000000	-1.722127000000
H	1.554355000000	-5.646112000000	-1.219184000000
H	4.031223000000	-6.210667000000	-1.481525000000
H	3.447668000000	-6.487305000000	0.154940000000
C	-4.784479000000	-1.482854000000	0.519703000000
C	-4.499240000000	-3.772277000000	-0.189035000000
C	-4.963512000000	-1.905397000000	1.968961000000
H	-4.278660000000	-0.521749000000	0.452074000000
H	-5.752052000000	-1.405475000000	0.005041000000
C	-4.619070000000	-4.282280000000	1.239739000000
H	-3.820212000000	-4.376301000000	-0.788505000000
H	-5.487959000000	-3.757509000000	-0.669342000000
C	-5.499767000000	-3.337420000000	2.066329000000
H	-3.997264000000	-1.831208000000	2.473963000000
H	-5.626915000000	-1.189137000000	2.456676000000
H	-3.618063000000	-4.340020000000	1.677326000000
H	-5.025513000000	-5.298630000000	1.216889000000
H	-5.537442000000	-3.657913000000	3.110901000000
H	-6.529204000000	-3.373728000000	1.685529000000
O	-3.963567000000	-2.427599000000	-0.222962000000
O	2.877667000000	-3.269182000000	0.790594000000
C	4.800274000000	-1.111004000000	-0.975570000000
C	5.047505000000	0.784610000000	0.477451000000
C	6.284167000000	-1.442184000000	-0.883961000000
H	4.180662000000	-1.997275000000	-1.092517000000
H	4.593588000000	-0.433187000000	-1.808592000000
C	6.538114000000	0.534939000000	0.641535000000
H	4.605390000000	1.207867000000	1.375867000000
H	4.835638000000	1.448590000000	-0.362113000000
C	7.102612000000	-0.176701000000	-0.594545000000
H	6.440368000000	-2.175860000000	-0.085231000000
H	6.598568000000	-1.910164000000	-1.822806000000
H	6.698943000000	-0.070561000000	1.539115000000
H	7.034629000000	1.497661000000	0.798151000000
H	8.157296000000	-0.427391000000	-0.448574000000
H	7.041245000000	0.498235000000	-1.454864000000
O	4.345038000000	-0.471183000000	0.242706000000
Ca	-1.658782000000	1.377630000000	2.494968000000

I	1.453807000000	2.045436000000	1.280822000000
I	-2.206096000000	1.439364000000	-0.907621000000
Ca	0.865731000000	1.991977000000	-1.860882000000
C	-4.083034000000	1.279041000000	2.753562000000
C	-5.102752000000	1.644056000000	1.848293000000
C	-4.545264000000	0.915048000000	4.038625000000
C	-6.462147000000	1.632711000000	2.174191000000
H	-4.831758000000	1.947131000000	0.836779000000
C	-5.898346000000	0.894416000000	4.391991000000
H	-3.821252000000	0.633106000000	4.803685000000
C	-6.867349000000	1.251019000000	3.454052000000
H	-7.206368000000	1.921794000000	1.435594000000
H	-6.199166000000	0.600803000000	5.394581000000
H	-7.920347000000	1.237748000000	3.717581000000
C	3.238341000000	2.483035000000	-2.321130000000
C	3.837364000000	3.520349000000	-1.568913000000
C	4.129460000000	1.816128000000	-3.188758000000
C	5.187842000000	3.868769000000	-1.664343000000
H	3.232996000000	4.068996000000	-0.845789000000
C	5.485630000000	2.139422000000	-3.305526000000
H	3.766379000000	0.986784000000	-3.796624000000
C	6.023073000000	3.173278000000	-2.539170000000
H	5.592161000000	4.671809000000	-1.053386000000
H	6.124691000000	1.584562000000	-3.988090000000
H	7.074146000000	3.430868000000	-2.620555000000
C	-1.060144000000	2.412500000000	-4.626225000000
C	0.930964000000	1.161010000000	-5.141266000000
C	-1.952188000000	1.335093000000	-5.226416000000
H	-1.532105000000	2.895363000000	-3.772155000000
H	-0.803621000000	3.179110000000	-5.371062000000
C	0.122707000000	0.039773000000	-5.781405000000
H	1.817154000000	0.783826000000	-4.635048000000
H	1.244986000000	1.904303000000	-5.886437000000
C	-1.202653000000	0.580964000000	-6.332632000000
H	-2.229398000000	0.647441000000	-4.423008000000
H	-2.869043000000	1.796459000000	-5.607052000000
H	-0.068947000000	-0.721681000000	-5.019445000000
H	0.721476000000	-0.426260000000	-6.570040000000
H	-1.814567000000	-0.231384000000	-6.734069000000
H	-1.001192000000	1.263232000000	-7.168432000000
C	-2.185362000000	4.318656000000	3.929387000000
C	-1.599285000000	4.650521000000	1.624685000000
C	-3.633761000000	4.722011000000	3.678486000000
H	-2.089633000000	3.546539000000	4.691770000000

H	-1.571464000000	5.182520000000	4.220098000000
C	-3.026508000000	5.032669000000	1.250606000000
H	-1.081269000000	4.125018000000	0.822749000000
H	-1.006392000000	5.536060000000	1.892443000000
C	-3.740131000000	5.653135000000	2.461418000000
H	-4.218816000000	3.815996000000	3.505257000000
H	-4.028082000000	5.207069000000	4.577261000000
H	-3.552392000000	4.128512000000	0.929210000000
H	-3.010339000000	5.727630000000	0.404521000000
H	-4.789641000000	5.847694000000	2.225195000000
H	-3.278411000000	6.622225000000	2.694113000000
O	-1.595318000000	3.744753000000	2.737007000000
O	0.161482000000	1.838411000000	-4.125742000000
C	1.066931000000	4.961975000000	-3.346340000000
C	-0.867666000000	5.076076000000	-1.935702000000
C	1.640110000000	6.244809000000	-2.759483000000
H	1.853383000000	4.260328000000	-3.620979000000
H	0.440443000000	5.170692000000	-4.224768000000
C	-0.377737000000	6.349106000000	-1.257641000000
H	-1.456730000000	4.442059000000	-1.275910000000
H	-1.485581000000	5.315949000000	-2.812953000000
C	0.524592000000	7.145189000000	-2.211087000000
H	2.337089000000	5.974432000000	-1.961604000000
H	2.219786000000	6.759354000000	-3.532052000000
H	0.180429000000	6.071686000000	-0.357660000000
H	-1.239272000000	6.944118000000	-0.939300000000
H	0.948326000000	8.015171000000	-1.702489000000
H	-0.080223000000	7.526998000000	-3.043580000000
C	-4.294044000000	-0.913133000000	-3.283260000000
C	-2.653678000000	-2.311424000000	-4.342118000000
C	-5.351486000000	-2.006375000000	-3.356968000000
H	-4.402139000000	-0.287553000000	-2.398132000000
H	-4.334288000000	-0.264259000000	-4.167630000000
C	-3.616282000000	-3.486744000000	-4.429735000000
H	-1.621541000000	-2.630532000000	-4.202522000000
H	-2.706134000000	-1.689337000000	-5.244088000000
C	-5.062341000000	-2.977159000000	-4.511096000000
H	-5.349608000000	-2.545461000000	-2.408745000000
H	-6.335826000000	-1.540996000000	-3.469159000000
H	-3.471631000000	-4.113732000000	-3.545051000000
H	-3.361702000000	-4.095998000000	-5.302358000000
H	-5.765651000000	-3.813771000000	-4.490142000000
H	-5.212353000000	-2.460185000000	-5.467763000000
O	-2.965000000000	-1.477445000000	-3.204414000000

O	0.245864000000	4.272256000000	-2.370801000000
F	-1.028085000000	1.429342000000	4.598216000000
C	0.793710000000	0.991574000000	4.968797000000
H	1.092672000000	1.584364000000	4.115836000000
H	0.855317000000	1.503180000000	5.923967000000
C	0.915526000000	-0.405239000000	4.911953000000
H	0.418948000000	-0.816314000000	4.033853000000
H	2.069675000000	-0.602613000000	4.341904000000
C	0.655086000000	-1.237425000000	6.158611000000
H	1.244542000000	-0.841937000000	6.994092000000
H	-0.398850000000	-1.136821000000	6.443957000000
C	0.985233000000	-2.719149000000	5.948316000000
H	0.419644000000	-3.123481000000	5.102795000000
H	0.735626000000	-3.311387000000	6.832756000000
H	2.048123000000	-2.857700000000	5.737067000000

THP

(E_{el} = -271.8561745 a.u.; G = -271.738775 a.u.)

0 1

O	0.000030000000	-1.399511000000	-0.284886000000
C	1.181614000000	-0.770768000000	0.201495000000
C	-1.181581000000	-0.770818000000	0.201495000000
H	-1.215845000000	-0.842471000000	1.302058000000
H	-2.016676000000	-1.347556000000	-0.200564000000
H	2.016735000000	-1.347470000000	-0.200564000000
H	1.215882000000	-0.842421000000	1.302058000000
C	1.257970000000	0.696879000000	-0.224395000000
C	-1.258000000000	0.696825000000	-0.224395000000
H	-2.163351000000	1.155480000000	0.186802000000
C	-0.000032000000	1.447634000000	0.236592000000
H	-0.000033000000	1.512757000000	1.332300000000
H	-0.000054000000	2.473941000000	-0.141550000000
H	2.163300000000	1.155574000000	0.186801000000
H	1.333227000000	0.739897000000	-1.316505000000
H	-1.333260000000	0.739842000000	-1.316506000000

nBuF

(E_{el} = -257.7722970 a.u.; G = -257.677259 a.u.)

0 1

C	2.497918000000	-0.296865000000	0.000061000000
H	2.550465000000	-0.941009000000	0.882991000000
H	2.550992000000	-0.940710000000	-0.883032000000
H	3.383304000000	0.344163000000	0.000431000000
C	1.209392000000	0.530265000000	-0.000214000000

H	1.197453000000	1.188182000000	-0.877527000000
H	1.197555000000	1.189037000000	0.876434000000
C	-0.051595000000	-0.341125000000	0.000117000000
H	-0.058099000000	-0.993679000000	-0.879668000000
H	-0.057626000000	-0.993762000000	0.879831000000
C	-1.325920000000	0.480690000000	0.000262000000
H	-1.392394000000	1.113768000000	0.891679000000
H	-1.392047000000	1.114386000000	-0.890745000000
F	-2.439819000000	-0.368685000000	-0.000195000000

Ca-Tetra_THF

(E_{el} = -2980.868506 a.u.; G = -2979.712567 a.u.)

0 1

C	3.874778000000	-5.550342000000	0.789168000000
C	2.744456000000	-4.733031000000	0.681541000000
C	2.515626000000	-3.606037000000	1.501154000000
C	3.548283000000	-3.350563000000	2.430866000000
C	4.693893000000	-4.143608000000	2.557125000000
C	4.856789000000	-5.260537000000	1.737534000000
H	3.994636000000	-6.409342000000	0.133620000000
H	2.015002000000	-4.987076000000	-0.087782000000
H	3.465651000000	-2.482773000000	3.086354000000
H	5.457000000000	-3.894679000000	3.290844000000
H	5.736755000000	-5.889100000000	1.829826000000
Ca	0.448731000000	-2.275055000000	1.548550000000
I	2.005409000000	0.539507000000	1.865777000000
O	0.346181000000	-2.528473000000	3.910009000000
C	0.518198000000	-1.519497000000	4.921857000000
C	0.732982000000	-3.793583000000	4.503673000000
C	1.820354000000	-1.909102000000	5.616664000000
H	-0.342011000000	-1.544398000000	5.603128000000
H	0.556767000000	-0.557062000000	4.415834000000
C	1.820315000000	-3.457005000000	5.544883000000
H	-0.153597000000	-4.239607000000	4.966266000000
H	1.088136000000	-4.428548000000	3.693938000000
H	2.662259000000	-1.499042000000	5.056241000000
H	1.873253000000	-1.530350000000	6.638826000000
H	1.579169000000	-3.903804000000	6.511266000000
H	2.790668000000	-3.836181000000	5.225538000000
O	-1.080199000000	-4.049233000000	1.611654000000
C	-2.284854000000	-4.147758000000	2.419254000000
C	-1.021643000000	-5.164656000000	0.666504000000
C	-3.203799000000	-5.072387000000	1.635537000000
H	-2.675309000000	-3.140478000000	2.555612000000

H	-2.010771000000	-4.567645000000	3.393914000000
C	-2.207596000000	-6.061961000000	1.015011000000
H	-1.109394000000	-4.743688000000	-0.335434000000
H	-0.049538000000	-5.644657000000	0.782812000000
H	-3.947736000000	-5.554542000000	2.272357000000
H	-3.719525000000	-4.515036000000	0.853519000000
H	-2.611112000000	-6.556233000000	0.131243000000
H	-1.914005000000	-6.825217000000	1.742402000000
C	-3.733088000000	5.973773000000	0.243347000000
C	-2.625078000000	5.126205000000	0.342414000000
C	-2.567340000000	4.021310000000	1.219464000000
C	-3.730159000000	3.837141000000	2.000282000000
C	-4.851814000000	4.668211000000	1.924445000000
C	-4.855635000000	5.747575000000	1.040002000000
H	-3.725189000000	6.807917000000	-0.453734000000
H	-1.775229000000	5.332917000000	-0.309154000000
H	-3.779684000000	2.989870000000	2.685206000000
H	-5.722457000000	4.475504000000	2.546948000000
H	-5.720068000000	6.400532000000	0.971666000000
Ca	-0.622438000000	2.543971000000	1.410012000000
I	-2.204955000000	-0.250027000000	1.680059000000
O	-0.654383000000	2.887373000000	3.766790000000
C	-1.007877000000	1.952976000000	4.803403000000
C	-0.977798000000	4.210549000000	4.267377000000
C	-2.326442000000	2.488814000000	5.357054000000
H	-0.212831000000	1.941330000000	5.560277000000
H	-1.089035000000	0.970631000000	4.342334000000
C	-2.194363000000	4.024672000000	5.195360000000
H	-0.104282000000	4.592985000000	4.805930000000
H	-1.184161000000	4.835292000000	3.399915000000
H	-3.151498000000	2.110439000000	4.751485000000
H	-2.493731000000	2.181958000000	6.390941000000
H	-2.026833000000	4.518780000000	6.154210000000
H	-3.090191000000	4.448411000000	4.742468000000
O	1.043299000000	4.200778000000	1.465676000000
C	1.495459000000	4.918981000000	0.268874000000
C	2.041714000000	4.333931000000	2.507153000000
C	2.903678000000	5.430207000000	0.587975000000
H	0.774201000000	5.711434000000	0.060583000000
H	1.504275000000	4.203202000000	-0.551274000000
C	3.343962000000	4.525613000000	1.748979000000
H	1.793719000000	5.206301000000	3.124247000000
H	1.998092000000	3.433200000000	3.117971000000
H	3.560750000000	5.349086000000	-0.276247000000

H	2.872244000000	6.475158000000	0.910633000000
H	4.130086000000	4.967800000000	2.363987000000
H	3.691765000000	3.565585000000	1.362832000000
C	-5.814119000000	-3.881908000000	-0.861996000000
C	-4.987116000000	-2.753461000000	-0.865614000000
C	-3.681014000000	-2.747237000000	-1.404470000000
C	-3.266277000000	-3.986358000000	-1.941799000000
C	-4.072641000000	-5.128818000000	-1.955824000000
C	-5.357068000000	-5.079705000000	-1.412401000000
H	-6.810496000000	-3.831771000000	-0.430118000000
H	-5.380363000000	-1.838656000000	-0.419922000000
H	-2.267570000000	-4.067630000000	-2.372259000000
H	-3.704066000000	-6.056179000000	-2.388092000000
H	-5.990755000000	-5.960768000000	-1.416734000000
Ca	-2.422528000000	-0.651751000000	-1.521556000000
I	0.403528000000	-2.153279000000	-1.665382000000
O	-4.270427000000	0.758785000000	-1.496542000000
C	-4.383773000000	1.944549000000	-0.650319000000
C	-5.370241000000	0.710177000000	-2.444010000000
C	-5.357877000000	2.851692000000	-1.382768000000
H	-3.392126000000	2.370762000000	-0.524026000000
H	-4.757165000000	1.634398000000	0.327888000000
C	-6.316385000000	1.835356000000	-2.022872000000
H	-4.954453000000	0.871844000000	-3.442477000000
H	-5.810182000000	-0.287644000000	-2.396857000000
H	-5.838115000000	3.556403000000	-0.704364000000
H	-4.831217000000	3.425595000000	-2.150264000000
H	-7.032824000000	1.471555000000	-1.280574000000
H	-6.876654000000	2.237685000000	-2.868816000000
O	-2.759893000000	-0.595223000000	-3.912397000000
C	-3.564503000000	-1.589996000000	-4.592380000000
C	-1.755267000000	-0.210035000000	-4.870865000000
C	-2.552755000000	-2.447343000000	-5.368133000000
H	-4.256218000000	-1.066216000000	-5.263296000000
H	-4.118956000000	-2.134365000000	-3.831734000000
C	-1.301423000000	-1.533184000000	-5.498217000000
H	-2.213622000000	0.458050000000	-5.610735000000
H	-0.986509000000	0.341429000000	-4.333848000000
H	-2.316129000000	-3.348511000000	-4.802024000000
H	-2.952096000000	-2.750660000000	-6.337316000000
H	-0.977408000000	-1.399901000000	-6.531999000000
H	-0.469790000000	-1.950464000000	-4.928730000000
C	5.763106000000	3.955646000000	-1.467295000000
C	4.978039000000	2.864758000000	-1.079151000000

C	3.693030000000	2.599653000000	-1.600903000000
C	3.253198000000	3.546753000000	-2.554411000000
C	4.014034000000	4.646673000000	-2.962798000000
C	5.282721000000	4.853827000000	-2.420018000000
H	6.745799000000	4.107844000000	-1.028253000000
H	5.399979000000	2.195327000000	-0.328797000000
H	2.264430000000	3.430817000000	-2.999072000000
H	3.619694000000	5.343429000000	-3.698380000000
H	5.883245000000	5.703185000000	-2.729303000000
Ca	2.423834000000	0.507539000000	-1.315454000000
I	-0.423627000000	2.017434000000	-1.787345000000
O	2.982189000000	0.006045000000	-3.582449000000
C	4.194654000000	0.519805000000	-4.191592000000
C	2.007090000000	-0.092942000000	-4.636135000000
C	3.729965000000	1.437938000000	-5.342096000000
H	4.778648000000	-0.332742000000	-4.555502000000
H	4.744764000000	1.044059000000	-3.413101000000
C	2.202148000000	1.192626000000	-5.434249000000
H	2.211232000000	-0.990763000000	-5.233041000000
H	1.034615000000	-0.199668000000	-4.162552000000
H	4.235661000000	1.175075000000	-6.273276000000
H	3.947483000000	2.480568000000	-5.113288000000
H	1.844873000000	1.103453000000	-6.461700000000
H	1.656877000000	2.004196000000	-4.948265000000
O	4.128414000000	-1.023310000000	-0.882372000000
C	5.106766000000	-0.919860000000	0.183027000000
C	4.325854000000	-2.286272000000	-1.589078000000
C	6.318268000000	-1.655229000000	-0.367072000000
H	4.706217000000	-1.403802000000	1.076299000000
H	5.262915000000	0.140675000000	0.376553000000
C	5.663087000000	-2.849175000000	-1.083158000000
H	4.320794000000	-2.045873000000	-2.653065000000
H	3.487157000000	-2.942123000000	-1.358573000000
H	6.856002000000	-1.015583000000	-1.073069000000
H	7.007413000000	-1.963939000000	0.420852000000
H	6.275660000000	-3.240399000000	-1.897393000000
H	5.477746000000	-3.655230000000	-0.372878000000

Intl_THF

(E_{el} = -2748.298434 a.u.; G = -2747.253022 a.u.)

0 1

C	3.179686000000	-5.185311000000	-2.546226000000
C	3.031041000000	-3.899129000000	-2.016721000000
C	2.221434000000	-2.903459000000	-2.605366000000

C	1.553933000000	-3.319136000000	-3.779151000000
C	1.678291000000	-4.599060000000	-4.329592000000
C	2.501341000000	-5.541177000000	-3.712710000000
H	3.820000000000	-5.911447000000	-2.051463000000
H	3.566282000000	-3.673102000000	-1.093959000000
H	0.887175000000	-2.620061000000	-4.285763000000
H	1.136061000000	-4.863800000000	-5.234099000000
H	2.611253000000	-6.536139000000	-4.132159000000
Ca	1.971156000000	-0.618858000000	-1.759461000000
I	-1.234176000000	-0.664148000000	-2.126680000000
O	2.215507000000	0.352607000000	-3.902431000000
C	1.220948000000	1.119816000000	-4.610435000000
C	3.035017000000	-0.308769000000	-4.902395000000
C	0.800099000000	0.195783000000	-5.746925000000
H	1.676372000000	2.050232000000	-4.972129000000
H	0.426563000000	1.354456000000	-3.904708000000
C	2.121287000000	-0.514062000000	-6.130494000000
H	3.887905000000	0.339197000000	-5.127734000000
H	3.384525000000	-1.240427000000	-4.459735000000
H	0.071106000000	-0.522356000000	-5.365861000000
H	0.348653000000	0.735779000000	-6.580823000000
H	2.568233000000	-0.065824000000	-7.020016000000
H	1.963318000000	-1.574058000000	-6.328711000000
O	4.224619000000	-0.067575000000	-1.482198000000
C	4.874602000000	1.159651000000	-1.915485000000
C	5.159432000000	-0.880148000000	-0.703466000000
C	6.101205000000	1.287210000000	-1.024414000000
H	4.158368000000	1.972067000000	-1.802540000000
H	5.138966000000	1.049941000000	-2.973205000000
C	6.509623000000	-0.179094000000	-0.825898000000
H	4.801874000000	-0.890669000000	0.326372000000
H	5.139063000000	-1.889812000000	-1.115156000000
H	6.884402000000	1.894081000000	-1.482309000000
H	5.825430000000	1.733878000000	-0.069092000000
H	7.119570000000	-0.323559000000	0.066357000000
H	7.062270000000	-0.550902000000	-1.694171000000
C	-3.957586000000	6.103662000000	1.096258000000
C	-3.637669000000	4.817654000000	0.650943000000
C	-2.317986000000	4.388711000000	0.389003000000
C	-1.328179000000	5.365253000000	0.635313000000
C	-1.618460000000	6.658902000000	1.079447000000
C	-2.941950000000	7.035959000000	1.307462000000
H	-4.993047000000	6.381265000000	1.277708000000
H	-4.465442000000	4.123194000000	0.493384000000

H	-0.280800000000	5.115693000000	0.463053000000
H	-0.816693000000	7.374159000000	1.246041000000
H	-3.177848000000	8.038872000000	1.649143000000
Ca	-1.905176000000	2.248136000000	-0.676873000000
I	1.315064000000	2.517812000000	-0.730691000000
O	-2.181077000000	3.350724000000	-2.803274000000
C	-1.105700000000	4.009740000000	-3.507641000000
C	-3.307705000000	4.267599000000	-2.870325000000
C	-1.192325000000	5.466490000000	-3.055232000000
H	-1.273862000000	3.898250000000	-4.586783000000
H	-0.177251000000	3.513332000000	-3.231811000000
C	-2.706459000000	5.682751000000	-2.800307000000
H	-3.831341000000	4.085204000000	-3.815580000000
H	-3.966348000000	4.034254000000	-2.036566000000
H	-0.640904000000	5.592928000000	-2.123052000000
H	-0.781089000000	6.150382000000	-3.799829000000
H	-3.160166000000	6.331547000000	-3.552147000000
H	-2.869945000000	6.118432000000	-1.815492000000
O	-4.129234000000	1.571234000000	-1.050731000000
C	-4.959028000000	0.999838000000	0.018856000000
C	-4.637316000000	1.133508000000	-2.338581000000
C	-6.031823000000	0.165889000000	-0.681311000000
H	-5.351392000000	1.824908000000	0.615242000000
H	-4.312279000000	0.377253000000	0.634423000000
C	-5.378792000000	-0.157220000000	-2.033060000000
H	-5.306595000000	1.907805000000	-2.731593000000
H	-3.784469000000	1.020826000000	-3.007243000000
H	-6.275445000000	-0.727476000000	-0.108639000000
H	-6.944349000000	0.751393000000	-0.829103000000
H	-6.100927000000	-0.420306000000	-2.808208000000
H	-4.667791000000	-0.977895000000	-1.917280000000
C	5.923870000000	3.285208000000	2.168819000000
C	4.554544000000	3.038060000000	2.027771000000
C	3.970419000000	1.767777000000	2.230468000000
C	4.888475000000	0.750087000000	2.575784000000
C	6.262899000000	0.967898000000	2.715862000000
C	6.786889000000	2.245119000000	2.515599000000
H	6.320298000000	4.283510000000	2.003962000000
H	3.920582000000	3.877357000000	1.741062000000
H	4.520651000000	-0.263415000000	2.740804000000
H	6.924384000000	0.147242000000	2.982395000000
H	7.851181000000	2.426718000000	2.624766000000
Ca	1.577418000000	1.333714000000	2.162501000000
I	1.825498000000	-1.661138000000	1.302124000000

O	1.511067000000	1.331232000000	4.537726000000
C	2.690144000000	1.643961000000	5.330843000000
C	0.809913000000	0.326265000000	5.304832000000
C	3.162786000000	0.287806000000	5.882043000000
H	2.383719000000	2.329657000000	6.127900000000
H	3.405890000000	2.127704000000	4.670400000000
C	1.917020000000	-0.633361000000	5.746397000000
H	0.321305000000	0.814796000000	6.155776000000
H	0.043897000000	-0.104942000000	4.664403000000
H	3.995115000000	-0.089752000000	5.287814000000
H	3.498015000000	0.380820000000	6.916196000000
H	1.664060000000	-1.148436000000	6.674563000000
H	2.082537000000	-1.385787000000	4.972201000000
C	-6.011006000000	-3.562627000000	0.154152000000
C	-4.668809000000	-3.233954000000	-0.064300000000
C	-3.903406000000	-2.444392000000	0.821104000000
C	-4.615585000000	-1.997907000000	1.958304000000
C	-5.956092000000	-2.309798000000	2.204371000000
C	-6.662001000000	-3.102480000000	1.298472000000
H	-6.549861000000	-4.174219000000	-0.564926000000
H	-4.207599000000	-3.617571000000	-0.974966000000
H	-4.107220000000	-1.367041000000	2.688210000000
H	-6.452209000000	-1.933686000000	3.095568000000
H	-7.702660000000	-3.351984000000	1.478466000000
Ca	-1.468635000000	-2.126747000000	0.713533000000
I	-1.607288000000	0.736519000000	2.207843000000
O	-1.271732000000	-3.460063000000	2.685498000000
C	-2.283453000000	-4.447810000000	3.016077000000
C	-0.755873000000	-2.975624000000	3.940579000000
C	-2.910417000000	-3.976721000000	4.345397000000
H	-1.787744000000	-5.419539000000	3.116252000000
H	-2.988478000000	-4.471251000000	2.187505000000
C	-2.003776000000	-2.804754000000	4.801027000000
H	-0.060888000000	-3.717681000000	4.353220000000
H	-0.208243000000	-2.059151000000	3.732879000000
H	-2.917039000000	-4.787032000000	5.076887000000
H	-3.936357000000	-3.644677000000	4.190305000000
H	-1.780637000000	-2.827931000000	5.869143000000
H	-2.472016000000	-1.846438000000	4.566450000000
O	-0.787354000000	-4.051058000000	-0.404219000000
C	-1.246832000000	-4.470652000000	-1.714407000000
C	0.203791000000	-5.009927000000	0.069009000000
C	-1.238800000000	-5.988094000000	-1.622434000000
H	-0.549541000000	-4.098722000000	-2.468453000000

H	-2.228677000000	-4.025582000000	-1.869955000000
C	0.050950000000	-6.255467000000	-0.823343000000
H	-0.018494000000	-5.185467000000	1.122068000000
H	1.190947000000	-4.557044000000	-0.024597000000
H	-2.121022000000	-6.332214000000	-1.075418000000
H	-1.229064000000	-6.461946000000	-2.605338000000
H	-0.003857000000	-7.174593000000	-0.237563000000
H	0.902148000000	-6.327117000000	-1.501178000000

Int2_THF

(E_{el} = -3006.112998 a.u.; G = -3004.952644 a.u.)

0 1

C	2.763672000000	-6.053965000000	0.710554000000
C	1.764861000000	-5.078383000000	0.624928000000
C	1.598682000000	-4.047039000000	1.574782000000
C	2.544653000000	-4.072861000000	2.624014000000
C	3.560514000000	-5.028568000000	2.732220000000
C	3.670748000000	-6.032946000000	1.770885000000
H	2.839878000000	-6.827947000000	-0.049406000000
H	1.097075000000	-5.121302000000	-0.235767000000
H	2.509025000000	-3.295836000000	3.387815000000
H	4.265212000000	-4.991065000000	3.559513000000
H	4.449935000000	-6.784875000000	1.845065000000
Ca	-0.080318000000	-2.248827000000	1.529942000000
I	2.081873000000	0.102576000000	1.939866000000
O	-0.421261000000	-2.536285000000	3.854684000000
C	-0.075845000000	-1.668708000000	4.949247000000
C	-0.524095000000	-3.881316000000	4.384450000000
C	0.918625000000	-2.480562000000	5.777715000000
H	-0.984532000000	-1.422833000000	5.513054000000
H	0.344954000000	-0.761084000000	4.519812000000
C	0.463517000000	-3.947215000000	5.566706000000
H	-1.558708000000	-4.047779000000	4.702404000000
H	-0.273455000000	-4.560120000000	3.570876000000
H	1.925815000000	-2.332387000000	5.385373000000
H	0.916497000000	-2.182928000000	6.827640000000
H	-0.025760000000	-4.348943000000	6.455841000000
H	1.311140000000	-4.588074000000	5.325018000000
O	-2.008831000000	-3.547309000000	1.324647000000
C	-3.326433000000	-3.306451000000	1.904784000000
C	-2.056676000000	-4.718606000000	0.464264000000
C	-4.215452000000	-4.452330000000	1.413748000000
H	-3.675785000000	-2.332227000000	1.568709000000
H	-3.195950000000	-3.296639000000	2.990254000000

C	-3.207041000000	-5.543351000000	1.021697000000
H	-2.251714000000	-4.387920000000	-0.558640000000
H	-1.080398000000	-5.198892000000	0.523069000000
H	-4.921593000000	-4.778252000000	2.179608000000
H	-4.780442000000	-4.130870000000	0.539173000000
H	-3.606331000000	-6.242754000000	0.285267000000
H	-2.876229000000	-6.110306000000	1.897432000000
C	-2.494142000000	6.348142000000	-0.329080000000
C	-1.489762000000	5.416621000000	-0.048225000000
C	-1.598031000000	4.439572000000	0.966337000000
C	-2.808283000000	4.485785000000	1.693561000000
C	-3.826925000000	5.409339000000	1.439574000000
C	-3.673469000000	6.346243000000	0.417069000000
H	-2.362559000000	7.072665000000	-1.128676000000
H	-0.593762000000	5.441544000000	-0.668760000000
H	-5.534559000000	3.511448000000	0.083257000000
H	-4.741557000000	5.395017000000	2.027657000000
H	-4.459153000000	7.065005000000	0.206637000000
Ca	0.066225000000	2.684870000000	1.324755000000
I	-2.165203000000	0.383778000000	1.569044000000
O	0.000065000000	3.057522000000	3.672763000000
C	-0.494021000000	2.154944000000	4.679383000000
C	-0.221804000000	4.405901000000	4.163554000000
C	-1.784385000000	2.812376000000	5.157534000000
H	0.251641000000	2.065774000000	5.480143000000
H	-0.637952000000	1.187056000000	4.203876000000
C	-1.465321000000	4.325550000000	5.074459000000
H	0.671890000000	4.719978000000	4.712488000000
H	-0.363991000000	5.039465000000	3.289410000000
H	-2.591542000000	2.549910000000	4.471030000000
H	-2.069188000000	2.491477000000	6.161035000000
H	-1.247405000000	4.741629000000	6.060006000000
H	-2.297768000000	4.883257000000	4.646020000000
O	2.062434000000	3.912390000000	1.483612000000
C	2.773917000000	4.463977000000	0.324945000000
C	2.980450000000	3.806205000000	2.600913000000
C	4.236615000000	4.609818000000	0.755615000000
H	2.296474000000	5.408010000000	0.055437000000
H	2.664257000000	3.750099000000	-0.489523000000
C	4.342126000000	3.645815000000	1.946849000000
H	2.916200000000	4.724307000000	3.197983000000
H	2.661743000000	2.958687000000	3.205826000000
H	4.916688000000	4.349254000000	-0.053523000000
H	4.445469000000	5.634947000000	1.075911000000

H	5.166043000000	3.885380000000	2.621752000000
H	4.462644000000	2.621622000000	1.588155000000
C	-6.350447000000	-2.271407000000	-0.765053000000
C	-5.234804000000	-1.431746000000	-0.684069000000
C	-4.027975000000	-1.668590000000	-1.376748000000
C	-4.021636000000	-2.858177000000	-2.138572000000
C	-5.118133000000	-3.722099000000	-2.233919000000
C	-6.298594000000	-3.422457000000	-1.552571000000
H	-7.258267000000	-2.030964000000	-0.217590000000
H	-5.315039000000	-0.550444000000	-0.048921000000
H	-3.118221000000	-3.129361000000	-2.686252000000
H	-5.056182000000	-4.624592000000	-2.837448000000
H	-7.159027000000	-4.079899000000	-1.625088000000
Ca	-2.216362000000	-0.038254000000	-1.611910000000
I	0.116118000000	-2.178731000000	-1.668094000000
O	-2.531490000000	-0.178120000000	-3.954275000000
C	-3.885777000000	-0.101072000000	-4.466195000000
C	-1.734538000000	-0.798608000000	-4.979438000000
C	-4.066630000000	-1.345540000000	-5.355567000000
H	-3.985908000000	0.832566000000	-5.029172000000
H	-4.553410000000	-0.084830000000	-3.606761000000
C	-2.630991000000	-1.901310000000	-5.543818000000
H	-1.477900000000	-0.045511000000	-5.735293000000
H	-0.825801000000	-1.166261000000	-4.506458000000
H	-4.701718000000	-2.078930000000	-4.859475000000
H	-4.527767000000	-1.076820000000	-6.307679000000
H	-2.394614000000	-2.125095000000	-6.585518000000
H	-2.499068000000	-2.813728000000	-4.960849000000
C	6.791831000000	2.381308000000	-1.079041000000
C	5.717059000000	1.537284000000	-0.779506000000
C	4.448731000000	1.640097000000	-1.390950000000
C	4.348678000000	2.684471000000	-2.338747000000
C	5.404873000000	3.541850000000	-2.661942000000
C	6.640151000000	3.389506000000	-2.030801000000
H	7.745797000000	2.255131000000	-0.573378000000
H	5.888048000000	0.764678000000	-0.029018000000
H	3.398076000000	2.847647000000	-2.847546000000
H	5.266606000000	4.329972000000	-3.398065000000
H	7.467872000000	4.048478000000	-2.272410000000
Ca	2.643337000000	-0.024032000000	-1.243220000000
I	0.292587000000	2.103276000000	-1.835422000000
O	3.008086000000	-0.477166000000	-3.551499000000
C	4.324251000000	-0.343649000000	-4.147057000000
C	2.050213000000	-0.206152000000	-4.593820000000

C	4.18092000000	0.71758900000	-5.25736200000
H	4.61747900000	-1.32000300000	-4.54848400000
H	5.00462000000	-0.04860500000	-3.35022500000
C	2.65550800000	0.97262500000	-5.35005600000
H	1.94342900000	-1.09936000000	-5.22241800000
H	1.09926100000	0.01340500000	-4.11262700000
H	4.58452400000	0.34464000000	-6.20073100000
H	4.71604300000	1.62814500000	-4.98994700000
H	2.29496200000	1.03445900000	-6.37831300000
H	2.39071400000	1.89876700000	-4.83704700000
O	3.89360600000	-1.94527100000	-0.82448700000
C	4.73790600000	-2.16448800000	0.33412200000
C	3.90276200000	-3.15916000000	-1.62847600000
C	5.87837800000	-3.00532300000	-0.21722900000
H	4.16201800000	-2.69528100000	1.09589700000
H	5.02963600000	-1.18519600000	0.71097500000
C	5.14490900000	-3.95646400000	-1.18405500000
H	3.92817600000	-2.83916100000	-2.67020000000
H	2.97704400000	-3.70268700000	-1.43851600000
H	6.58448500000	-2.36585200000	-0.75390600000
H	6.41553900000	-3.53891200000	0.56850100000
H	5.76858800000	-4.24890800000	-2.03048400000
H	4.83205100000	-4.85815800000	-0.65652500000
C	-6.36098500000	1.98926200000	-1.23544900000
H	-6.70343700000	2.69915400000	-1.99869900000
H	-5.99791300000	1.10520700000	-1.76664700000
C	-7.53191300000	1.59260800000	-0.33436400000
H	-7.94292100000	2.46299600000	0.18710600000
H	-7.21308700000	0.87073100000	0.42304800000
H	-8.33828800000	1.13188700000	-0.91059600000
C	-5.20337200000	2.61345900000	-0.45035900000
H	-4.83576900000	1.92098500000	0.31472400000
H	-2.98605600000	3.74765800000	2.47569900000
C	-4.04341700000	3.03978500000	-1.30868200000
H	-4.32702800000	3.70960700000	-2.12018300000
H	-3.20856800000	3.44714900000	-0.74461500000
F	-3.51517100000	1.85704400000	-1.98827100000

TSA_THF

(E_{el} = -3006.084265 a.u.; G = -3004.919677 a.u.)

0 1

C	-6.35406700000	2.41560600000	-1.48882200000
C	-5.32351000000	1.52627200000	-1.16527400000
C	-4.06126000000	1.52925300000	-1.79865200000

C	-3.910505000000	2.538933000000	-2.775537000000
C	-4.917517000000	3.449067000000	-3.114416000000
C	-6.155888000000	3.382226000000	-2.475498000000
H	-7.308376000000	2.360732000000	-0.971096000000
H	-5.519958000000	0.802301000000	-0.374326000000
H	-2.958237000000	2.627821000000	-3.299908000000
H	-4.740929000000	4.206314000000	-3.874715000000
H	-6.948790000000	4.076476000000	-2.734494000000
Ca	-2.353584000000	-0.229543000000	-1.574809000000
I	0.132019000000	1.884952000000	-1.912115000000
O	-2.467856000000	-0.569568000000	-3.926138000000
C	-1.450496000000	-0.279536000000	-4.900813000000
C	-3.744384000000	-0.468633000000	-4.605704000000
C	-2.030291000000	0.878467000000	-5.709505000000
H	-1.276426000000	-1.172385000000	-5.515071000000
H	-0.543042000000	-0.029758000000	-4.355308000000
C	-3.554214000000	0.596631000000	-5.704993000000
H	-3.987396000000	-1.451033000000	-5.024052000000
H	-4.482509000000	-0.191802000000	-3.855243000000
H	-1.813647000000	1.817475000000	-5.197351000000
H	-1.610111000000	0.932018000000	-6.715420000000
H	-3.896436000000	0.219114000000	-6.670437000000
H	-4.119270000000	1.497863000000	-5.469085000000
O	-3.763898000000	-2.099973000000	-1.573626000000
C	-3.560206000000	-3.341801000000	-2.303973000000
C	-4.898030000000	-2.241046000000	-0.659506000000
C	-4.310624000000	-4.394739000000	-1.502578000000
H	-2.487458000000	-3.515376000000	-2.371862000000
H	-3.972661000000	-3.216297000000	-3.311417000000
C	-5.514587000000	-3.600776000000	-0.977694000000
H	-4.503901000000	-2.200233000000	0.356194000000
H	-5.567239000000	-1.398177000000	-0.833656000000
H	-4.595324000000	-5.253875000000	-2.112699000000
H	-3.697702000000	-4.742942000000	-0.671273000000
H	-5.957477000000	-4.058212000000	-0.093041000000
H	-6.284682000000	-3.504712000000	-1.749612000000
C	6.871737000000	-1.425179000000	-0.911281000000
C	5.579975000000	-1.245415000000	-0.405998000000
C	4.458985000000	-1.925655000000	-0.921682000000
C	4.725276000000	-2.826240000000	-1.972578000000
C	6.006933000000	-3.038604000000	-2.480683000000
C	7.087766000000	-2.329322000000	-1.950954000000
H	7.708199000000	-0.875545000000	-0.489255000000
H	5.449439000000	-0.550743000000	0.423351000000

H	5.040614000000	-4.118673000000	0.499563000000
H	6.170630000000	-3.755334000000	-3.280813000000
H	8.088502000000	-2.487375000000	-2.338922000000
Ca	2.586600000000	-0.197283000000	-1.185716000000
I	0.226683000000	-2.321568000000	-1.589684000000
O	3.152437000000	-0.170087000000	-3.495126000000
C	2.317936000000	-0.664063000000	-4.564545000000
C	4.521403000000	-0.120426000000	-3.989034000000
C	3.178138000000	-1.729544000000	-5.229319000000
H	2.077007000000	0.162878000000	-5.244415000000
H	1.403844000000	-1.045306000000	-4.114190000000
C	4.591232000000	-1.112807000000	-5.168060000000
H	4.731971000000	0.903422000000	-4.306488000000
H	5.171006000000	-0.385990000000	-3.157532000000
H	3.132684000000	-2.645556000000	-4.637409000000
H	2.854828000000	-1.956655000000	-6.246525000000
H	4.825353000000	-0.586660000000	-6.096105000000
H	5.358152000000	-1.868213000000	-5.001871000000
O	3.869767000000	1.786857000000	-1.178534000000
C	4.390838000000	2.465463000000	0.017764000000
C	3.849029000000	2.735942000000	-2.277720000000
C	4.577186000000	3.934983000000	-0.370971000000
H	5.317287000000	1.966091000000	0.307932000000
H	3.646720000000	2.349270000000	0.801886000000
C	3.672125000000	4.082804000000	-1.602529000000
H	4.804589000000	2.673658000000	-2.811717000000
H	3.037620000000	2.446933000000	-2.943590000000
H	4.287424000000	4.598688000000	0.441756000000
H	5.618698000000	4.137532000000	-0.638110000000
H	3.955603000000	4.917562000000	-2.246354000000
H	2.633446000000	4.209008000000	-1.292410000000
C	-2.875769000000	-6.584191000000	1.208675000000
C	-1.857790000000	-5.625786000000	1.157828000000
C	-2.022148000000	-4.293007000000	1.597887000000
C	-3.310130000000	-4.000652000000	2.100937000000
C	-4.344647000000	-4.939530000000	2.166735000000
C	-4.129595000000	-6.242415000000	1.716110000000
H	-2.694559000000	-7.596021000000	0.854948000000
H	-0.892792000000	-5.937516000000	0.758266000000
H	-3.521226000000	-2.993332000000	2.460493000000
H	-5.315816000000	-4.659448000000	2.568605000000
H	-4.925025000000	-6.979554000000	1.761832000000
Ca	-0.146467000000	-2.719325000000	1.689996000000
I	-2.255554000000	-0.143447000000	1.594254000000

O	-0.232624000000	-2.708373000000	4.068922000000
C	-0.925049000000	-3.748058000000	4.802310000000
C	-0.250476000000	-1.555000000000	4.926928000000
C	-2.089934000000	-3.026793000000	5.502638000000
H	-0.220444000000	-4.185212000000	5.518749000000
H	-1.239479000000	-4.499101000000	4.080532000000
C	-1.672938000000	-1.528705000000	5.494618000000
H	0.504679000000	-1.685430000000	5.712202000000
H	0.022294000000	-0.694925000000	4.319174000000
H	-3.013488000000	-3.176063000000	4.943318000000
H	-2.238478000000	-3.410391000000	6.513523000000
H	-1.706626000000	-1.072889000000	6.486012000000
H	-2.323348000000	-0.957114000000	4.830472000000
C	2.381128000000	6.529399000000	1.321419000000
C	1.522883000000	5.495947000000	0.931152000000
C	1.492381000000	4.226710000000	1.548954000000
C	2.421495000000	4.080356000000	2.605229000000
C	3.291968000000	5.093706000000	3.018907000000
C	3.271886000000	6.332151000000	2.376342000000
H	2.358207000000	7.485659000000	0.805025000000
H	0.851277000000	5.701552000000	0.097077000000
H	2.479059000000	3.127689000000	3.132457000000
H	3.986732000000	4.919613000000	3.836879000000
H	3.941588000000	7.126910000000	2.688670000000
Ca	-0.227566000000	2.481241000000	1.242496000000
I	1.904336000000	0.158153000000	1.943089000000
O	-1.029995000000	3.038615000000	3.424184000000
C	-0.851794000000	4.375608000000	3.958313000000
C	-1.047433000000	2.153499000000	4.559612000000
C	0.028179000000	4.208518000000	5.215264000000
H	-1.841691000000	4.778602000000	4.199715000000
H	-0.386077000000	4.972869000000	3.177394000000
C	0.084440000000	2.675197000000	5.440043000000
H	-2.025182000000	2.222706000000	5.052936000000
H	-0.917806000000	1.142373000000	4.183283000000
H	-0.415990000000	4.724360000000	6.068745000000
H	1.023060000000	4.618446000000	5.044514000000
H	-0.036954000000	2.391508000000	6.486870000000
H	1.034536000000	2.273052000000	5.082019000000
O	-2.069907000000	3.742752000000	0.589012000000
C	-2.097960000000	4.709921000000	-0.491905000000
C	-3.399682000000	3.640295000000	1.187257000000
C	-3.200167000000	5.677967000000	-0.091144000000
H	-2.332689000000	4.188567000000	-1.421874000000

H	-1.104414000000	5.152199000000	-0.555527000000
C	-4.245894000000	4.727274000000	0.514283000000
H	-3.267094000000	3.788260000000	2.260496000000
H	-3.780554000000	2.637205000000	1.000253000000
H	-2.827074000000	6.385397000000	0.655550000000
H	-3.585682000000	6.239653000000	-0.943704000000
H	-4.910905000000	5.223575000000	1.223344000000
H	-4.852298000000	4.286722000000	-0.276780000000
C	4.783801000000	-3.388059000000	2.527570000000
H	5.158007000000	-2.382044000000	2.309477000000
H	3.953798000000	-3.271183000000	3.231049000000
C	5.895925000000	-4.230388000000	3.154053000000
H	6.742839000000	-4.334547000000	2.468096000000
H	5.539115000000	-5.236492000000	3.396367000000
H	6.267847000000	-3.777373000000	4.076997000000
C	4.241248000000	-4.001529000000	1.235715000000
H	3.840976000000	-5.002981000000	1.425653000000
H	3.901575000000	-3.396644000000	-2.400985000000
C	3.126621000000	-3.205819000000	0.636959000000
H	2.911742000000	-2.229700000000	1.021558000000
H	2.645978000000	-3.521881000000	-0.270058000000
F	1.705493000000	-3.874956000000	1.653997000000

ProdA_THF

(E_{el} = -3006.203140 a.u.; G = -3005.034866 a.u.)

0 1

C	6.068150000000	3.715382000000	-0.277415000000
C	4.703932000000	3.418904000000	-0.180357000000
C	4.104235000000	2.284776000000	-0.770734000000
C	5.014386000000	1.443329000000	-1.450984000000
C	6.382218000000	1.711217000000	-1.564263000000
C	6.916538000000	2.861494000000	-0.982326000000
H	6.470379000000	4.608377000000	0.193993000000
H	4.085504000000	4.115137000000	0.387176000000
H	4.644843000000	0.536365000000	-1.927892000000
H	7.031678000000	1.027612000000	-2.105813000000
H	7.975437000000	3.082852000000	-1.067516000000
Ca	1.669295000000	2.080079000000	-1.049765000000
I	2.113019000000	-1.198251000000	-1.449669000000
O	2.110849000000	2.679355000000	-3.335670000000
C	2.673657000000	1.756303000000	-4.298985000000
C	2.668227000000	3.985629000000	-3.615853000000
C	4.032241000000	2.344506000000	-4.736202000000
H	1.975818000000	1.666757000000	-5.138786000000

H	2.760487000000	0.789547000000	-3.803098000000
C	4.112970000000	3.710390000000	-4.016075000000
H	2.089858000000	4.445773000000	-4.426921000000
H	2.561868000000	4.580370000000	-2.710432000000
H	4.857655000000	1.701047000000	-4.433156000000
H	4.066491000000	2.458410000000	-5.821718000000
H	4.517051000000	4.498691000000	-4.653768000000
H	4.729027000000	3.628471000000	-3.121431000000
O	0.854039000000	4.305870000000	-0.911960000000
C	-0.194945000000	4.902053000000	-1.734752000000
C	1.107457000000	5.160955000000	0.251992000000
C	-0.834928000000	5.968298000000	-0.857952000000
H	-0.876389000000	4.107961000000	-2.033281000000
H	0.278078000000	5.329125000000	-2.625737000000
C	0.356461000000	6.457815000000	-0.024353000000
H	0.715151000000	4.647748000000	1.129352000000
H	2.187955000000	5.278625000000	0.342429000000
H	-1.301118000000	6.759436000000	-1.447604000000
H	-1.590234000000	5.524247000000	-0.209012000000
H	0.041836000000	6.943531000000	0.899124000000
H	0.978049000000	7.152439000000	-0.598679000000
C	-3.796463000000	-3.298061000000	-1.229454000000
C	-4.115854000000	-1.937720000000	-1.167011000000
C	-4.864711000000	-1.333236000000	-2.190756000000
C	-5.290454000000	-2.129345000000	-3.260042000000
C	-4.980540000000	-3.489131000000	-3.317895000000
C	-4.222489000000	-4.078715000000	-2.307333000000
H	-3.248347000000	-3.750898000000	-0.409756000000
H	-3.854191000000	-1.334834000000	-0.299367000000
H	-7.406698000000	-0.133327000000	-2.365687000000
H	-5.328608000000	-4.086867000000	-4.153763000000
H	-3.980189000000	-5.134670000000	-2.346593000000
Ca	-0.926075000000	-1.862986000000	-1.589886000000
I	-1.441995000000	1.192872000000	-1.833227000000
O	-0.848801000000	-1.803929000000	-3.949422000000
C	-0.087591000000	-0.831008000000	-4.713649000000
C	-2.001684000000	-2.137489000000	-4.756473000000
C	-1.123522000000	-0.031462000000	-5.529809000000
H	0.614457000000	-1.377934000000	-5.350997000000
H	0.470226000000	-0.231161000000	-4.000021000000
C	-2.455432000000	-0.791401000000	-5.309646000000
H	-1.687806000000	-2.829531000000	-5.547827000000
H	-2.729034000000	-2.631897000000	-4.116557000000
H	-1.196439000000	0.993703000000	-5.167158000000

H	-0.843949000000	-0.005778000000	-6.584707000000
H	-3.044630000000	-0.895656000000	-6.221793000000
H	-3.064195000000	-0.282614000000	-4.560642000000
O	-0.358866000000	-4.093340000000	-1.848693000000
C	-0.272953000000	-5.074207000000	-0.754694000000
C	0.447113000000	-4.544495000000	-2.978510000000
C	0.313537000000	-6.322717000000	-1.396537000000
H	-1.277711000000	-5.199892000000	-0.352703000000
H	0.381363000000	-4.666919000000	0.015763000000
C	1.255977000000	-5.722255000000	-2.448097000000
H	-0.237482000000	-4.836551000000	-3.780850000000
H	1.057024000000	-3.705039000000	-3.312092000000
H	0.835456000000	-6.933478000000	-0.661104000000
H	-0.468493000000	-6.921808000000	-1.873983000000
H	1.528325000000	-6.423249000000	-3.239130000000
H	2.166499000000	-5.366466000000	-1.961513000000
C	-4.013044000000	5.647044000000	1.245361000000
C	-3.697290000000	4.290361000000	1.112858000000
C	-2.558835000000	3.692621000000	1.701794000000
C	-1.760672000000	4.584729000000	2.452128000000
C	-2.057941000000	5.942052000000	2.612299000000
C	-3.189620000000	6.482513000000	2.000520000000
H	-4.900514000000	6.053511000000	0.766367000000
H	-4.373992000000	3.671866000000	0.522262000000
H	-0.859346000000	4.209699000000	2.939340000000
H	-1.411237000000	6.579154000000	3.211842000000
H	-3.428415000000	7.535295000000	2.114795000000
Ca	-2.234507000000	1.264494000000	1.376345000000
I	0.960774000000	1.647703000000	1.996264000000
O	-2.505424000000	0.632648000000	3.697519000000
C	-3.704886000000	-0.149481000000	3.923765000000
C	-2.573708000000	1.721322000000	4.647268000000
C	-4.805451000000	0.898574000000	4.118437000000
H	-3.547994000000	-0.768395000000	4.816485000000
H	-3.852068000000	-0.777420000000	3.048304000000
C	-4.051713000000	2.142420000000	4.670295000000
H	-2.234924000000	1.347924000000	5.622114000000
H	-1.899848000000	2.502298000000	4.300095000000
H	-5.247785000000	1.118725000000	3.146490000000
H	-5.590034000000	0.544539000000	4.789704000000
H	-4.369867000000	2.414247000000	5.678625000000
H	-4.197916000000	3.002520000000	4.016174000000
C	3.385110000000	-5.862509000000	0.602504000000
C	3.242030000000	-4.474874000000	0.708146000000

C	2.383392000000	-3.847669000000	1.637487000000
C	1.652095000000	-4.747972000000	2.445374000000
C	1.768148000000	-6.138604000000	2.359065000000
C	2.648165000000	-6.704372000000	1.435865000000
H	4.068520000000	-6.289300000000	-0.127843000000
H	3.818629000000	-3.860318000000	0.016548000000
H	0.933568000000	-4.352874000000	3.164265000000
H	1.176772000000	-6.780809000000	3.006995000000
H	2.755854000000	-7.782306000000	1.365457000000
Ca	1.932254000000	-1.429600000000	1.821000000000
I	-1.214285000000	-2.075344000000	1.450486000000
O	1.553678000000	-1.430581000000	4.149229000000
C	2.200953000000	-2.388289000000	5.025306000000
C	0.359036000000	-0.975470000000	4.829128000000
C	1.070494000000	-3.031102000000	5.860463000000
H	2.917645000000	-1.849779000000	5.653508000000
H	2.732119000000	-3.094643000000	4.387874000000
C	-0.200267000000	-2.253748000000	5.439940000000
H	0.645397000000	-0.238814000000	5.589715000000
H	-0.293425000000	-0.501040000000	4.099823000000
H	1.271086000000	-2.915445000000	6.927492000000
H	0.978688000000	-4.097204000000	5.651112000000
H	-0.874824000000	-2.056814000000	6.274889000000
H	-0.751990000000	-2.799505000000	4.671882000000
O	4.127174000000	-0.622946000000	1.889032000000
C	5.191627000000	-1.289062000000	1.154969000000
C	4.628582000000	0.627908000000	2.459843000000
C	6.473219000000	-0.764813000000	1.785823000000
H	5.113693000000	-1.005133000000	0.102077000000
H	5.034265000000	-2.361582000000	1.264454000000
C	6.108730000000	0.698910000000	2.077910000000
H	4.464786000000	0.570724000000	3.539062000000
H	4.050019000000	1.449130000000	2.041942000000
H	6.690243000000	-1.310295000000	2.709224000000
H	7.329492000000	-0.861143000000	1.116025000000
H	6.713519000000	1.137788000000	2.873359000000
H	6.229408000000	1.304541000000	1.180099000000
C	-7.004060000000	-0.274751000000	-0.238818000000
H	-6.898975000000	-1.365275000000	-0.278405000000
H	-6.231380000000	0.078702000000	0.449654000000
C	-8.399893000000	0.083765000000	0.276439000000
H	-9.183317000000	-0.275229000000	-0.400518000000
H	-8.517129000000	1.168426000000	0.370825000000
H	-8.585202000000	-0.354963000000	1.261225000000

C	-6.723112000000	0.308904000000	-1.628269000000
H	-6.932908000000	1.385181000000	-1.616106000000
H	-5.882233000000	-1.679743000000	-4.051574000000
C	-5.261203000000	0.119815000000	-2.087763000000
H	-4.609372000000	0.613507000000	-1.366120000000
H	-5.122070000000	0.605733000000	-3.060375000000
F	-4.063682000000	0.389146000000	0.917316000000

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