

Supporting Information

CO, CO₂ and CS₂ Activation by Divalent Ytterbium Hydrido Complex

Xianghui Shi,^{[a][†]} Thayalan Rajeshkumar,^{[c][†]} Laurent Maron^{*[c]} and Jianhua Cheng^{*[a][b]}

[†] X. Shi and T. Rajeshkumar contributed equally to this work.

[a] State Key Laboratory of Polymer Physics and Chemistry

Changchun Institute of Applied Chemistry

Chinese Academy of Sciences

No. 5625, Renmin Street, Changchun 130022 (China)

E-Mail: jhcheng@ciac.ac.cn

[b] University of Science and Technology of China

Hefei, Anhui 230026 (China)

[c] LPCNO, CNRS & INSA, UPS

Université de Toulouse 135 Avenue de Rangueil, 31077 Toulouse (France)

Email: laurent.maron@irsamc.ups-tlse.fr

Contents Page

1. Experimental section and NMR spectra.....	S3
2. X-ray crystallographic studies	S9
3. Tables of crystal data and structure refinement.....	S11
4. ORTEP drawing of complexes	S14
5. DFT calculations.....	S17
6. References	S76

General remarks

All reactions were carried out under a dry and oxygen-free nitrogen atmosphere using Schlenk techniques and a Vigor glovebox. The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves (4 Å) catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored using an O₂(GE)/H₂O (Xentaur) analyzer to ensure that both were always below 0.1 ppm. Toluene, hexane and Et₂O were purified by use of a Vigor VSPS-5 solvent purification system, and dried over fresh Na chips in the glovebox. Tetrahydrofuran (THF), pentane, and benzene-*d*₆ were distilled from Na/K alloy/benzophenone, degassed by the freeze-pump-thaw method (three times), and dried over fresh Na chips in the glovebox. [(Tp^{Ad,iPr})Yb(H)(THF)]¹ was prepared according to literature procedures. The commercially available reagents were used without purification.

Samples for NMR spectroscopic measurements were prepared in the glovebox by use of J. Young valve NMR tubes. ¹H and ¹³C NMR spectra were recorded on a Bruker AV400 or AV500 spectrometer and referenced to the resonances of the solvent used. The elemental analyses were performed on Elementar Vario EL cube (WO₃ was used as pro-oxidant) at National Analytical Research Centre of Changchun Institute of Applied Chemistry (CIAC).

Synthesis of $[(\text{Tp}^{\text{Ad},i\text{Pr}})\text{Yb}]_2(\text{cis-OCH=CHO})$ (**2**)

A solution of $[(\text{Tp}^{\text{Ad},i\text{Pr}})\text{Yb}(\text{H})(\text{THF})]$ (**1**) (86 mg, 0.087 mmol) in hexane (10 mL)/THF (1 mL) was charged into J. Young valve NMR tube. The tube was frozen in liquid nitrogen, evacuated and backfilled with CO (1 atm). Warmed up to room temperature, no color change was observed. After 30 minutes, the resulting solution was filtered and all volatiles were removed under reduced pressure to give complex **2** (74 mg, 0.039 mmol, 90% yield) as red-orange powder. Single crystals of complex **2** suitable for X-ray analysis were grown from a concentrated hexane/benzene solution at $-30\text{ }^{\circ}\text{C}$ as red-orange crystals.

^1H NMR (400 MHz, C_6D_6 , $25\text{ }^{\circ}\text{C}$): δ = 1.27 (d, J = 7 Hz, 36H, $\text{CH}(\text{CH}_3)_2$), 1.74, 1.83 (dd, J = 55, 12 Hz, 36H, AdCH_2), 2.04 (br, 18 H, AdCH), 2.13 (br, 36 H, AdCH_2), 3.64 (sept, J = 7 Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 5.98 (s, 6H, 4-*pz-H*), 7.27 (s, 2H, OHC=CHO) ppm. ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , $25\text{ }^{\circ}\text{C}$): δ = 23.55 (s, $\text{CH}(\text{CH}_3)_2$), 26.84 (s, $\text{CH}(\text{CH}_3)_2$), 28.90 (s, $\text{Ad-}\gamma$), 34.21 (s, $\text{Ad-}\alpha$), 36.84 (s, $\text{Ad-}\delta$), 42.16 (s, $\text{Ad-}\beta$), 98.11 (s, *pz-4C*), 133.54 (s, OHC=CHO), 157.11 (s, *pz-3C*), 163.65 (s, *pz-5C*) ppm. Anal. calcd. for (**2**) $\text{C}_{98}\text{H}_{142}\text{B}_2\text{N}_{12}\text{O}_2\text{Yb}_2$ (1887.93): C, 62.34; H, 7.58; N, 8.90; found: C, 62.72; H, 7.03; N, 8.51.

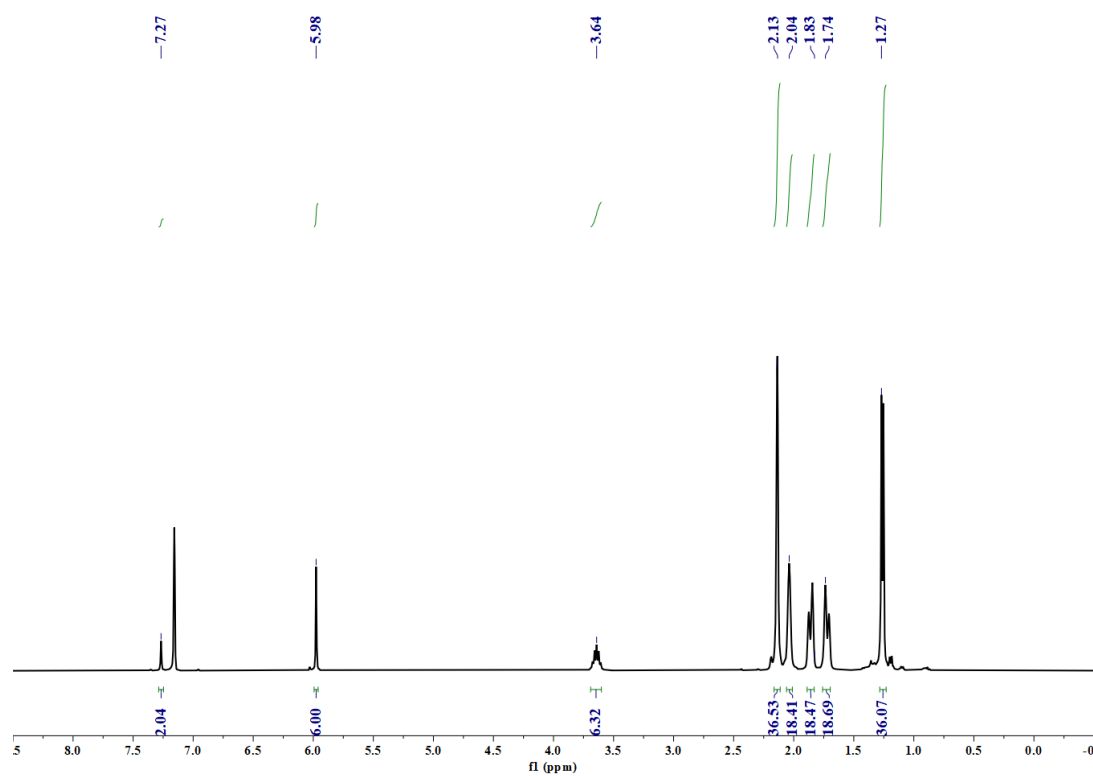


Figure S1. ^1H NMR spectrum (500 MHz) of $[(\text{Tp}^{\text{Ad,IPr}})\text{Yb}]_2(\text{cis-OCH=CHO})$ (**2**) in C_6D_6 at 25 °C.

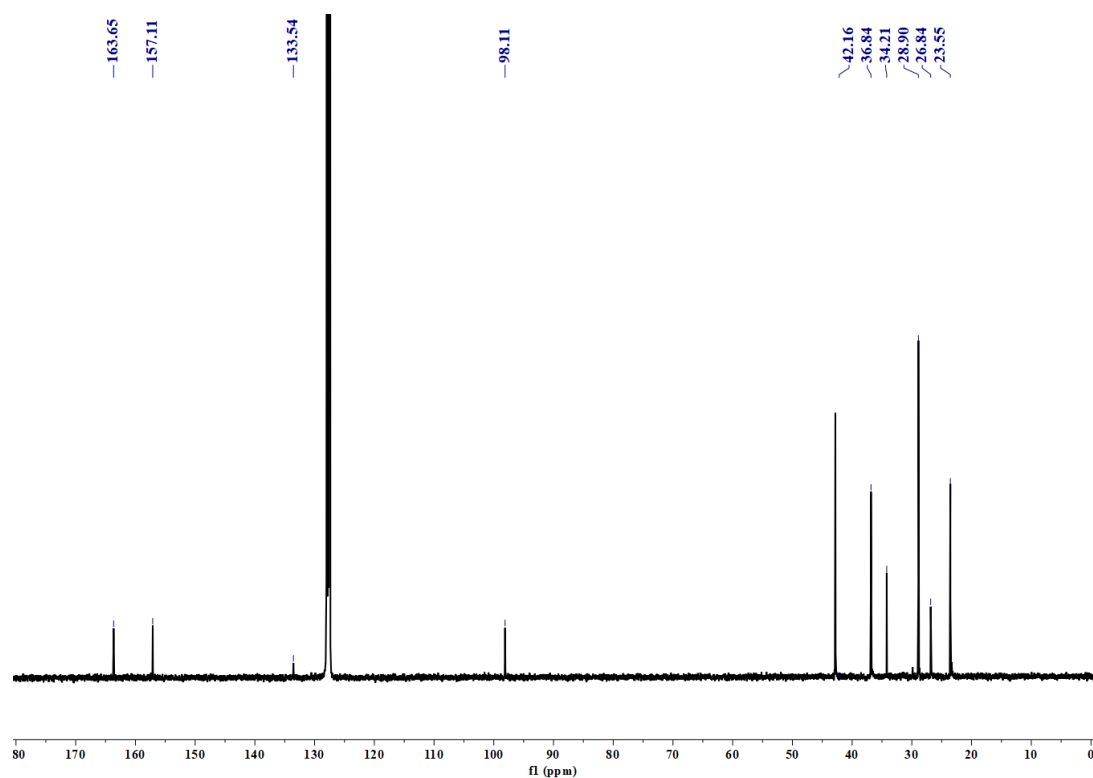


Figure S2. $^{13}\text{C} \{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Tp}^{\text{Ad,IPr}})\text{Yb}]_2(\text{cis-OCH=CHO})$ (**2**) in C_6D_6 at 25 °C.

Synthesis of $[(\text{Tp}^{\text{Ad},\text{Pr}})\text{Yb}(\kappa^2\text{-O}_2\text{CH})(\text{THF})]$ (**3**)

A solution of $[(\text{Tp}^{\text{Ad},\text{Pr}})\text{Yb}(\text{H})(\text{THF})]$ (**1**) (100 mg, 0.101 mmol) in hexane (10 mL)/THF (1 mL) was charged into J. Young valve NMR tube. The tube was frozen in liquid nitrogen, evacuated and backfilled with CO_2 (1 atm). Warmed up to room temperature, the solution changed from red-brown to pale-yellow in 5 minutes. After 30 minutes, the resulting solution was filtered. The filtrate was volatilized at room temperature overnight to give complex **3** (68 mg, 0.066 mmol, 65% yield) as pale-yellow crystals. Single crystals of complex **3** suitable for X-ray analysis were grown from benzene/pentane solution at room temperature.

^1H NMR (500 MHz, C_6D_6 , 25 °C): δ = 1.19 (d, $^3J_{\text{HH}}$ = 7 Hz, 18H, $\text{CH}(\text{CH}_3)_2$), 1.31 (m, 4 H, THF), 1.75, 1.90 (dd, $^3J_{\text{HH}}$ = 89, 12 Hz, 18H, AdCH_2), 2.10 (br, 9 H, AdCH), 2.14 (br, 18 H, AdCH_2), 3.35 (m, 4 H, THF), 3.62 (sept, $^3J_{\text{HH}}$ = 7 Hz, 3H, $\text{CH}(\text{CH}_3)_2$), 3.00 (s, 3 H, 4-pz-H), 9.47 (s, 1 H, OCHO) ppm. ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): δ = 23.15 (s, $\text{CH}(\text{CH}_3)_2$), 25.35 (s, THF), 26.73 (s, $\text{CH}(\text{CH}_3)_2$), 28.89 (s, Ad- γ), 34.17 (s, Ad- α), 36.64 (s, Ad- δ), 42.82 (s, Ad- β), 67.83 (s, THF), 97.69 (s, pz-4C), 156.37 (s, pz-3C), 163.15 (s, pz-5C), 173.24 (s, OCHO) ppm. Anal. calcd. for (**3**) $\text{C}_{53}\text{H}_{79}\text{B}_1\text{N}_6\text{O}_3\text{Yb}_1$ (1032.07): C, 61.68; H, 7.72; N, 8.14; found: C, 61.92; H, 7.83; N, 7.91.

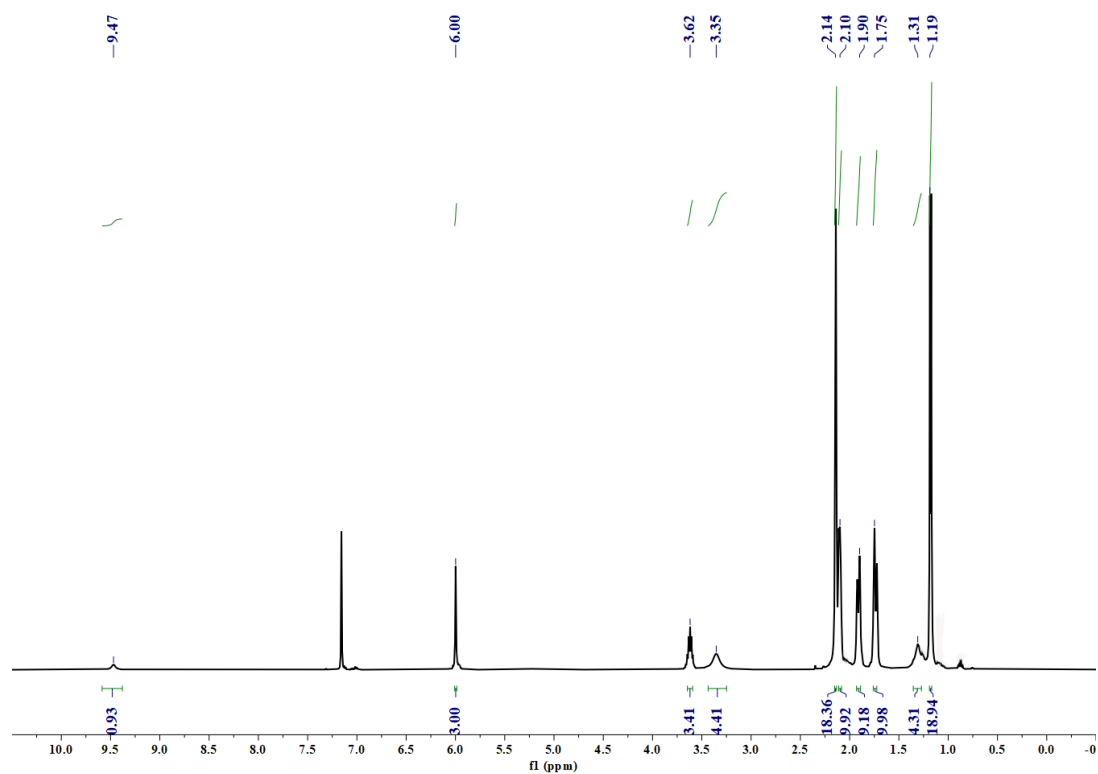


Figure S3. ¹H NMR spectrum (500 MHz) of [(Tp^{Ad,Pr})Yb(κ²-O₂CH)(THF)] (**3**) in C₆D₆ at 25 °C.

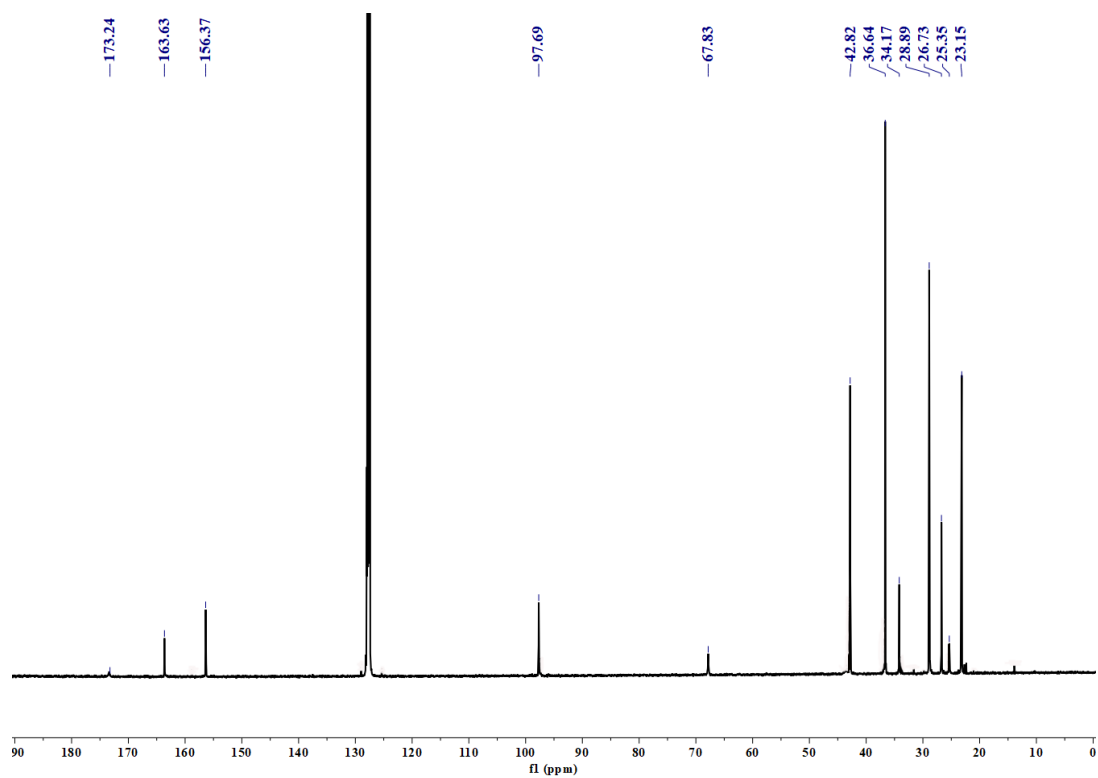


Figure S4. ¹³C {¹H} NMR spectrum (125 MHz) of [(Tp^{Ad,Pr})Yb(κ²-O₂CH)(THF)] (**3**) in C₆D₆ at 25 °C.

Synthesis of $[(\text{Tp}^{\text{Ad},i\text{Pr}})\text{Yb}^{\text{III}}]_2(\text{C}_2\text{S}_4)$ (**4**)

To a stirring solution of $[(\text{Tp}^{\text{Ad},i\text{Pr}})\text{Yb}(\text{H})(\text{THF})]$ (**1**) (100 mg, 0.101 mmol) in hexane (10 mL)/THF (1 mL) was added carbon disulfide (8 mg, 0.101 mmol). Upon addition, the solution immediately turned dark-green, with concomitant release of H_2 gas. After 30 minutes, the solution was filtered. The filtrate was concentrated to 2 mL and kept at $-30\text{ }^\circ\text{C}$ to give complex **4** (48 mg, 0.02 mmol, 45 % yield) as yellow-greenish crystals. Single crystals of complex **4** suitable for X-ray analysis were grown from a concentrated hexane solution at $-30\text{ }^\circ\text{C}$.

^1H NMR (500 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$): $\delta = 1.18, 1.33, 1.77, 2.16, 10.18, 11.98, 16.18$ ppm. Due to the paramagnetic nature of complex **4**, no useful information could be obtained from the NMR spectra. Anal. calcd. for (**4**) $\text{C}_{106}\text{H}_{156}\text{B}_2\text{N}_{12}\text{O}_2\text{S}_4\text{Yb}_2$ (2126.36): C, 59.87; H, 7.39 N, 7.90; found: C, 60.35; H, 7.03; N, 7.11.

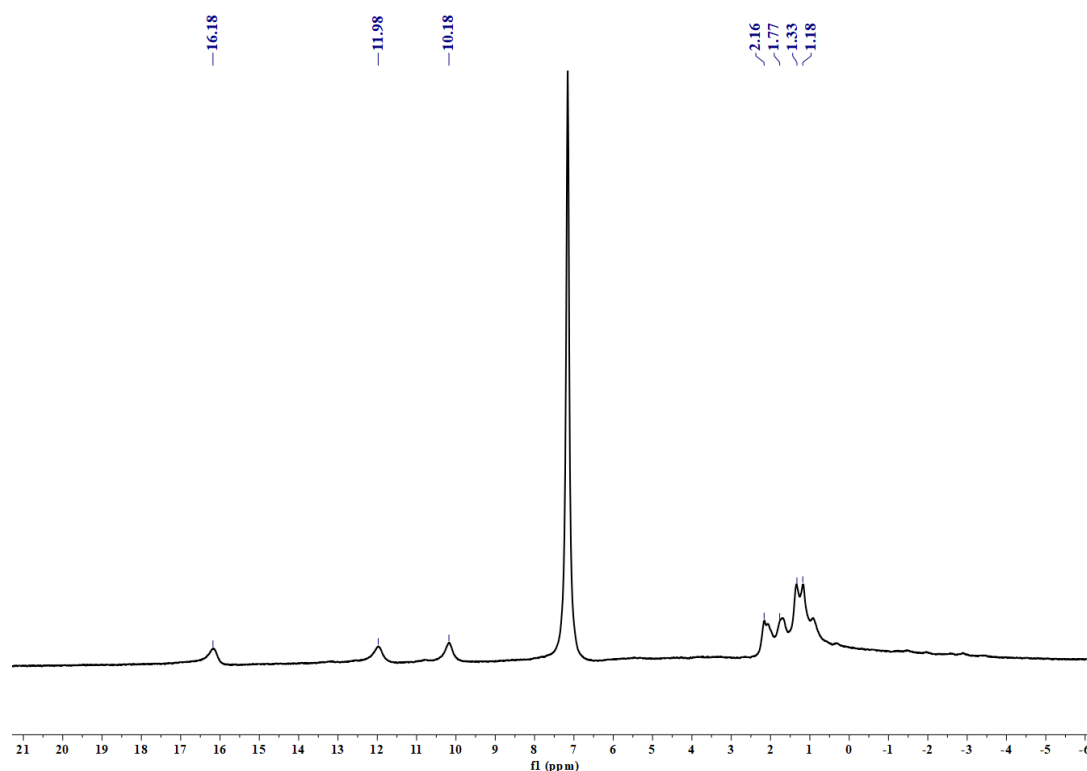


Figure S5. ^1H NMR spectrum (500 MHz) of $[(\text{Tp}^{\text{Ad},i\text{Pr}})\text{Yb}^{\text{III}}]_2(\text{C}_2\text{S}_4)$ (**4**) in C_6D_6 at $25\text{ }^\circ\text{C}$.

X-ray Crystallographic Studies

Single crystals suitable for X-ray analysis were obtained as described in the preparation. The crystals were manipulated in the glovebox under a microscope in the glovebox. Data collection was performed at - 80 °C on D8 Venture diffractometer with a CCD area detector, using graphite monochromated Mo K_{α} radiation ($\lambda = 0.71073$ Å). The determination of the crystal class and unit cell parameters was carried out by the SMART program packages². The raw frame data were processed using SAINT³ and absorption corrections using SADABS⁴ to yield the reflection data file. The structures were solved by using SHELXS-2018,⁵ SUPERFLIP⁶⁻⁷ or Sir 97⁸ in the WinGX program package.⁹ Refinements were performed on F^2 anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method using SHELXL-2018 program.⁵

Refinement of **2**: The SQUEEZE¹⁰ routine of the program PLATON¹¹ was implemented to remove the contributions of three disordered benzene to the observed structure factors. The hydrogen atoms (H1 and H2) in the *cis*-OCH=CHO ligand were located by difference Fourier syntheses, and refined. Two of the six adamantyl groups in the Tp^{Ad,iPr} ligand were highly disordered. C18~C26 and C18'~C26' disordered over two sites with occupancies 0.649:0.351. C38~C46 and C38'~C46' disordered over two sites with occupancies 0.632:0.368.

Refinement of **3**: The hydrogen atom (H1) in the formate ligand was located by difference Fourier syntheses, and refined. One of the three adamantyl groups in the Tp^{Ad,iPr} ligand was highly disordered. C18~C26 and C18'~C26' disordered over two sites with occupancies 0.784:0.216.

Refinement of **4**: The SQUEEZE¹⁰ routine of the program PLATON¹¹ was implemented to remove the contributions of the disordered hexane to the observed structure factors.

Other hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. The residual electron densities were of no chemical significance. Crystal data and analysis results are listed in Table **S1-3**.

CCDC number 2080818 (**2**), 2080817 (**3**) and 2080819 (**4**) contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge on

application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement for complex **2**

CCDC number	2080818
Empirical formula	$C_{98}H_{142}B_2N_{12}O_2Yb_2 \cdot (3 \times \text{Benzene})$
Formula weight	1887.93
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	13.283(2) Å
b	13.301(3) Å
c	31.912(6) Å
α	94.556(6) °
β	99.241(6) °
γ	108.981(6) °
Volume	5209.5(18) Å ³
Z, Calculated density	2, 1.204 Mg/m ³
Absorption coefficient	1.832 mm ⁻¹
F(000)	1960
Crystal size	0.200 x 0.150 x 0.130 mm
Theta range for data collection	1.944 to 25.000 °
Limiting indices	-15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -37 ≤ l ≤ 37
Reflections collected / unique	122928 / 18206 [R(int) = 0.0956]
Completeness to theta	(25.000) 99.2 %
Absorption correction	Empirical
Max. and min. transmission	0.788 and 0.726
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	18206 / 101 / 1081
Goodness-of-fit on F ²	1.036
Final R indices [I > 2σ(I)]	R1 = 0.0489, wR2 = 0.1146
R indices (all data)	R1 = 0.0661, wR2 = 0.1237
Largest diff. peak and hole	2.147 and -1.484 e. Å ⁻³

Table S2. Crystal data and structure refinement for complex **3**

CCDC number	2080817
Empirical formula	C ₅₃ H ₇₉ B ₁ N ₆ O ₃ Yb ₁
Formula weight	1032.07
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	11.7981(11) Å
b	14.1667(13) Å
c	16.5848(13) Å
α	77.268(2) °
β	86.284(2) °
γ	68.546(3) °
Volume	2516.1(4) Å ³
Z, Calculated density	2, 1.362 Mg/m ³
Absorption coefficient	1.906 mm ⁻¹
F(000)	1076
Crystal size	0.200 x 0.160 x 0.130 mm
Theta range for data collection	2.675 to 24.999 °
Limiting indices	-14<= <i>h</i> <=14, -16<= <i>k</i> <=16, -19<= <i>l</i> <=19
Reflections collected / unique	98366 / 8794 [R(int) = 0.0466]
Completeness to theta	(24.999) 99.2 %
Absorption correction	Empirical
Max. and min. transmission	0.781 and 0.700
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8794 / 37 / 571
Goodness-of-fit on F ²	1.037
Final R indices [I>2σ(I)]	R1 = 0.0228, wR2 = 0.0541
R indices (all data)	R1 = 0.0253, wR2 = 0.0556
Largest diff. peak and hole	0.933 and -0.500 e. Å ⁻³

Table S3. Crystal data and structure refinement for complex **4**

CCDC number	2080819
Empirical formula	C ₁₀₆ H ₁₅₆ B ₂ N ₁₂ O ₂ S ₄ Yb ₂ • (Hexane)
Formula weight	2126.37
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	13.2709(12) Å
b	15.0463(14) Å
c	15.3231(15) Å
α	88.839(3) °
β	73.545(2) °
γ	75.808(2) °
Volume	2840.8(5) Å ³
Z, Calculated density	2, 1.243 Mg/m ³
Absorption coefficient	1.759 mm ⁻¹
F(000)	1106
Crystal size	0.180 x 0.140 x 0.120 mm
Theta range for data collection	2.085 to 24.997 °
Limiting indices	-15<=h<=15, -17<=k<=17, -18<=l<=18
Reflections collected / unique	114056 / 9931 [R(int) = 0.0523]
Completeness to theta	(24.997) 99.2 %
Absorption correction	Empirical
Max. and min. transmission	0.810 and 0.744
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9931 / 6 / 602
Goodness-of-fit on F ²	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0306, wR2 = 0.0719
R indices (all data)	R1 = 0.0346, wR2 = 0.0738
Largest diff. peak and hole	1.390 and -0.672 e. Å ⁻³

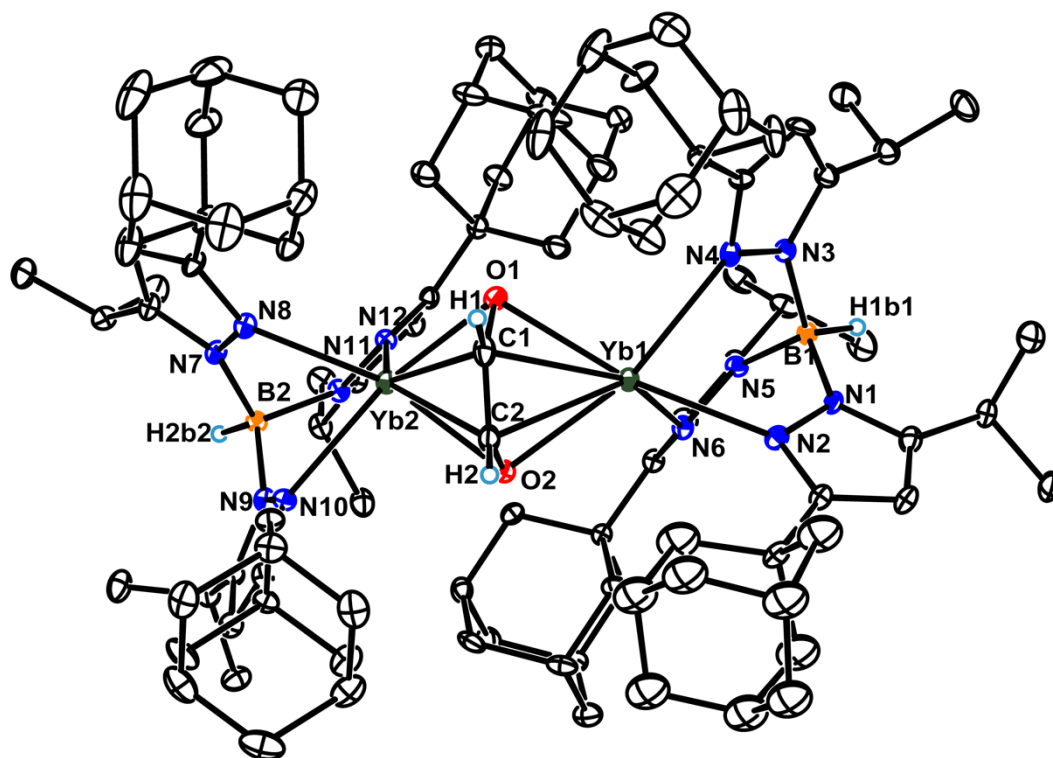


Figure S6. ORTEP drawing of $[(\text{Tp}^{\text{Ad,Pr}})\text{Yb}]_2(\text{cis-OCH=CHO})$ (**2**) with thermal ellipsoids drawn at the 20% probability level. All the hydrogen atoms in pyrazolyls are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: Yb1–O1 2.469(4), Yb1–C1 2.700(6), Yb1–C2 2.676(6), Yb1–O2 2.430(4), Yb1–N2 2.507(5), Yb1–N4 2.543(5), Yb1–N6 2.471(5), Yb2–O1 2.411(4), Yb2–C1 2.681(6), Yb2–C2 2.696(7), Yb2–O2 2.448(4), Yb2–N8 2.485(5), Yb2–N10 2.506(5), Yb2–N12 2.466(4), O1–C1 1.358(8), C1–C2 1.357(10), C2–O2 1.349(8), O1–C1–C2 119.9(6), C1–C2–O2 120.5(6).

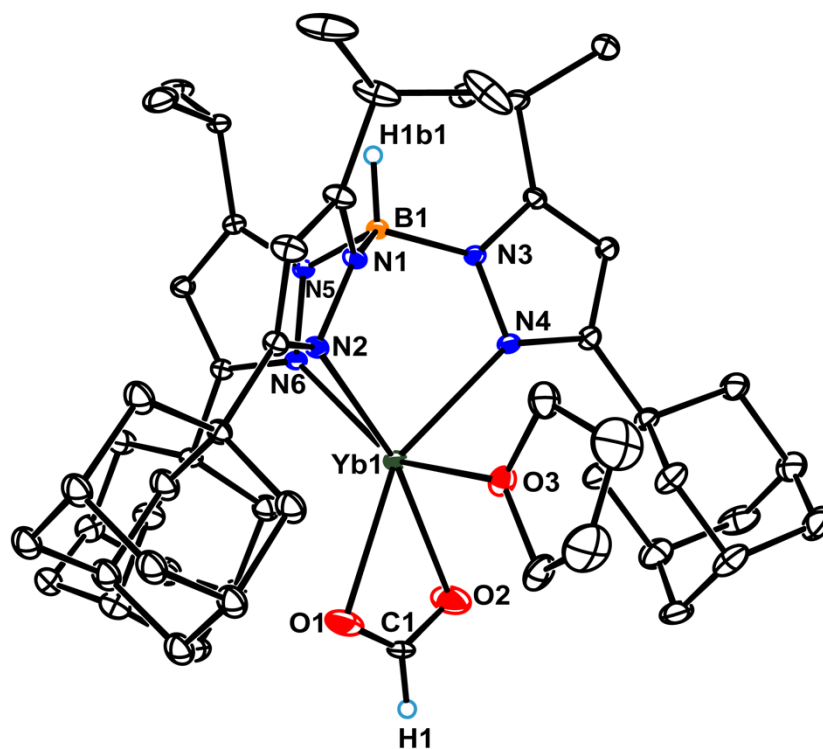


Figure S7. ORTEP drawing of $[(\text{Tp}^{\text{Ad},i\text{Pr}})\text{Yb}(\kappa^2\text{-O}_2\text{CH})(\text{THF})]$ (**3**) with thermal ellipsoids drawn at the 20% probability level. All the hydrogen atoms in pyrazolyls and THF are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: O1–C1 1.182(5), C1–O2 1.245(5), Yb1–O1 2.462(2), Yb1–O2 2.441(2), Yb1–O3 2.459(2), Yb1–N2 2.478(2), Yb1–N4 2.484(2), Yb1–N6 2.501(2), O1–C1–O2 125.5(3).

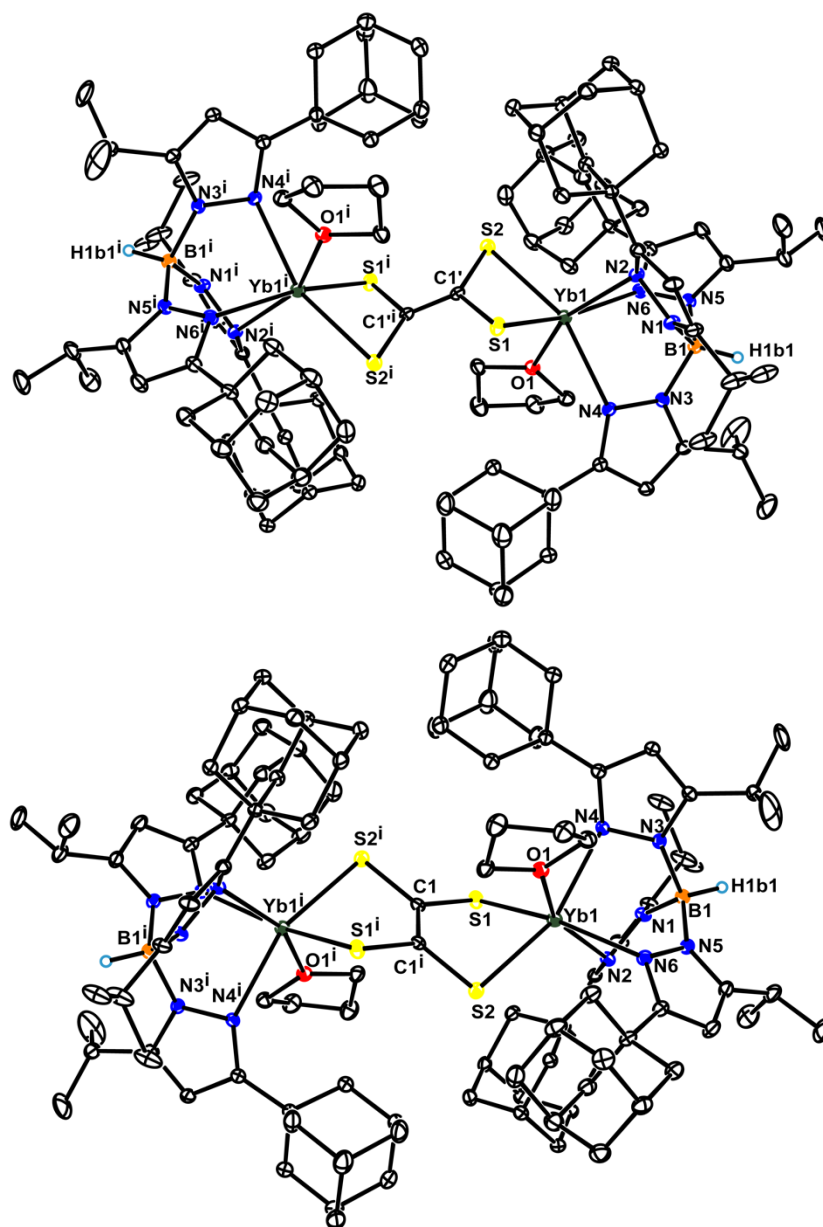


Figure S8. ORTEP drawing of $[(\text{Tp}^{\text{Ad},i\text{Pr}})\text{Yb}^{\text{III}}]_2(\text{C}_2\text{S}_4)$ (**4**) with thermal ellipsoids drawn at the 20% probability level. Two independent molecules were found in the unit cell. Except H1b1, all the hydrogen atoms are omitted for clarity. Selected interatomic distances [Å]: Yb1–S1 2.580(1), Yb1–S2 2.585(1), Yb1–O1 2.357(2), Yb1–N2 2.458(3), Yb1–N4 2.465(3), Yb1–N6 2.501(3), C1–S2ⁱ 1.776(5), C1–S1 1.807(5), C1ⁱ–C1 1.349(9), C1'–S2 1.796(13), C1'–S1 1.887(13), C1'–C1ⁱ 1.32(3).

Computational details

The optimization of reactants, transition states, IRC and products were carried out by employing DFT hybrid functional (B3PW91)¹² along with small core pseudopotential Stuttgart basis set¹³ for ytterbium atom and People basis set¹⁴⁻¹⁶ (6-31G**) for the rest of the atoms. Frequency calculations were performed to locate saddle points for transition state structures, minima for rest of the structures and for obtaining thermal corrections over the energies. All the calculations were performed using Gaussian 09 suite of programs.¹⁷

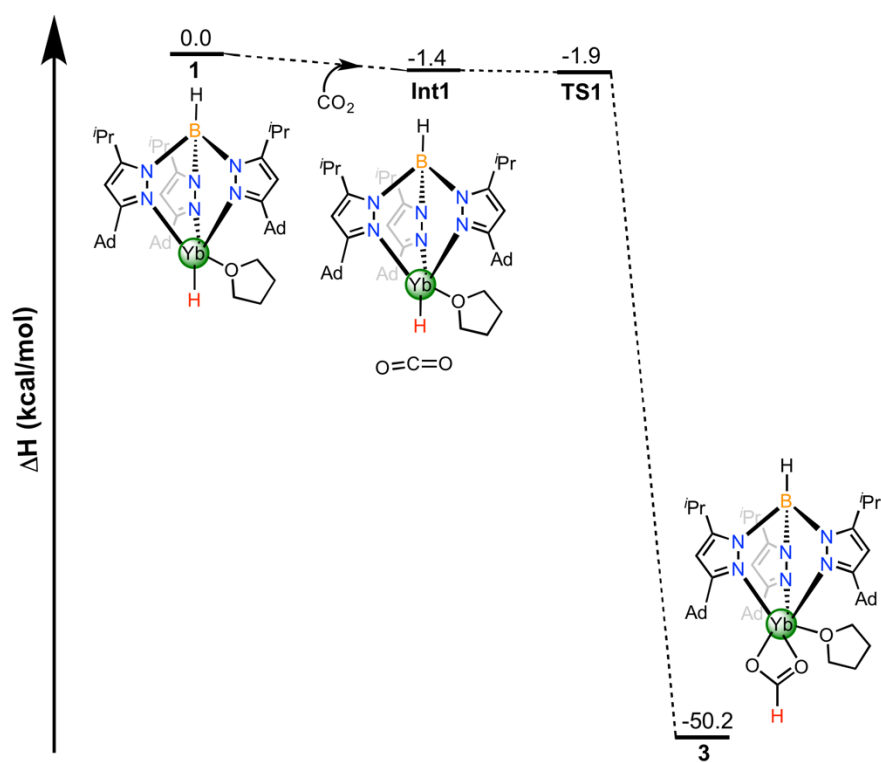


Figure S9. Computed enthalpy profile for the reaction of **1** with CO₂.

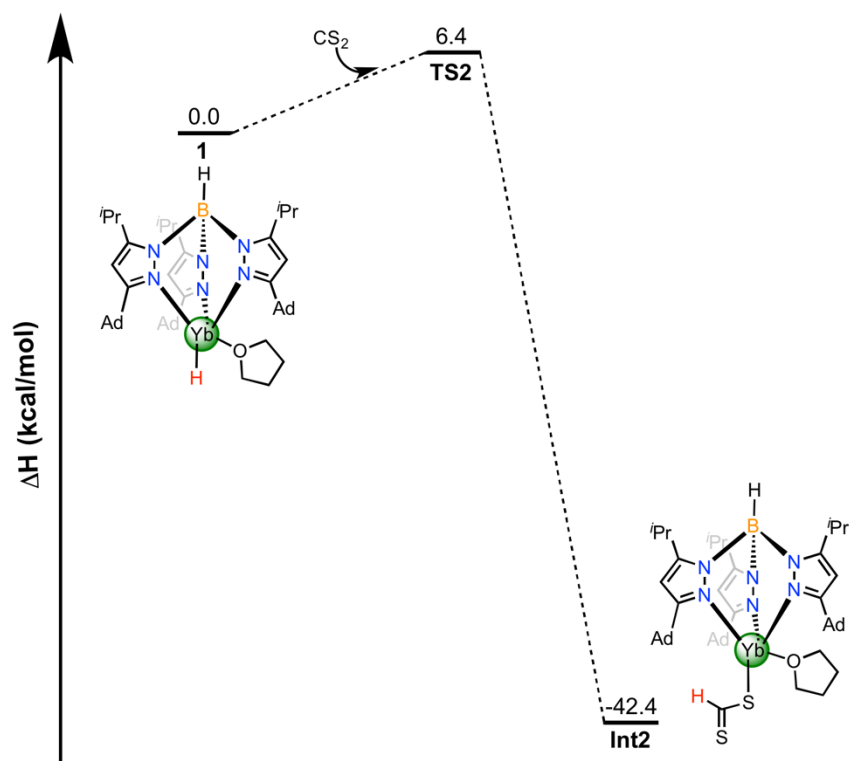


Figure S10. Computed enthalpy profile at room temperature for the insertion reaction of CS_2 with **1**

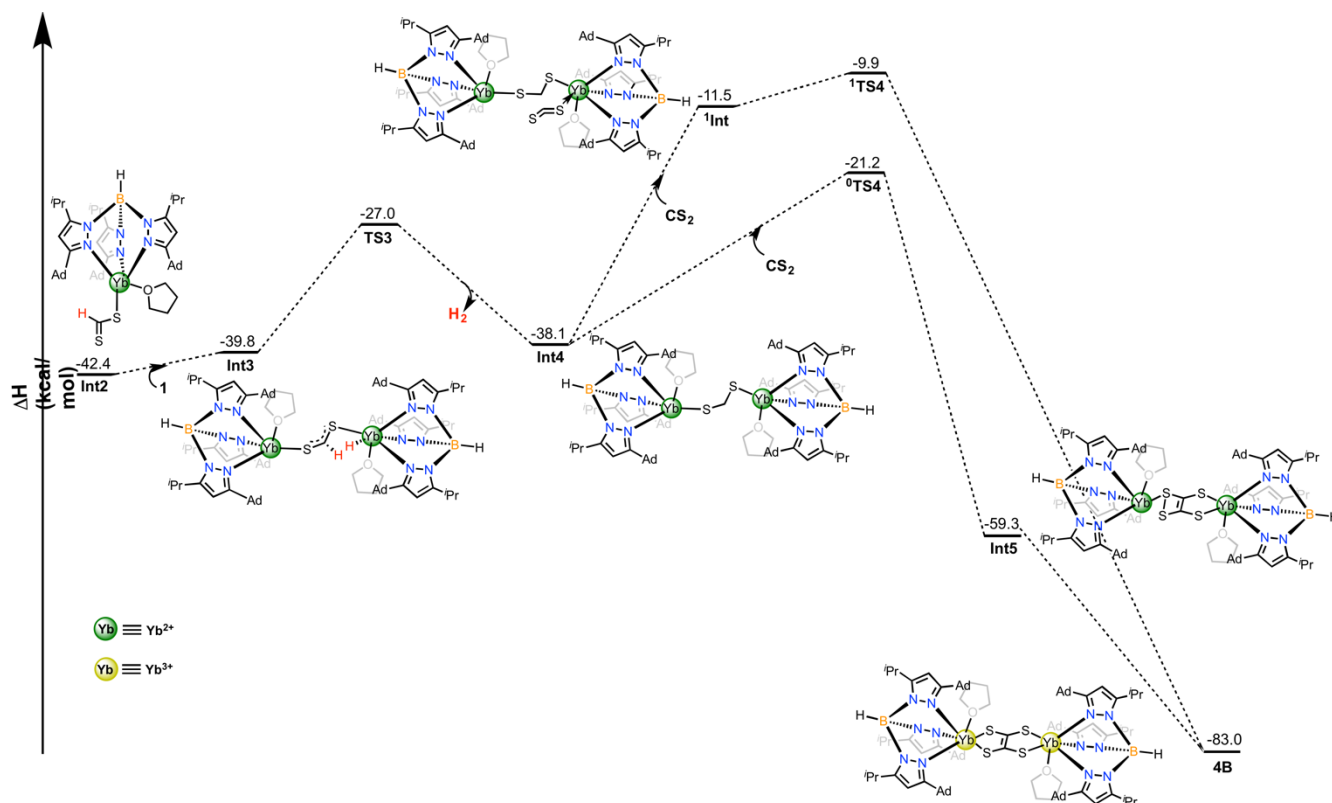


Figure S11. Computed enthalpy profile at room temperature for the H_2 release and C-C coupling reaction for both spin states ($s = 0, 1$) for **1**

Optimized coordinates

1

C	7.413781000	1.399405000	0.209286000
H	6.851644000	2.337568000	0.138288000
H	6.866656000	0.712623000	0.861311000
C	7.737491000	0.815924000	-1.163751000
H	6.959542000	1.033751000	-1.900409000
H	7.850077000	-0.272330000	-1.103202000
C	9.083900000	1.469789000	-1.487227000
H	9.664063000	0.920933000	-2.233943000
H	8.937078000	2.491758000	-1.853881000
C	9.759597000	1.482532000	-0.123020000
H	10.249245000	0.524424000	0.092967000
H	10.493588000	2.277495000	0.024841000
C	2.600724000	4.437716000	2.215382000
H	1.569770000	4.128793000	2.415474000
H	2.760557000	5.414592000	2.681441000
H	2.701486000	4.558645000	1.131038000
C	3.337881000	2.025655000	2.087465000
H	2.306578000	1.694442000	2.252015000
H	3.502743000	2.090900000	1.006108000
H	4.011539000	1.262473000	2.486817000
C	3.580521000	3.390855000	2.751688000
H	3.395106000	3.275579000	3.826703000
C	5.010306000	3.828192000	2.579656000
C	5.534726000	4.743035000	1.677323000
H	4.980504000	5.341148000	0.969190000
C	6.922646000	4.752966000	1.907566000
C	7.955227000	5.654386000	1.276092000
C	7.658472000	7.119812000	1.691108000
H	7.690482000	7.196512000	2.785486000
H	6.639382000	7.388386000	1.383995000
C	7.896096000	5.569684000	-0.266818000
H	8.104162000	4.537677000	-0.578593000
H	6.882769000	5.809508000	-0.614678000
C	9.386466000	5.308689000	1.729079000
H	9.638856000	4.279867000	1.434933000
H	9.453408000	5.363059000	2.823223000
C	10.327761000	6.162329000	-0.434960000
H	10.578917000	5.141903000	-0.754768000
H	11.065244000	6.831090000	-0.898506000
C	10.405348000	6.269048000	1.095701000
H	11.410263000	5.991371000	1.435826000
C	10.088914000	7.710304000	1.522951000
H	10.824153000	8.402155000	1.090559000
H	10.163677000	7.805296000	2.614241000
C	8.673533000	8.081384000	1.055883000
H	8.438304000	9.108117000	1.365506000
C	8.592019000	7.971961000	-0.474507000
H	9.299930000	8.669415000	-0.941863000
H	7.588815000	8.255544000	-0.820811000
C	8.911925000	6.531318000	-0.903111000
H	8.849555000	6.449630000	-1.996414000
C	3.161293000	-1.047769000	5.274325000
H	2.200085000	-0.876748000	5.770053000

H	2.978986000	-1.146779000	4.200033000
H	3.551302000	-2.003743000	5.640203000
C	4.372559000	0.221505000	7.091636000
H	3.430923000	0.389831000	7.626023000
H	4.824051000	-0.698152000	7.479253000
H	5.052257000	1.046785000	7.320721000
C	4.125660000	0.103160000	5.578972000
H	3.654791000	1.032452000	5.241520000
C	5.428890000	-0.056880000	4.840750000
C	6.089529000	-1.235876000	4.533256000
H	5.745396000	-2.239761000	4.732857000
C	7.294448000	-0.851951000	3.923666000
C	8.394762000	-1.767478000	3.447037000
C	8.836699000	-2.694058000	4.608252000
H	7.972840000	-3.260085000	4.979151000
H	9.194519000	-2.079400000	5.444232000
C	7.886839000	-2.658315000	2.285927000
H	7.564886000	-2.019799000	1.452052000
H	7.001592000	-3.219205000	2.612480000
C	9.630435000	-0.992427000	2.957482000
H	10.028394000	-0.362234000	3.766000000
H	9.347889000	-0.331629000	2.127457000
C	10.733885000	-1.954436000	2.490447000
H	11.593454000	-1.363815000	2.151444000
C	10.203871000	-2.822773000	1.339183000
H	9.923209000	-2.190798000	0.485042000
H	10.990369000	-3.502947000	0.985883000
C	8.986480000	-3.625864000	1.821947000
H	8.599842000	-4.243151000	1.000206000
C	9.402819000	-4.528421000	2.993900000
H	8.544901000	-5.123572000	3.335070000
H	10.173973000	-5.238599000	2.666815000
C	9.936529000	-3.660963000	4.144334000
H	10.227983000	-4.302952000	4.985815000
C	11.152946000	-2.858304000	3.659443000
H	11.557037000	-2.249674000	4.478817000
H	11.953973000	-3.539084000	3.341711000
C	4.942276000	5.497786000	6.388000000
H	3.930523000	5.822372000	6.656293000
H	5.631225000	6.323036000	6.598395000
H	4.968349000	5.307170000	5.311612000
C	5.248301000	4.517334000	8.694503000
H	4.225064000	4.795201000	8.967424000
H	5.530939000	3.636870000	9.279459000
H	5.902386000	5.344493000	8.991243000
C	5.340057000	4.247880000	7.189903000
H	4.622035000	3.455576000	6.947614000
C	6.713674000	3.771191000	6.796319000
C	7.921488000	3.999714000	7.439489000
H	8.063568000	4.517449000	8.375123000
C	8.906224000	3.407245000	6.631867000
C	10.400854000	3.366596000	6.856661000
C	11.131758000	4.307242000	5.865636000
H	10.935137000	3.983698000	4.834177000
H	10.741157000	5.328060000	5.976953000
C	10.954710000	1.935532000	6.663098000
H	10.437615000	1.247397000	7.345234000

H	10.750595000	1.596747000	5.639137000
C	10.737349000	3.827167000	8.291758000
H	10.364435000	4.848353000	8.448049000
H	10.221729000	3.182197000	9.016211000
C	12.252977000	3.793052000	8.537611000
H	12.455870000	4.122082000	9.565568000
C	12.951365000	4.735359000	7.545245000
H	12.604129000	5.766780000	7.697211000
H	14.035508000	4.733417000	7.722572000
C	12.648515000	4.277312000	6.111385000
H	13.138285000	4.949631000	5.394862000
C	13.162194000	2.843949000	5.904085000
H	12.946751000	2.519835000	4.878066000
H	14.251310000	2.809833000	6.045778000
C	12.471485000	1.904862000	6.905631000
H	12.835446000	0.879288000	6.759171000
C	12.773049000	2.361395000	8.340574000
H	12.296628000	1.684595000	9.063314000
H	13.854271000	2.323316000	8.530838000
B	5.988444000	2.496925000	4.628172000
N	6.051916000	3.324971000	3.301395000
N	7.222890000	3.884386000	2.878818000
N	6.213241000	0.972166000	4.412777000
N	7.355540000	0.484229000	3.846509000
N	6.987419000	3.065419000	5.664928000
N	8.329118000	2.849737000	5.558353000
O	8.689566000	1.686194000	0.823661000
Yb	9.035414000	2.228256000	3.250885000
H	4.883896000	2.630861000	5.070364000
H	11.130403000	2.241024000	2.937045000

Int1

C	7.212491000	9.653727000	5.650278000
C	10.735577000	9.691521000	7.676021000
H	10.396668000	8.656447000	7.811092000
H	9.894606000	10.283669000	7.310861000
C	11.398780000	10.225919000	8.937251000
H	11.396852000	11.321548000	8.937804000
H	10.897346000	9.884896000	9.847000000
C	12.825392000	9.689394000	8.792277000
H	12.867821000	8.638382000	9.098491000
H	13.560551000	10.243294000	9.382293000
C	13.072192000	9.821273000	7.291964000
H	13.496628000	10.796097000	7.026761000
H	13.711748000	9.035212000	6.881343000
C	17.057724000	10.224225000	5.416494000
H	18.122534000	9.971150000	5.368075000
H	16.839289000	10.570541000	6.432891000
H	16.480089000	9.313044000	5.238187000
C	17.564194000	12.567968000	4.624851000
H	18.627829000	12.324353000	4.538323000
H	17.334329000	13.352881000	3.898103000
H	17.402359000	12.976552000	5.628563000
C	16.714417000	11.316531000	4.390579000
H	16.958000000	10.925590000	3.394804000
C	15.242996000	11.632809000	4.408603000
C	14.595864000	12.723203000	4.973661000

H	15.060589000	13.565939000	5.463460000
C	13.223647000	12.514716000	4.742208000
C	12.078017000	13.449323000	5.044078000
C	12.137067000	13.949048000	6.505804000
H	13.105647000	14.429460000	6.696215000
H	12.069365000	13.090004000	7.186448000
C	12.179738000	14.682324000	4.107385000
H	13.151926000	15.171320000	4.251776000
H	12.146505000	14.343902000	3.063847000
C	10.708150000	12.782942000	4.810053000
H	10.642594000	12.429814000	3.771973000
H	10.599133000	11.910927000	5.470196000
C	9.564884000	13.770652000	5.091019000
H	8.609375000	13.260661000	4.923780000
C	9.689988000	14.978765000	4.150593000
H	9.610966000	14.653474000	3.104759000
H	8.866025000	15.682401000	4.329396000
C	11.039807000	15.672966000	4.387466000
H	11.137890000	16.533238000	3.712462000
C	11.123776000	16.148148000	5.846145000
H	10.325044000	16.872384000	6.054417000
H	12.077095000	16.665284000	6.020913000
C	10.996505000	14.939857000	6.787081000
H	11.062100000	15.276589000	7.830141000
C	9.646496000	14.246976000	6.549014000
H	8.822806000	14.940114000	6.765430000
H	9.529848000	13.393564000	7.229926000
C	16.361525000	6.912054000	1.149536000
H	17.308112000	7.003270000	0.605263000
H	16.002211000	5.883471000	1.036728000
H	15.627766000	7.572928000	0.679942000
C	17.594522000	6.330847000	3.276517000
H	18.558603000	6.438111000	2.768570000
H	17.739106000	6.561041000	4.336341000
H	17.299075000	5.279153000	3.196991000
C	16.553490000	7.254930000	2.635726000
H	16.933134000	8.280026000	2.698322000
C	15.237964000	7.196279000	3.367281000
C	14.653475000	6.090601000	3.968430000
H	15.078391000	5.101988000	4.045275000
C	13.405589000	6.522107000	4.439997000
C	12.343208000	5.702300000	5.138330000
C	10.992115000	5.797978000	4.389016000
H	11.128069000	5.474842000	3.349004000
H	10.637372000	6.838515000	4.357450000
C	12.131776000	6.182864000	6.593433000
H	11.844674000	7.240704000	6.587986000
H	13.082722000	6.109912000	7.139511000
C	12.759875000	4.215543000	5.185002000
H	13.715339000	4.118268000	5.717959000
H	12.922039000	3.846329000	4.163671000
C	11.688682000	3.366166000	5.885258000
H	12.018938000	2.319261000	5.903360000
C	10.363435000	3.478501000	5.117401000
H	10.486156000	3.097577000	4.094562000
H	9.593828000	2.860204000	5.598630000
C	9.919563000	4.947671000	5.086036000

H	8.976772000	5.042670000	4.533655000
C	9.726693000	5.460900000	6.521091000
H	8.943519000	4.881282000	7.027827000
H	9.388828000	6.505054000	6.493962000
C	11.051404000	5.340786000	7.291031000
H	10.917108000	5.706790000	8.318148000
C	11.493445000	3.870090000	7.323434000
H	12.429208000	3.767853000	7.889935000
H	10.739559000	3.259566000	7.838134000
C	15.252486000	10.465011000	-1.603521000
H	16.263030000	10.740635000	-1.922099000
H	15.068606000	9.430174000	-1.907700000
H	14.551325000	11.107039000	-2.147766000
C	15.365805000	12.102655000	0.314916000
H	16.361267000	12.423644000	-0.012068000
H	14.626003000	12.764326000	-0.148590000
H	15.299988000	12.235504000	1.398309000
C	15.108442000	10.641810000	-0.089243000
H	15.873820000	10.023440000	0.394035000
C	13.759017000	10.180177000	0.395414000
C	12.567455000	10.113934000	-0.311920000
H	12.428534000	10.332631000	-1.358998000
C	11.594899000	9.693958000	0.609892000
C	10.122698000	9.450268000	0.366444000
C	9.714972000	8.028851000	0.822266000
H	9.917654000	7.913426000	1.894339000
H	10.330155000	7.287091000	0.295538000
C	9.252855000	10.474292000	1.136506000
H	9.537938000	11.492801000	0.839626000
H	9.433135000	10.379800000	2.216835000
C	9.803921000	9.586556000	-1.138273000
H	10.414112000	8.873377000	-1.708762000
H	10.078130000	10.592697000	-1.483281000
C	8.313251000	9.336983000	-1.409071000
H	8.123453000	9.438690000	-2.485888000
C	7.476251000	10.367770000	-0.636573000
H	6.407307000	10.211746000	-0.835188000
H	7.720379000	11.383274000	-0.977894000
C	7.759956000	10.228085000	0.865932000
H	7.170136000	10.966182000	1.425125000
C	7.389016000	8.811839000	1.333074000
H	7.577055000	8.711230000	2.408564000
H	6.318140000	8.630656000	1.168238000
C	8.222268000	7.782478000	0.554045000
H	7.961785000	6.769950000	0.888877000
C	7.939555000	7.919763000	-0.949079000
H	8.517163000	7.175726000	-1.514741000
H	6.878310000	7.724124000	-1.153815000
B	14.479863000	9.650599000	2.854492000
N	14.285171000	10.822472000	3.873908000
N	13.049769000	11.360904000	4.090292000
N	14.367303000	8.235054000	3.494714000
N	13.245343000	7.824606000	4.155583000
N	13.488497000	9.803652000	1.675024000
N	12.162938000	9.514743000	1.811003000
O	7.589144000	10.631172000	6.177673000
O	6.692619000	8.707826000	5.202393000

O	11.771103000	9.714537000	6.668994000
Yb	11.427545000	9.495698000	4.195484000
H	9.351332000	9.158831000	4.531125000
H	15.589867000	9.751120000	2.418647000

TS1

C	7.436768000	9.612976000	5.540322000
C	10.745433000	9.704558000	7.694163000
H	10.403253000	8.671144000	7.833598000
H	9.904150000	10.300888000	7.336660000
C	11.423469000	10.236616000	8.948337000
H	11.426205000	11.332232000	8.948499000
H	10.929385000	9.898086000	9.862999000
C	12.846245000	9.693938000	8.789812000
H	12.887162000	8.642723000	9.095514000
H	13.589382000	10.244731000	9.372685000
C	13.079256000	9.825050000	7.287418000
H	13.503083000	10.799064000	7.018324000
H	13.713064000	9.037548000	6.870756000
C	17.054904000	10.227489000	5.416445000
H	18.119771000	9.974956000	5.366873000
H	16.837720000	10.575018000	6.432687000
H	16.477590000	9.315697000	5.240197000
C	17.559153000	12.570366000	4.620771000
H	18.622756000	12.327011000	4.533331000
H	17.328166000	13.354019000	3.893025000
H	17.398356000	12.980468000	5.624021000
C	16.709635000	11.318213000	4.389520000
H	16.951952000	10.925954000	3.393926000
C	15.238093000	11.633831000	4.409115000
C	14.591143000	12.726394000	4.970259000
H	15.056070000	13.571627000	5.455513000
C	13.218624000	12.516303000	4.741896000
C	12.072640000	13.451523000	5.040174000
C	12.130227000	13.955868000	6.500364000
H	13.098719000	14.436731000	6.690209000
H	12.061607000	13.098997000	7.183648000
C	12.175559000	14.681493000	4.099555000
H	13.147684000	15.170779000	4.243429000
H	12.143416000	14.339734000	3.057045000
C	10.702856000	12.784605000	4.806860000
H	10.638656000	12.428096000	3.769701000
H	10.591894000	11.915819000	5.470897000
C	9.559293000	13.773356000	5.082919000
H	8.604517000	13.262115000	4.916962000
C	9.685914000	14.978396000	4.138827000
H	9.608146000	14.650013000	3.093819000
H	8.861809000	15.682663000	4.314316000
C	11.035501000	15.673204000	4.375160000
H	11.134738000	16.531300000	3.697553000
C	11.117987000	16.152933000	5.832441000
H	10.319127000	16.877908000	6.037516000
H	12.071189000	16.670537000	6.006584000
C	10.989358000	14.947640000	6.777053000
H	11.053876000	15.287669000	7.819106000
C	9.639569000	14.254201000	6.539468000
H	8.815781000	14.948183000	6.752672000

H	9.521549000	13.402775000	7.222501000
C	16.346352000	6.903508000	1.159342000
H	17.293339000	6.991251000	0.615236000
H	15.983352000	5.876227000	1.046558000
H	15.615107000	7.567038000	0.689559000
C	17.577555000	6.318449000	3.286364000
H	18.541956000	6.422756000	2.778450000
H	17.722850000	6.548164000	4.346192000
H	17.278863000	5.267686000	3.206762000
C	16.539476000	7.245802000	2.645518000
H	16.922329000	8.269714000	2.708129000
C	15.223813000	7.191329000	3.377123000
C	14.636329000	6.087909000	3.979590000
H	15.058525000	5.098233000	4.057457000
C	13.389732000	6.523056000	4.450953000
C	12.325576000	5.706639000	5.150584000
C	10.974332000	5.804586000	4.401817000
H	11.109062000	5.479815000	3.362116000
H	10.622153000	6.846013000	4.369277000
C	12.116006000	6.189170000	6.605344000
H	11.831593000	7.247752000	6.599193000
H	13.067086000	6.114456000	7.150952000
C	12.738688000	4.218903000	5.198550000
H	13.694129000	4.119936000	5.731227000
H	12.899500000	3.848260000	4.177517000
C	11.665758000	3.372870000	5.900178000
H	11.993573000	2.325224000	5.919123000
C	10.340458000	3.487649000	5.132770000
H	10.461815000	3.105372000	4.110264000
H	9.569570000	2.871736000	5.614918000
C	9.899917000	4.957806000	5.100356000
H	8.957060000	5.054829000	4.548596000
C	9.709021000	5.472625000	6.535079000
H	8.925166000	4.894698000	7.042544000
H	9.371986000	6.516899000	6.507576000
C	11.033919000	5.350420000	7.304294000
H	10.901134000	5.717815000	8.331080000
C	11.472600000	3.878740000	7.337956000
H	12.408452000	3.774785000	7.904009000
H	10.717544000	3.270604000	7.853703000
C	15.243967000	10.461327000	-1.594594000
H	16.255117000	10.734407000	-1.913406000
H	15.057950000	9.426495000	-1.897476000
H	14.544285000	11.104151000	-2.139784000
C	15.360114000	12.101246000	0.321827000
H	16.356148000	12.420024000	-0.005518000
H	14.621568000	12.763655000	-0.142604000
H	15.294464000	12.235688000	1.405042000
C	15.100247000	10.640343000	-0.080508000
H	15.864440000	10.021158000	0.403513000
C	13.750027000	10.181578000	0.404658000
C	12.557557000	10.121633000	-0.301665000
H	12.418100000	10.345432000	-1.347563000
C	11.584631000	9.701362000	0.619340000
C	10.113907000	9.452301000	0.372012000
C	9.732713000	8.000315000	0.748716000
H	9.948841000	7.827467000	1.810369000

H	10.356220000	7.300658000	0.176124000
C	9.231797000	10.416286000	1.202033000
H	9.497369000	11.454625000	0.961104000
H	9.416646000	10.266059000	2.275552000
C	9.783807000	9.666940000	-1.121134000
H	10.399797000	8.994584000	-1.733385000
H	10.042581000	10.694232000	-1.411441000
C	8.295734000	9.408907000	-1.397717000
H	8.097907000	9.567581000	-2.466146000
C	7.446345000	10.380203000	-0.564253000
H	6.378994000	10.217793000	-0.766064000
H	7.671677000	11.417335000	-0.848625000
C	7.741299000	10.160267000	0.926365000
H	7.143231000	10.855243000	1.529956000
C	7.395916000	8.713904000	1.313966000
H	7.586253000	8.557168000	2.382194000
H	6.327597000	8.524923000	1.141966000
C	8.242541000	7.744193000	0.475201000
H	8.000844000	6.709920000	0.752849000
C	7.948774000	7.961822000	-1.016639000
H	8.535460000	7.260965000	-1.626359000
H	6.889831000	7.759740000	-1.226681000
B	14.472023000	9.646968000	2.861825000
N	14.279954000	10.820539000	3.879549000
N	13.044641000	11.359408000	4.095619000
N	14.356133000	8.232572000	3.503513000
N	13.233147000	7.825848000	4.165063000
N	13.479690000	9.801552000	1.683136000
N	12.153035000	9.516504000	1.819711000
O	7.755058000	10.629259000	6.042958000
O	6.874404000	8.653918000	5.167441000
O	11.771802000	9.720913000	6.676670000
Yb	11.423330000	9.499061000	4.205783000
H	9.346399000	9.142351000	4.554687000
H	15.581924000	9.744272000	2.425252000

3

C	8.658884000	9.533963000	4.977446000
C	10.828855000	9.792403000	7.784836000
H	10.413645000	8.787208000	7.933488000
H	10.024894000	10.464714000	7.476573000
C	11.605899000	10.261212000	9.007543000
H	11.668804000	11.354392000	9.023744000
H	11.147078000	9.930860000	9.943352000
C	12.986274000	9.648321000	8.757415000
H	12.989623000	8.589662000	9.039388000
H	13.788896000	10.148157000	9.306305000
C	13.136758000	9.801380000	7.247807000
H	13.568279000	10.770933000	6.973468000
H	13.722444000	9.006617000	6.778906000
C	16.917347000	10.081562000	5.411587000
H	17.968555000	9.776012000	5.367618000
H	16.718016000	10.456558000	6.421770000
H	16.296724000	9.196165000	5.249011000
C	17.544423000	12.379067000	4.574423000
H	18.593122000	12.076607000	4.490792000
H	17.355015000	13.160984000	3.832985000

H	17.407543000	12.815403000	5.570128000
C	16.627592000	11.170972000	4.366255000
H	16.847262000	10.748660000	3.377520000
C	15.175672000	11.567350000	4.379226000
C	14.593202000	12.711241000	4.905716000
H	15.109153000	13.540174000	5.365019000
C	13.211443000	12.585295000	4.670545000
C	12.119921000	13.588175000	4.977093000
C	11.416898000	13.263839000	6.317927000
H	12.164147000	13.255960000	7.124197000
H	10.979847000	12.261442000	6.261481000
C	12.722747000	15.007346000	5.088130000
H	13.472940000	15.031515000	5.889851000
H	13.242973000	15.260344000	4.154848000
C	11.054083000	13.600615000	3.857008000
H	11.538898000	13.823287000	2.897700000
H	10.599586000	12.609015000	3.764901000
C	9.960618000	14.635559000	4.161494000
H	9.219134000	14.617697000	3.352338000
C	10.586685000	16.033961000	4.259352000
H	11.059608000	16.305209000	3.305678000
H	9.810475000	16.785663000	4.456905000
C	11.629542000	16.044508000	5.386770000
H	12.090275000	17.038845000	5.456351000
C	10.947054000	15.697187000	6.718733000
H	10.174348000	16.441983000	6.952212000
H	11.679331000	15.729040000	7.537510000
C	10.321011000	14.298451000	6.619557000
H	9.838091000	14.041805000	7.572187000
C	9.278195000	14.276852000	5.490965000
H	8.474625000	14.993786000	5.708620000
H	8.824449000	13.281198000	5.418991000
C	16.108009000	6.937048000	1.037467000
H	17.023648000	7.030020000	0.442832000
H	15.734745000	5.912924000	0.929304000
H	15.354666000	7.610515000	0.619770000
C	17.454690000	6.313382000	3.080836000
H	18.389949000	6.426784000	2.522865000
H	17.658294000	6.522151000	4.135387000
H	17.150014000	5.264648000	2.996821000
C	16.385413000	7.254170000	2.515865000
H	16.776001000	8.275612000	2.573143000
C	15.112859000	7.191032000	3.319843000
C	14.581899000	6.091100000	3.975398000
H	15.031171000	5.113834000	4.054751000
C	13.353740000	6.511161000	4.506902000
C	12.342640000	5.657077000	5.241638000
C	11.105179000	5.407549000	4.341971000
H	11.431492000	4.938554000	3.404333000
H	10.636548000	6.362519000	4.080468000
C	11.871507000	6.318027000	6.555195000
H	11.436070000	7.299744000	6.342817000
H	12.741388000	6.487297000	7.205476000
C	12.956906000	4.283603000	5.593888000
H	13.846851000	4.426704000	6.221894000
H	13.288542000	3.781564000	4.675693000
C	11.935793000	3.393680000	6.318463000

H	12.407424000	2.431181000	6.556868000
C	10.722538000	3.163689000	5.404742000
H	11.034753000	2.647987000	4.486406000
H	9.991889000	2.513081000	5.904088000
C	10.081918000	4.516297000	5.062556000
H	9.217779000	4.362279000	4.403686000
C	9.625353000	5.214113000	6.353128000
H	8.872766000	4.601056000	6.867682000
H	9.157462000	6.174469000	6.105890000
C	10.838903000	5.432608000	7.270833000
H	10.516674000	5.931966000	8.194939000
C	11.478908000	4.079977000	7.614209000
H	12.335293000	4.224529000	8.287334000
H	10.758590000	3.443134000	8.145073000
C	14.964309000	10.552192000	-1.621177000
H	15.960451000	10.858583000	-1.956393000
H	14.794873000	9.522642000	-1.950821000
H	14.236366000	11.194435000	-2.128869000
C	15.092934000	12.137049000	0.339944000
H	16.072174000	12.488068000	-0.004667000
H	14.327153000	12.795107000	-0.084863000
H	15.054374000	12.238688000	1.427877000
C	14.855641000	10.682946000	-0.099407000
H	15.645923000	10.067648000	0.346500000
C	13.528913000	10.179045000	0.405366000
C	12.329059000	10.078675000	-0.283154000
H	12.167936000	10.294321000	-1.327565000
C	11.384379000	9.627493000	0.651975000
C	9.920294000	9.329000000	0.418853000
C	9.563527000	7.907356000	0.914377000
H	9.772598000	7.822856000	1.987178000
H	10.204648000	7.175186000	0.406179000
C	9.015956000	10.350846000	1.149747000
H	9.255116000	11.363382000	0.798456000
H	9.217496000	10.339636000	2.227921000
C	9.595138000	9.408387000	-1.089399000
H	10.229696000	8.700989000	-1.639805000
H	9.832473000	10.412817000	-1.464722000
C	8.113774000	9.098812000	-1.350298000
H	7.919455000	9.164416000	-2.429017000
C	7.239252000	10.118694000	-0.605034000
H	6.176729000	9.916084000	-0.795793000
H	7.443094000	11.132650000	-0.975223000
C	7.532123000	10.035600000	0.900447000
H	6.916341000	10.767667000	1.438881000
C	7.212430000	8.619069000	1.404506000
H	7.404982000	8.543298000	2.481251000
H	6.147985000	8.396908000	1.248395000
C	8.081312000	7.598276000	0.653946000
H	7.857793000	6.587347000	1.018647000
C	7.791475000	7.682580000	-0.851283000
H	8.395352000	6.944010000	-1.395878000
H	6.737899000	7.442736000	-1.048688000
B	14.318472000	9.631380000	2.833473000
N	14.172024000	10.802220000	3.862925000
N	12.967779000	11.419824000	4.056253000
N	14.232335000	8.217638000	3.474944000

N	13.153042000	7.805967000	4.205897000
N	13.290055000	9.790625000	1.687419000
N	11.974953000	9.464694000	1.845468000
O	9.235135000	10.654058000	4.897440000
O	9.209095000	8.429275000	4.702057000
O	11.794482000	9.739349000	6.714738000
Yb	11.331570000	9.535751000	4.261036000
H	7.602595000	9.515263000	5.313281000
H	15.410665000	9.728599000	2.354039000

TS2

C	7.087707000	9.926005000	5.451021000
C	10.643394000	9.843889000	7.697076000
H	10.158358000	8.861490000	7.734868000
H	9.892261000	10.575171000	7.392572000
C	11.363650000	10.172046000	8.998811000
H	11.470951000	11.255846000	9.118686000
H	10.833089000	9.785926000	9.873203000
C	12.732152000	9.521782000	8.780389000
H	12.675599000	8.443388000	8.966817000
H	13.517708000	9.934816000	9.418965000
C	12.982447000	9.797781000	7.302130000
H	13.451469000	10.775882000	7.141422000
H	13.583062000	9.033225000	6.802460000
C	16.877105000	10.288498000	5.499686000
H	17.939912000	10.026451000	5.455025000
H	16.654655000	10.620758000	6.519884000
H	16.292847000	9.385406000	5.302737000
C	17.412258000	12.638986000	4.748609000
H	18.474010000	12.386203000	4.665137000
H	17.194767000	13.437751000	4.033302000
H	17.247870000	13.032981000	5.757698000
C	16.551566000	11.400018000	4.488685000
H	16.797926000	11.022326000	3.488502000
C	15.083466000	11.731602000	4.500721000
C	14.441695000	12.812005000	5.089056000
H	14.908742000	13.634756000	5.609792000
C	13.070600000	12.630404000	4.830253000
C	11.943036000	13.576846000	5.161219000
C	11.890542000	13.861905000	6.680704000
H	12.861288000	14.246678000	7.020154000
H	11.715498000	12.919730000	7.216275000
C	12.190377000	14.920744000	4.425706000
H	13.167228000	15.325893000	4.719891000
H	12.236625000	14.735927000	3.344697000
C	10.570895000	13.034525000	4.717985000
H	10.586654000	12.825601000	3.640079000
H	10.343577000	12.088684000	5.232377000
C	9.457687000	14.044373000	5.040123000
H	8.498039000	13.623248000	4.719361000
C	9.726791000	15.362880000	4.300308000
H	9.729458000	15.194241000	3.215167000
H	8.924742000	16.083229000	4.509638000
C	11.080792000	15.931647000	4.749734000
H	11.284495000	16.870500000	4.218218000
C	11.053153000	16.190735000	6.263980000
H	10.275595000	16.927011000	6.507123000

H	12.010819000	16.617784000	6.591820000
C	10.779477000	14.872614000	7.005058000
H	10.763716000	15.054895000	8.087791000
C	9.425346000	14.305341000	6.553581000
H	8.619894000	15.010714000	6.797197000
H	9.204023000	13.373749000	7.091018000
C	16.196116000	7.141361000	1.146673000
H	17.145099000	7.239685000	0.607949000
H	15.817707000	6.126005000	0.986434000
H	15.476148000	7.837429000	0.707713000
C	17.418678000	6.441989000	3.243585000
H	18.384596000	6.557571000	2.741215000
H	17.566336000	6.619519000	4.313086000
H	17.106376000	5.400119000	3.113878000
C	16.393250000	7.411411000	2.647075000
H	16.789350000	8.426690000	2.756451000
C	15.077520000	7.342204000	3.377178000
C	14.493797000	6.236571000	3.975460000
H	14.917494000	5.246582000	4.055130000
C	13.243250000	6.669997000	4.444141000
C	12.196027000	5.828917000	5.130837000
C	10.891271000	6.606038000	5.381178000
H	10.477491000	6.958313000	4.423837000
H	11.096818000	7.484952000	6.006347000
C	12.728272000	5.317605000	6.492961000
H	12.975178000	6.176191000	7.131951000
H	13.662212000	4.762523000	6.336635000
C	11.860313000	4.597774000	4.251019000
H	12.774631000	4.023777000	4.054333000
H	11.487537000	4.940538000	3.276964000
C	10.818017000	3.704078000	4.940078000
H	10.601865000	2.842681000	4.294784000
C	9.531714000	4.508154000	5.180618000
H	9.110091000	4.844902000	4.224362000
H	8.772194000	3.874963000	5.657885000
C	9.845648000	5.717613000	6.073313000
H	8.936290000	6.307559000	6.235331000
C	10.400721000	5.227767000	7.419571000
H	9.653336000	4.606520000	7.930500000
H	10.606394000	6.082621000	8.078421000
C	11.687169000	4.422664000	7.182196000
H	12.090471000	4.075357000	8.142561000
C	11.375554000	3.214265000	6.285576000
H	12.284703000	2.619180000	6.124424000
H	10.647431000	2.557050000	6.779221000
C	15.045202000	10.847713000	-1.536494000
H	16.039709000	11.190289000	-1.839887000
H	14.914282000	9.821415000	-1.892704000
H	14.311164000	11.480036000	-2.047899000
C	15.081214000	12.390159000	0.462121000
H	16.058553000	12.775336000	0.150388000
H	14.308472000	13.037133000	0.032915000
H	15.013483000	12.465382000	1.550778000
C	14.895078000	10.940789000	-0.015613000
H	15.690386000	10.336791000	0.437423000
C	13.571810000	10.387948000	0.444339000
C	12.393924000	10.257782000	-0.274072000

H	12.245984000	10.486164000	-1.318896000
C	11.446130000	9.751778000	0.632490000
C	10.022794000	9.357501000	0.326418000
C	9.273198000	8.836290000	1.565674000
H	9.214000000	9.610223000	2.346552000
H	9.815762000	7.978864000	1.989640000
C	9.235462000	10.559095000	-0.250339000
H	9.754863000	10.950890000	-1.134557000
H	9.214414000	11.369359000	0.490223000
C	10.035725000	8.229604000	-0.739005000
H	10.597076000	7.370888000	-0.347721000
H	10.570507000	8.575553000	-1.632822000
C	8.605536000	7.811689000	-1.109227000
H	8.647921000	7.015886000	-1.864669000
C	7.852013000	9.024406000	-1.677250000
H	6.832422000	8.734759000	-1.964684000
H	8.350129000	9.384966000	-2.587702000
C	7.804416000	10.139376000	-0.620938000
H	7.269216000	11.008422000	-1.025595000
C	7.082765000	9.623994000	0.632836000
H	7.021609000	10.414458000	1.390996000
H	6.051797000	9.338109000	0.385059000
C	7.841032000	8.414310000	1.199939000
H	7.337337000	8.057201000	2.106005000
C	7.884419000	7.298064000	0.146044000
H	8.405351000	6.417434000	0.546005000
H	6.864529000	6.978452000	-0.106546000
B	14.317514000	9.802920000	2.885307000
N	14.123738000	10.951429000	3.927661000
N	12.890742000	11.498434000	4.140994000
N	14.205697000	8.381460000	3.505829000
N	13.082726000	7.970284000	4.164064000
N	13.317951000	9.968353000	1.715205000
N	12.011562000	9.592875000	1.835224000
S	6.587135000	11.060991000	4.473384000
S	7.040190000	8.841039000	6.600860000
O	11.676775000	9.811947000	6.685594000
Yb	11.247822000	9.651299000	4.224369000
H	9.163496000	9.735158000	4.798621000
H	15.425750000	9.911242000	2.444070000

Int2

C	-3.844561000	-0.917942000	1.180876000
C	-1.224777000	0.142042000	3.731528000
H	-1.614218000	-0.878384000	3.829275000
H	-2.029845000	0.776409000	3.355133000
C	-0.569131000	0.615957000	5.018475000
H	-0.522484000	1.710286000	5.046709000
H	-1.109242000	0.275914000	5.905798000
C	0.835503000	0.019776000	4.895933000
H	0.822521000	-1.040401000	5.172400000
H	1.579071000	0.522174000	5.520481000
C	1.129075000	0.183347000	3.407782000
H	1.594695000	1.150073000	3.184497000
H	1.753525000	-0.611604000	2.990660000
C	5.269008000	0.604671000	1.600049000
H	6.326547000	0.321921000	1.559579000

H	5.056232000	0.970455000	2.610696000
H	4.667249000	-0.292742000	1.431716000
C	5.843198000	2.923371000	0.779837000
H	6.899856000	2.649874000	0.698144000
H	5.635985000	3.705815000	0.043764000
H	5.691354000	3.347547000	1.778523000
C	4.960513000	1.692471000	0.558087000
H	5.196084000	1.282608000	-0.431776000
C	3.498314000	2.048391000	0.568457000
C	2.877766000	3.148164000	1.143412000
H	3.361638000	3.972359000	1.645576000
C	1.502612000	2.983172000	0.903789000
C	0.398477000	3.962957000	1.214136000
C	0.486317000	4.451733000	2.678756000
H	1.474352000	4.891639000	2.866721000
H	0.386852000	3.592851000	3.355943000
C	0.548624000	5.195793000	0.283150000
H	1.540688000	5.643771000	0.425606000
H	0.496195000	4.865157000	-0.762189000
C	-0.996497000	3.357503000	0.985845000
H	-1.084379000	3.011695000	-0.053917000
H	-1.136887000	2.488790000	1.642735000
C	-2.098265000	4.387602000	1.276169000
H	-3.072566000	3.914325000	1.109225000
C	-1.927761000	5.594122000	0.341017000
H	-2.026238000	5.277948000	-0.705975000
H	-2.720603000	6.330455000	0.527600000
C	-0.548962000	6.230455000	0.574426000
H	-0.417936000	7.089438000	-0.096584000
C	-0.438146000	6.693875000	2.035140000
H	-1.205214000	7.449291000	2.250852000
H	0.536525000	7.170432000	2.207889000
C	-0.611136000	5.487099000	2.970732000
H	-0.525646000	5.815051000	4.015042000
C	-1.989789000	4.851733000	2.736255000
H	-2.783103000	5.576639000	2.960970000
H	-2.137851000	4.000119000	3.413432000
C	4.552833000	-2.567135000	-2.697844000
H	5.508327000	-2.489371000	-3.228152000
H	4.156262000	-3.575516000	-2.857816000
H	3.850798000	-1.858723000	-3.145975000
C	5.746342000	-3.281215000	-0.589394000
H	6.718259000	-3.181962000	-1.083356000
H	5.887676000	-3.104677000	0.481111000
H	5.418283000	-4.317936000	-0.721088000
C	4.742882000	-2.295810000	-1.196691000
H	5.156314000	-1.287440000	-1.087028000
C	3.420375000	-2.340410000	-0.476819000
C	2.825973000	-3.427902000	0.142121000
H	3.245340000	-4.416700000	0.250347000
C	1.571748000	-2.981034000	0.586416000
C	0.528286000	-3.815288000	1.287962000
C	-0.817267000	-3.082746000	1.443899000
H	-1.198075000	-2.803612000	0.448413000
H	-0.670931000	-2.163711000	2.028120000
C	1.030686000	-4.218873000	2.697532000
H	1.216079000	-3.312995000	3.290455000

H	1.993210000	-4.738537000	2.606764000
C	0.278021000	-5.112282000	0.476370000
H	1.222384000	-5.655692000	0.348393000
H	-0.072317000	-4.847665000	-0.529910000
C	-0.748000000	-6.009884000	1.183122000
H	-0.900543000	-6.917817000	0.585269000
C	-2.075462000	-5.252200000	1.326179000
H	-2.473996000	-4.995969000	0.335389000
H	-2.825953000	-5.886618000	1.815103000
C	-1.849891000	-3.977452000	2.152202000
H	-2.792418000	-3.428223000	2.256787000
C	-1.323517000	-4.359067000	3.544233000
H	-2.063690000	-4.980286000	4.064665000
H	-1.182695000	-3.457693000	4.156237000
C	0.004298000	-5.116792000	3.404457000
H	0.386363000	-5.385689000	4.398048000
C	-0.219891000	-6.390724000	2.574953000
H	0.719652000	-6.952417000	2.482638000
H	-0.936643000	-7.049014000	3.083214000
C	3.500415000	1.166221000	-5.412301000
H	4.500126000	1.510985000	-5.695126000
H	3.380423000	0.138629000	-5.768505000
H	2.775785000	1.795074000	-5.941001000
C	3.488169000	2.714929000	-3.418592000
H	4.469522000	3.103317000	-3.712923000
H	2.721288000	3.356867000	-3.865434000
H	3.399267000	2.794500000	-2.331775000
C	3.318475000	1.263059000	-3.895065000
H	4.107160000	0.663917000	-3.424344000
C	1.988430000	0.705635000	-3.460810000
C	0.831509000	0.557442000	-4.208882000
H	0.715239000	0.775664000	-5.258941000
C	-0.136557000	0.044846000	-3.329001000
C	-1.562879000	-0.326897000	-3.666805000
C	-2.134183000	-1.384844000	-2.699804000
H	-2.153167000	-0.981545000	-1.676944000
H	-1.487558000	-2.272036000	-2.698594000
C	-2.480708000	0.921385000	-3.621326000
H	-2.084866000	1.688960000	-4.299631000
H	-2.469241000	1.346369000	-2.609309000
C	-1.614236000	-0.910028000	-5.100768000
H	-0.959095000	-1.789075000	-5.161296000
H	-1.225276000	-0.173388000	-5.814737000
C	-3.050913000	-1.283483000	-5.492100000
H	-3.048698000	-1.691287000	-6.511578000
C	-3.933345000	-0.026683000	-5.439244000
H	-4.961461000	-0.274358000	-5.735231000
H	-3.566162000	0.721290000	-6.155404000
C	-3.919225000	0.547501000	-4.014753000
H	-4.546137000	1.447462000	-3.971495000
C	-4.459731000	-0.504519000	-3.034639000
H	-4.472950000	-0.099424000	-2.015864000
H	-5.494249000	-0.765270000	-3.294982000
C	-3.573553000	-1.758919000	-3.091573000
H	-3.952380000	-2.507872000	-2.384065000
C	-3.589031000	-2.336976000	-4.513573000
H	-2.974304000	-3.246187000	-4.562721000

H	-4.611300000	-2.626221000	-4.791379000
B	2.693562000	0.113782000	-1.015659000
N	2.522954000	1.272957000	0.018157000
N	1.298408000	1.838831000	0.236854000
N	2.551661000	-1.295991000	-0.382834000
N	1.418225000	-1.686050000	0.273341000
N	1.705740000	0.291865000	-2.195263000
N	0.398235000	-0.096068000	-2.106843000
S	-3.102111000	0.549685000	0.675110000
S	-4.833430000	-1.165108000	2.479532000
O	-0.157990000	0.141494000	2.746532000
Yb	-0.370761000	0.030309000	0.265306000
H	-3.638525000	-1.778272000	0.533839000
H	3.804949000	0.195894000	-1.451515000

Int3

C	-0.582471000	-0.285288000	0.266537000
C	2.309990000	0.771398000	3.145940000
H	2.675583000	1.453042000	2.371047000
H	1.826516000	-0.077154000	2.654364000
C	3.392330000	0.359909000	4.140193000
H	3.162205000	-0.618397000	4.576623000
H	4.380063000	0.298770000	3.674862000
C	3.291480000	1.452851000	5.206731000
H	3.814212000	2.357337000	4.878048000
H	3.702089000	1.153505000	6.175196000
C	1.789311000	1.696868000	5.263578000
H	1.284303000	0.996062000	5.938651000
H	1.515738000	2.715784000	5.547710000
C	-5.430601000	1.881339000	6.144371000
H	-5.962074000	1.798129000	7.099147000
H	-5.870086000	1.160908000	5.445954000
H	-4.387439000	1.597537000	6.304080000
C	-7.017956000	3.702660000	5.410887000
H	-7.541267000	3.650555000	6.371210000
H	-7.119061000	4.720319000	5.021373000
H	-7.530392000	3.022843000	4.721027000
C	-5.549328000	3.309101000	5.587148000
H	-5.103212000	3.989725000	6.323332000
C	-4.778800000	3.458724000	4.303089000
C	-5.252666000	3.510825000	3.001829000
H	-6.286338000	3.490550000	2.690093000
C	-4.113546000	3.626894000	2.184421000
C	-4.093954000	3.848368000	0.692377000
C	-4.706787000	2.641541000	-0.055994000
H	-4.117637000	1.742069000	0.161303000
H	-5.723868000	2.455890000	0.314187000
C	-2.670510000	4.091979000	0.159300000
H	-2.219821000	4.941045000	0.687191000
H	-2.030810000	3.220157000	0.353224000
C	-4.950143000	5.101564000	0.368230000
H	-5.971164000	4.959489000	0.744696000
H	-4.535517000	5.968655000	0.898687000
C	-4.983231000	5.367238000	-1.144082000
H	-5.597893000	6.255982000	-1.340498000
C	-5.589107000	4.151982000	-1.862510000
H	-5.631072000	4.335651000	-2.945176000

H	-6.622257000	3.990379000	-1.525895000
C	-4.736834000	2.907823000	-1.569149000
H	-5.170635000	2.036361000	-2.078830000
C	-3.304532000	3.144618000	-2.071816000
H	-2.688896000	2.257536000	-1.873534000
H	-3.306851000	3.309064000	-3.158708000
C	-2.701143000	4.360536000	-1.352917000
H	-1.674961000	4.523827000	-1.703534000
C	-3.553101000	5.602727000	-1.649594000
H	-3.119319000	6.483780000	-1.158250000
H	-3.561323000	5.808891000	-2.729045000
C	-0.005502000	3.933553000	8.246069000
H	0.164102000	4.413848000	7.278822000
H	0.045671000	4.704071000	9.023625000
H	0.808806000	3.221976000	8.423691000
C	-1.611184000	2.599529000	9.666374000
H	-2.578498000	2.090287000	9.713002000
H	-0.832872000	1.871163000	9.920363000
H	-1.595942000	3.376584000	10.437624000
C	-1.365432000	3.216419000	8.286664000
H	-2.142004000	3.971265000	8.111278000
C	-1.475063000	2.189237000	7.192799000
C	-1.292832000	0.817680000	7.265042000
H	-1.078020000	0.244966000	8.153765000
C	-1.484277000	0.333530000	5.956958000
C	-1.515896000	-1.120708000	5.531106000
C	-1.359905000	-2.031153000	6.770486000
H	-0.400254000	-1.824427000	7.264221000
H	-2.150784000	-1.801529000	7.496828000
C	-2.873603000	-1.448232000	4.862800000
H	-3.004981000	-0.812590000	3.980740000
H	-3.686065000	-1.202861000	5.559843000
C	-0.386576000	-1.473709000	4.537437000
H	-0.478093000	-0.847895000	3.643388000
H	0.585335000	-1.249721000	4.997550000
C	-1.428969000	-3.513637000	6.379208000
H	-1.316378000	-4.127637000	7.283003000
C	-2.785486000	-3.806252000	5.721430000
H	-2.852752000	-4.869432000	5.452789000
H	-3.599029000	-3.602214000	6.431012000
C	-2.940850000	-2.931653000	4.467894000
H	-3.911365000	-3.131412000	3.994808000
C	-1.809946000	-3.250372000	3.478945000
H	-1.858091000	-4.306610000	3.179051000
H	-1.920106000	-2.647069000	2.569903000
C	-0.455517000	-2.957555000	4.141526000
H	0.352428000	-3.174357000	3.431299000
C	-0.296386000	-3.833011000	5.392590000
H	-0.322708000	-4.896463000	5.117910000
H	0.678129000	-3.649091000	5.866711000
C	-1.909853000	8.118445000	6.876085000
H	-2.669422000	8.543527000	7.540398000
H	-1.017888000	7.900614000	7.471425000
H	-1.647540000	8.889859000	6.143706000
C	-2.451503000	6.861294000	6.189200000
H	-2.753907000	6.155071000	6.971192000
C	-3.698671000	7.194260000	5.354383000

H	-4.471799000	7.650663000	5.982938000
H	-3.446929000	7.902037000	4.557023000
H	-4.118333000	6.299643000	4.886943000
C	-1.396714000	6.196752000	5.343949000
C	-0.293127000	6.775890000	4.738285000
H	0.017569000	7.805270000	4.821340000
C	0.338517000	5.747612000	4.019729000
C	1.578484000	5.880049000	3.162740000
C	1.205626000	5.890300000	1.658731000
H	0.713530000	4.944078000	1.396239000
H	0.494471000	6.705593000	1.468142000
C	2.564625000	4.719481000	3.411924000
H	2.073631000	3.767540000	3.182161000
H	2.837896000	4.702812000	4.476511000
C	2.302190000	7.205842000	3.487218000
H	1.627673000	8.051061000	3.298795000
H	2.562979000	7.233225000	4.553962000
C	3.565157000	7.368919000	2.628468000
H	4.056218000	8.316044000	2.889346000
C	3.168457000	7.382505000	1.144517000
H	4.059739000	7.516449000	0.515845000
H	2.502494000	8.232465000	0.941180000
C	2.465919000	6.062895000	0.796179000
H	2.174517000	6.067417000	-0.262758000
C	3.416229000	4.885016000	1.061291000
H	2.909628000	3.944714000	0.809857000
H	4.310951000	4.968635000	0.428164000
C	3.821813000	4.880035000	2.543277000
H	4.502480000	4.038789000	2.734731000
C	4.524236000	6.199275000	2.893231000
H	5.436876000	6.315165000	2.292541000
H	4.833216000	6.196122000	3.947738000
B	-2.434117000	3.807263000	5.399204000
N	-3.421083000	3.541350000	4.239170000
N	-3.009365000	3.621925000	2.940878000
N	-1.762555000	2.488267000	5.895950000
N	-1.749165000	1.356615000	5.127243000
N	-1.398128000	4.882136000	4.998889000
N	-0.340831000	4.598799000	4.182797000
O	1.314475000	1.472132000	3.922139000
S	-1.831181000	0.086246000	1.311287000
S	-0.363703000	-1.790267000	-0.505195000
Yb	-0.754581000	2.417048000	2.878389000
H	-3.071667000	4.246606000	6.318895000
C	-2.266597000	-0.611539000	-3.357953000
H	-2.829977000	-1.298184000	-2.716396000
H	-1.793863000	0.137294000	-2.719626000
C	-3.126240000	-0.025488000	-4.470833000
H	-2.723852000	0.938226000	-4.800767000
H	-4.159419000	0.132143000	-4.151685000
C	-2.982690000	-1.071600000	-5.577758000
H	-3.639707000	-1.927069000	-5.384982000
H	-3.213269000	-0.684611000	-6.573933000
C	-1.521765000	-1.476425000	-5.440207000
H	-0.856503000	-0.800243000	-5.989837000
H	-1.313859000	-2.504711000	-5.744891000
C	5.764559000	-3.009482000	-6.456413000

H	6.306958000	-3.122879000	-7.401541000
H	6.408454000	-2.463089000	-5.758805000
H	4.877017000	-2.398025000	-6.640494000
C	6.643591000	-5.245900000	-5.682050000
H	7.153715000	-5.395710000	-6.638952000
H	6.396271000	-6.228701000	-5.269577000
H	7.355760000	-4.763102000	-5.003989000
C	5.392574000	-4.385596000	-5.880482000
H	4.752181000	-4.890715000	-6.613220000
C	4.612990000	-4.239725000	-4.599718000
C	5.068644000	-4.367716000	-3.297228000
H	6.063206000	-4.651150000	-2.990988000
C	3.969634000	-4.076141000	-2.473720000
C	3.939882000	-4.075807000	-0.963364000
C	4.314211000	-2.675605000	-0.416217000
H	3.593759000	-1.932659000	-0.784934000
H	5.298738000	-2.384796000	-0.805449000
C	2.552098000	-4.462630000	-0.412750000
H	2.261094000	-5.445877000	-0.803884000
H	1.794035000	-3.741077000	-0.749021000
C	4.970344000	-5.092845000	-0.416690000
H	5.973135000	-4.835008000	-0.779750000
H	4.737904000	-6.093342000	-0.804506000
C	4.975906000	-5.100715000	1.118811000
H	5.716423000	-5.831557000	1.469181000
C	5.349026000	-3.701087000	1.630608000
H	5.371921000	-3.694322000	2.728467000
H	6.357019000	-3.430058000	1.288278000
C	4.320569000	-2.680709000	1.119988000
H	4.585226000	-1.677717000	1.479053000
C	2.925039000	-3.064088000	1.632939000
H	2.178362000	-2.337863000	1.288782000
H	2.911361000	-3.050588000	2.730815000
C	2.555706000	-4.465774000	1.123629000
H	1.553223000	-4.731880000	1.480580000
C	3.582345000	-5.485997000	1.634896000
H	3.318753000	-6.496168000	1.293557000
H	3.577001000	-5.507989000	2.732704000
C	0.622262000	-2.769433000	-8.850749000
H	0.260149000	-3.481730000	-8.104151000
H	0.650919000	-3.275449000	-9.821853000
H	-0.103296000	-1.951239000	-8.918829000
C	2.524456000	-1.272503000	-9.566921000
H	3.514853000	-0.877783000	-9.321583000
H	1.844705000	-0.424204000	-9.703162000
H	2.593647000	-1.793796000	-10.526804000
C	2.012825000	-2.225732000	-8.483776000
H	2.701330000	-3.078303000	-8.431878000
C	1.996714000	-1.568575000	-7.129617000
C	1.976382000	-0.215786000	-6.822558000
H	2.019460000	0.605099000	-7.522429000
C	1.933495000	-0.140351000	-5.418879000
C	2.044172000	1.098114000	-4.566921000
C	1.036892000	2.178381000	-5.022927000
H	0.014177000	1.793303000	-4.911961000
H	1.181294000	2.392087000	-6.090105000
C	3.477541000	1.669385000	-4.739112000

H	4.206292000	0.909876000	-4.427232000
H	3.662955000	1.869528000	-5.802387000
C	1.817782000	0.815532000	-3.068195000
H	2.533836000	0.054142000	-2.725326000
H	0.800820000	0.422791000	-2.912055000
C	1.213031000	3.463505000	-4.199830000
H	0.485938000	4.210915000	-4.543380000
C	2.638629000	4.004608000	-4.391009000
H	2.765012000	4.934420000	-3.821453000
H	2.813862000	4.249355000	-5.447711000
C	3.653576000	2.953307000	-3.916861000
H	4.673800000	3.332917000	-4.060412000
C	3.417231000	2.640627000	-2.432480000
H	3.555800000	3.544149000	-1.826290000
H	4.152991000	1.905012000	-2.079782000
C	1.992227000	2.101114000	-2.240976000
H	1.809959000	1.892449000	-1.179704000
C	0.979899000	3.152203000	-2.715383000
H	1.082089000	4.061071000	-2.110224000
H	-0.041693000	2.784413000	-2.556808000
C	0.558957000	-7.164386000	-8.212579000
H	1.133438000	-7.549947000	-9.061025000
H	-0.232875000	-6.517712000	-8.602354000
H	0.084400000	-8.021825000	-7.723417000
C	1.481493000	-6.409767000	-7.249658000
H	1.962989000	-5.602425000	-7.811201000
C	2.585048000	-7.335287000	-6.712543000
H	3.180361000	-7.745024000	-7.535888000
H	2.147507000	-8.173332000	-6.159340000
H	3.255709000	-6.802901000	-6.032469000
C	0.708771000	-5.794435000	-6.112215000
C	-0.412285000	-6.303138000	-5.477008000
H	-0.944868000	-7.206409000	-5.733180000
C	-0.702306000	-5.411575000	-4.433365000
C	-1.817242000	-5.554344000	-3.428680000
C	-1.767250000	-4.480969000	-2.329112000
H	-1.839237000	-3.482955000	-2.782078000
H	-0.808393000	-4.547363000	-1.792109000
C	-3.188818000	-5.457294000	-4.143391000
H	-3.272470000	-4.479284000	-4.636386000
H	-3.244449000	-6.215368000	-4.935173000
C	-1.725185000	-6.943985000	-2.747720000
H	-0.755790000	-7.035193000	-2.240525000
H	-1.757949000	-7.732428000	-3.510062000
C	-2.874244000	-7.135784000	-1.747461000
H	-2.782833000	-8.126723000	-1.283992000
C	-2.799827000	-6.047533000	-0.666287000
H	-3.606919000	-6.183104000	0.065456000
H	-1.854071000	-6.124600000	-0.113972000
C	-2.914775000	-4.664753000	-1.324216000
H	-2.839004000	-3.879237000	-0.564219000
C	-4.259302000	-4.561894000	-2.060770000
H	-4.367978000	-3.567551000	-2.515117000
H	-5.086320000	-4.674615000	-1.347724000
C	-4.337664000	-5.649499000	-3.142775000
H	-5.294566000	-5.575449000	-3.675988000
C	-4.217353000	-7.034007000	-2.487020000

H	-5.047253000	-7.192392000	-1.785922000
H	-4.289519000	-7.820564000	-3.250520000
B	2.301003000	-3.756673000	-5.708509000
N	3.299086000	-3.893457000	-4.534237000
N	2.903893000	-3.776271000	-3.231907000
N	1.960121000	-2.253332000	-5.952073000
N	1.908298000	-1.375914000	-4.906069000
N	1.049733000	-4.642365000	-5.471345000
N	0.183254000	-4.403595000	-4.441796000
O	-1.224058000	-1.363962000	-4.028431000
Yb	0.774306000	-2.451947000	-3.025642000
H	2.838216000	-4.158766000	-6.698397000
H	0.156239000	0.509833000	0.109537000
H	0.529799000	2.526505000	1.122253000

TS3

C	6.569992000	0.278457000	0.712414000
C	9.120908000	0.809763000	3.094675000
H	9.589306000	1.601961000	2.497344000
H	8.767480000	0.032505000	2.414287000
C	10.044313000	0.321348000	4.201069000
H	9.744368000	-0.677070000	4.536242000
H	11.088686000	0.274813000	3.880483000
C	9.793788000	1.356211000	5.301084000
H	10.371179000	2.265948000	5.104256000
H	10.056077000	0.999346000	6.301028000
C	8.297958000	1.625718000	5.162344000
H	7.700844000	0.952038000	5.785461000
H	8.012456000	2.656956000	5.384558000
C	1.159362000	1.296700000	5.624268000
H	0.606489000	1.089511000	6.547535000
H	0.736192000	0.674811000	4.827710000
H	2.199240000	0.993555000	5.769555000
C	-0.412175000	3.202070000	5.096112000
H	-0.960026000	3.027490000	6.027898000
H	-0.504953000	4.261880000	4.839575000
H	-0.906936000	2.618968000	4.311308000
C	1.052221000	2.785467000	5.255879000
H	1.480003000	3.363390000	6.085064000
C	1.855371000	3.099098000	4.023401000
C	1.423319000	3.285704000	2.720117000
H	0.401274000	3.275630000	2.371255000
C	2.584813000	3.529923000	1.963341000
C	2.645857000	3.982622000	0.524956000
C	2.022636000	2.940296000	-0.431038000
H	2.590567000	2.004180000	-0.362401000
H	0.994323000	2.716094000	-0.117678000
C	4.086207000	4.274829000	0.065027000
H	4.549211000	5.000981000	0.743395000
H	4.685770000	3.356006000	0.119337000
C	1.826923000	5.297289000	0.407378000
H	0.795413000	5.118100000	0.736381000
H	2.250201000	6.046597000	1.088725000
C	1.833135000	5.822150000	-1.034665000
H	1.244522000	6.748048000	-1.083789000
C	1.212214000	4.766246000	-1.961618000
H	1.195268000	5.133728000	-2.996880000

H	0.169575000	4.576858000	-1.672085000
C	2.029445000	3.468174000	-1.875100000
H	1.585578000	2.712386000	-2.537671000
C	3.475309000	3.753759000	-2.309267000
H	4.067950000	2.831360000	-2.269093000
H	3.494675000	4.109347000	-3.349021000
C	4.094717000	4.805367000	-1.377138000
H	5.131624000	4.999488000	-1.679192000
C	3.279498000	6.103733000	-1.465073000
H	3.721820000	6.872734000	-0.817870000
H	3.301386000	6.496560000	-2.490988000
C	6.251378000	3.576270000	8.299873000
H	6.467179000	4.114354000	7.373220000
H	6.205170000	4.305923000	9.116073000
H	7.085829000	2.895647000	8.502897000
C	4.610949000	2.097860000	9.525528000
H	3.670905000	1.540676000	9.470203000
H	5.404153000	1.396554000	9.807828000
H	4.524705000	2.835199000	10.330155000
C	4.931137000	2.794529000	8.200235000
H	4.132000000	3.518330000	7.997482000
C	4.961171000	1.818443000	7.055475000
C	5.179979000	0.450386000	7.087245000
H	5.322708000	-0.155174000	7.968386000
C	5.125585000	0.018887000	5.749471000
C	5.219453000	-1.408912000	5.257542000
C	4.931154000	-2.382384000	6.425418000
H	5.664801000	-2.229472000	7.228123000
H	3.941848000	-2.164430000	6.848879000
C	4.184432000	-1.677416000	4.143218000
H	4.358789000	-1.001487000	3.299381000
H	3.178506000	-1.455744000	4.523147000
C	6.630802000	-1.732127000	4.712454000
H	6.868629000	-1.055820000	3.883611000
H	7.371912000	-1.549701000	5.503069000
C	4.999892000	-3.842381000	5.955745000
H	4.785612000	-4.502157000	6.807201000
C	3.967091000	-4.077797000	4.844251000
H	4.001930000	-5.124690000	4.512706000
H	2.953573000	-3.896257000	5.227169000
C	4.266715000	-3.135505000	3.669886000
H	3.529246000	-3.291081000	2.872066000
C	5.676475000	-3.420639000	3.129141000
H	5.738512000	-4.458043000	2.773702000
H	5.892416000	-2.767847000	2.274140000
C	6.708235000	-3.192068000	4.242800000
H	7.716344000	-3.391047000	3.857556000
C	6.408929000	-4.133451000	5.418350000
H	6.481260000	-5.180079000	5.092512000
H	7.152288000	-3.994959000	6.215733000
C	4.565575000	7.751983000	6.853565000
H	3.789518000	8.140647000	7.521097000
H	5.457478000	7.542007000	7.451766000
H	4.814293000	8.548225000	6.143392000
C	4.061817000	6.498986000	6.131023000
H	3.770374000	5.767553000	6.893460000
C	2.814357000	6.822026000	5.292740000

H	2.024220000	7.243148000	5.924776000
H	3.056123000	7.556038000	4.516304000
H	2.421318000	5.929657000	4.798605000
C	5.140350000	5.881564000	5.279545000
C	6.235468000	6.502966000	4.704575000
H	6.521119000	7.536009000	4.822920000
C	6.898754000	5.512263000	3.961826000
C	8.147663000	5.719564000	3.130243000
C	7.797904000	5.788063000	1.622860000
H	7.320878000	4.848914000	1.316328000
H	7.074017000	6.597280000	1.456873000
C	9.165809000	4.582618000	3.348332000
H	8.703021000	3.627811000	3.080265000
H	9.425614000	4.534526000	4.414989000
C	8.829857000	7.052970000	3.516234000
H	8.135496000	7.886352000	3.349163000
H	9.074746000	7.047163000	4.586941000
C	10.099846000	7.284129000	2.683259000
H	10.558520000	8.234183000	2.988248000
C	9.725591000	7.345116000	1.194677000
H	10.622140000	7.527530000	0.586285000
H	9.039677000	8.183885000	1.012951000
C	9.064714000	6.021268000	0.784900000
H	8.788362000	6.059693000	-0.277214000
C	10.047274000	4.863682000	1.019254000
H	9.581823000	3.916552000	0.719186000
H	10.947363000	5.000022000	0.403825000
C	10.429873000	4.810287000	2.506228000
H	11.130764000	3.981212000	2.675449000
C	11.089504000	6.133892000	2.917453000
H	12.006955000	6.299796000	2.336347000
H	11.382903000	6.098244000	3.975689000
B	4.137983000	3.487387000	5.235507000
N	3.212111000	3.227243000	4.019390000
N	3.662863000	3.464781000	2.752215000
N	4.788113000	2.167306000	5.751692000
N	4.908790000	1.071991000	4.942875000
N	5.174455000	4.577892000	4.894350000
N	6.245544000	4.340990000	4.079168000
O	7.973967000	1.359530000	3.778027000
S	4.881245000	0.202044000	0.747637000
S	7.629499000	-0.765458000	-0.150862000
Yb	5.831538000	2.088521000	2.723311000
H	3.451671000	3.908249000	6.127512000
C	4.726650000	-0.075990000	-2.934194000
H	4.234410000	-0.596987000	-2.107186000
H	5.330868000	0.726766000	-2.504105000
C	3.746697000	0.396835000	-4.004441000
H	4.121430000	1.298061000	-4.501155000
H	2.765271000	0.629817000	-3.584787000
C	3.725515000	-0.777837000	-4.984238000
H	3.069788000	-1.574584000	-4.616246000
H	3.392482000	-0.498913000	-5.987631000
C	5.177414000	-1.228332000	-4.960588000
H	5.803116000	-0.626253000	-5.631012000
H	5.326845000	-2.285469000	-5.189394000
C	12.190830000	-2.946761000	-6.488752000

H	12.635775000	-3.088059000	-7.480026000
H	12.906899000	-2.393371000	-5.871531000
H	11.296302000	-2.327672000	-6.598717000
C	13.124214000	-5.171152000	-5.747072000
H	13.540090000	-5.346737000	-6.744406000
H	12.911371000	-6.142305000	-5.290139000
H	13.900509000	-4.678715000	-5.151260000
C	11.865399000	-4.305148000	-5.845902000
H	11.154161000	-4.822261000	-6.500761000
C	11.212678000	-4.121616000	-4.500980000
C	11.789016000	-4.226207000	-3.245898000
H	12.804888000	-4.517441000	-3.030907000
C	10.775583000	-3.910574000	-2.326334000
C	10.884811000	-3.947972000	-0.818288000
C	11.302879000	-2.571752000	-0.244249000
H	10.547922000	-1.816570000	-0.499139000
H	12.246808000	-2.255569000	-0.707827000
C	9.552812000	-4.367768000	-0.159883000
H	9.225895000	-5.331508000	-0.570892000
H	8.768697000	-3.633795000	-0.394340000
C	11.966350000	-4.981365000	-0.416656000
H	12.930304000	-4.695234000	-0.855614000
H	11.705559000	-5.964318000	-0.830466000
C	12.115460000	-5.063430000	1.107548000
H	12.887781000	-5.804804000	1.351710000
C	12.531336000	-3.686691000	1.647094000
H	12.660308000	-3.730379000	2.736915000
H	13.501147000	-3.394300000	1.221560000
C	11.455639000	-2.652694000	1.283753000
H	11.746798000	-1.665016000	1.664080000
C	10.116821000	-3.072932000	1.909150000
H	9.343068000	-2.332992000	1.672530000
H	10.212361000	-3.115484000	3.002821000
C	9.704220000	-4.449262000	1.366816000
H	8.741620000	-4.742836000	1.804258000
C	10.776645000	-5.486342000	1.727968000
H	10.487277000	-6.479641000	1.358556000
H	10.871278000	-5.566015000	2.819222000
C	6.888159000	-2.880833000	-8.451537000
H	6.565593000	-3.502490000	-7.611695000
H	6.802856000	-3.473018000	-9.369182000
H	6.197107000	-2.034277000	-8.531352000
C	8.777419000	-1.550385000	-9.467552000
H	9.805170000	-1.193645000	-9.351925000
H	8.129233000	-0.678815000	-9.610583000
H	8.725487000	-2.150766000	-10.381253000
C	8.330001000	-2.381758000	-8.262474000
H	8.981635000	-3.262111000	-8.198893000
C	8.471896000	-1.613162000	-6.976084000
C	8.546852000	-0.240688000	-6.789224000
H	8.563893000	0.516322000	-7.558848000
C	8.630590000	-0.046350000	-5.398943000
C	8.843752000	1.255349000	-4.670219000
C	7.829991000	2.325150000	-5.138792000
H	6.809823000	1.973072000	-4.935573000
H	7.908352000	2.462369000	-6.225244000
C	10.273247000	1.777551000	-4.977235000

H	11.007237000	1.025894000	-4.659061000
H	10.393349000	1.899921000	-6.061714000
C	8.712334000	1.089875000	-3.147515000
H	9.431172000	0.340199000	-2.789525000
H	7.703956000	0.731938000	-2.897129000
C	8.082739000	3.660425000	-4.421691000
H	7.349223000	4.399109000	-4.770568000
C	9.503092000	4.151958000	-4.741288000
H	9.686444000	5.116546000	-4.249745000
H	9.613153000	4.318222000	-5.821783000
C	10.525716000	3.111460000	-4.259535000
H	11.541355000	3.456686000	-4.493986000
C	10.381394000	2.912331000	-2.743346000
H	10.579248000	3.855346000	-2.217669000
H	11.122449000	2.185303000	-2.385182000
C	8.961708000	2.420215000	-2.424905000
H	8.847859000	2.260551000	-1.346926000
C	7.940292000	3.460567000	-2.906000000
H	8.098194000	4.411794000	-2.381715000
H	6.923041000	3.129839000	-2.659189000
C	6.746431000	-7.290135000	-7.347171000
H	7.230437000	-7.776360000	-8.200259000
H	5.906560000	-6.698124000	-7.723125000
H	6.342903000	-8.081758000	-6.706675000
C	7.756984000	-6.421899000	-6.591712000
H	8.165429000	-5.691782000	-7.298867000
C	8.924007000	-7.274689000	-6.068188000
H	9.427476000	-7.788296000	-6.894702000
H	8.560076000	-8.033865000	-5.367531000
H	9.661293000	-6.662420000	-5.541915000
C	7.102949000	-5.666120000	-5.464769000
C	6.007926000	-6.047524000	-4.706549000
H	5.409054000	-6.936115000	-4.838699000
C	5.845753000	-5.048864000	-3.733793000
C	4.799413000	-5.021865000	-2.648064000
C	5.023403000	-3.881177000	-1.639847000
H	4.997563000	-2.915271000	-2.162200000
H	6.010755000	-3.992026000	-1.164885000
C	3.391299000	-4.852154000	-3.273036000
H	3.354502000	-3.908561000	-3.833287000
H	3.214425000	-5.656591000	-3.998663000
C	4.821297000	-6.364304000	-1.874733000
H	5.813698000	-6.509173000	-1.428310000
H	4.664709000	-7.195776000	-2.573324000
C	3.736882000	-6.382799000	-0.787207000
H	3.778272000	-7.343264000	-0.257130000
C	3.987137000	-5.233771000	0.199032000
H	3.231657000	-5.246937000	0.995335000
H	4.963621000	-5.360207000	0.683246000
C	3.940595000	-3.893185000	-0.548603000
H	4.129975000	-3.065547000	0.144159000
C	2.558885000	-3.720370000	-1.196889000
H	2.502091000	-2.753440000	-1.714587000
H	1.781163000	-3.709350000	-0.422216000
C	2.307151000	-4.868639000	-2.184716000
H	1.323523000	-4.744823000	-2.656744000
C	2.355582000	-6.209701000	-1.436620000

H	1.571837000	-6.240258000	-0.668226000
H	2.155555000	-7.037676000	-2.130423000
B	8.806098000	-3.682393000	-5.396540000
N	9.913375000	-3.763017000	-4.317803000
N	9.645116000	-3.609455000	-2.986136000
N	8.507095000	-2.192525000	-5.743172000
N	8.590848000	-1.231422000	-4.776852000
N	7.551641000	-4.482845000	-4.961623000
N	6.781480000	-4.102270000	-3.899571000
O	5.613002000	-1.012625000	-3.599717000
Yb	7.619651000	-2.113583000	-2.667963000
H	9.223959000	-4.196198000	-6.393419000
H	7.143757000	1.593968000	0.983024000
H	7.331476000	2.564127000	1.081555000

Int4

C	0.065220000	0.643995000	0.664193000
C	2.550244000	0.752226000	3.169953000
H	3.023342000	1.487527000	2.507815000
H	2.186338000	-0.073528000	2.559437000
C	3.478629000	0.345628000	4.305709000
H	3.174150000	-0.621462000	4.720405000
H	4.521206000	0.267979000	3.985473000
C	3.236532000	1.464242000	5.321643000
H	3.803351000	2.359772000	5.043325000
H	3.513794000	1.191788000	6.343770000
C	1.737745000	1.708208000	5.177919000
H	1.154462000	1.060662000	5.841033000
H	1.441150000	2.746394000	5.343108000
C	-5.185809000	1.246759000	6.680399000
H	-5.601932000	1.237834000	7.694199000
H	-5.693242000	0.469328000	6.098757000
H	-4.127025000	0.982360000	6.742111000
C	-6.877031000	2.993317000	6.003766000
H	-7.276752000	3.022681000	7.022695000
H	-7.042416000	3.972616000	5.544189000
H	-7.460832000	2.253592000	5.444684000
C	-5.391263000	2.623878000	6.028238000
H	-4.870502000	3.365637000	6.646275000
C	-4.788107000	2.668860000	4.649787000
C	-5.421361000	2.561108000	3.423410000
H	-6.483514000	2.473730000	3.250018000
C	-4.399987000	2.627825000	2.459361000
C	-4.606503000	2.717787000	0.968780000
C	-5.351936000	1.471165000	0.438090000
H	-4.740329000	0.578793000	0.622760000
H	-6.290073000	1.335692000	0.991622000
C	-3.290143000	2.875736000	0.187742000
H	-2.745556000	3.753030000	0.558585000
H	-2.647043000	1.999587000	0.347921000
C	-5.487587000	3.965640000	0.687232000
H	-6.429729000	3.883357000	1.243363000
H	-4.974892000	4.859579000	1.065690000
C	-5.776111000	4.109220000	-0.812432000
H	-6.400543000	4.997435000	-0.977097000
C	-6.514995000	2.857689000	-1.309158000
H	-6.743654000	2.951823000	-2.379688000

H	-7.475383000	2.754647000	-0.785937000
C	-5.642209000	1.618066000	-1.063081000
H	-6.165406000	0.721432000	-1.419826000
C	-4.314882000	1.773330000	-1.818368000
H	-3.695715000	0.881926000	-1.658114000
H	-4.505292000	1.851847000	-2.898316000
C	-3.576181000	3.023420000	-1.315813000
H	-2.621830000	3.130976000	-1.847147000
C	-4.448816000	4.262128000	-1.568181000
H	-3.926570000	5.167793000	-1.232242000
H	-4.636270000	4.380500000	-2.644574000
C	0.006769000	3.540912000	8.187746000
H	0.037932000	4.053866000	7.222925000
H	0.013960000	4.299333000	8.978425000
H	0.919738000	2.943103000	8.287515000
C	-1.296439000	1.992784000	9.693711000
H	-2.186917000	1.366975000	9.805815000
H	-0.415983000	1.365573000	9.873177000
H	-1.317930000	2.759303000	10.475007000
C	-1.238298000	2.648467000	8.311631000
H	-2.119017000	3.295881000	8.209991000
C	-1.301320000	1.623655000	7.210718000
C	-1.091669000	0.256216000	7.286603000
H	-0.870134000	-0.309199000	8.178007000
C	-1.285981000	-0.239229000	5.982491000
C	-1.302282000	-1.693671000	5.561824000
C	-1.500058000	-2.584849000	6.811260000
H	-0.671144000	-2.429306000	7.514792000
H	-2.421318000	-2.289018000	7.330271000
C	-2.471620000	-1.963202000	4.586638000
H	-2.350667000	-1.347006000	3.689062000
H	-3.414149000	-1.659611000	5.060659000
C	0.017195000	-2.121281000	4.877104000
H	0.179238000	-1.509988000	3.981032000
H	0.857801000	-1.935794000	5.560857000
C	-1.559594000	-4.069315000	6.426980000
H	-1.705320000	-4.668389000	7.335905000
C	-2.727849000	-4.304647000	5.458839000
H	-2.787323000	-5.368492000	5.190988000
H	-3.677949000	-4.043157000	5.944441000
C	-2.522084000	-3.449046000	4.200644000
H	-3.355168000	-3.608131000	3.503825000
C	-1.201993000	-3.846069000	3.522121000
H	-1.234452000	-4.903983000	3.225951000
H	-1.055757000	-3.253996000	2.610161000
C	-0.035918000	-3.609786000	4.493858000
H	0.908718000	-3.888175000	4.010328000
C	-0.239278000	-4.466730000	5.751623000
H	-0.256179000	-5.531783000	5.483196000
H	0.598220000	-4.325580000	6.448894000
C	-1.741406000	7.546539000	6.670977000
H	-2.385963000	7.960794000	7.453191000
H	-0.748412000	7.379547000	7.099205000
H	-1.648757000	8.307104000	5.887990000
C	-2.344242000	6.249739000	6.122156000
H	-2.472694000	5.559266000	6.963405000
C	-3.731693000	6.510407000	5.514104000

H	-4.403607000	6.950125000	6.259811000
H	-3.654979000	7.207553000	4.672560000
H	-4.184875000	5.587329000	5.142920000
C	-1.429363000	5.597298000	5.118207000
C	-0.491188000	6.204228000	4.299866000
H	-0.236562000	7.252009000	4.284579000
C	0.048166000	5.179900000	3.505159000
C	1.127426000	5.326489000	2.456818000
C	0.718520000	4.669184000	1.119594000
H	0.544422000	3.591958000	1.250682000
H	-0.225180000	5.108810000	0.770549000
C	2.449465000	4.681392000	2.935789000
H	2.274079000	3.617570000	3.128399000
H	2.751393000	5.140047000	3.887546000
C	1.400569000	6.824922000	2.192476000
H	0.475156000	7.315953000	1.863070000
H	1.707884000	7.312015000	3.127324000
C	2.500344000	7.010919000	1.138826000
H	2.665566000	8.084859000	0.979605000
C	2.061513000	6.352252000	-0.176849000
H	2.833332000	6.492742000	-0.945877000
H	1.146249000	6.831169000	-0.550811000
C	1.819488000	4.855984000	0.064899000
H	1.502075000	4.367896000	-0.863937000
C	3.116184000	4.202505000	0.564700000
H	2.955726000	3.125546000	0.699296000
H	3.909292000	4.318072000	-0.186365000
C	3.552727000	4.861428000	1.881534000
H	4.477420000	4.390965000	2.242817000
C	3.797587000	6.358290000	1.639543000
H	4.600057000	6.495725000	0.902171000
H	4.129061000	6.844649000	2.567268000
B	-2.349795000	3.183184000	5.408040000
N	-3.454887000	2.792184000	4.402203000
N	-3.208683000	2.740119000	3.060439000
N	-1.594543000	1.913943000	5.911927000
N	-1.566084000	0.776860000	5.151733000
N	-1.425989000	4.270554000	4.815106000
N	-0.525963000	4.008087000	3.823943000
O	1.412359000	1.364198000	3.811403000
S	-0.989521000	-0.622171000	1.145838000
S	1.088103000	0.501474000	-0.724949000
Yb	-0.857191000	1.650790000	2.806596000
H	-2.886912000	3.667201000	6.365136000
C	-1.086470000	1.204632000	-3.694270000
H	-1.817211000	0.912324000	-2.934666000
H	-0.343859000	1.851787000	-3.222083000
C	-1.752484000	1.807719000	-4.925715000
H	-1.062459000	2.478544000	-5.449636000
H	-2.649105000	2.377644000	-4.669659000
C	-2.038645000	0.570065000	-5.778708000
H	-2.933009000	0.052344000	-5.414318000
H	-2.182764000	0.795874000	-6.838775000
C	-0.794666000	-0.269517000	-5.530071000
H	0.032959000	0.027773000	-6.184960000
H	-0.950105000	-1.346756000	-5.620261000
C	5.808876000	-3.470842000	-6.257420000

H	6.294509000	-3.780133000	-7.189692000
H	6.570673000	-3.022819000	-5.610224000
H	5.073141000	-2.697192000	-6.493355000
C	6.196659000	-5.768242000	-5.286592000
H	6.647757000	-6.105972000	-6.225173000
H	5.750169000	-6.635551000	-4.790884000
H	7.006035000	-5.393550000	-4.650480000
C	5.157551000	-4.677946000	-5.562547000
H	4.409515000	-5.093658000	-6.247936000
C	4.452108000	-4.255783000	-4.300732000
C	4.888458000	-4.373345000	-2.990365000
H	5.796734000	-4.849192000	-2.656154000
C	3.894061000	-3.777301000	-2.199708000
C	3.844560000	-3.703038000	-0.694385000
C	4.183233000	-2.282603000	-0.184044000
H	3.466184000	-1.553606000	-0.586338000
H	5.178064000	-1.992264000	-0.547874000
C	2.442267000	-4.097132000	-0.178288000
H	2.184281000	-5.096665000	-0.551470000
H	1.687192000	-3.405871000	-0.576768000
C	4.872912000	-4.685466000	-0.088525000
H	5.881452000	-4.419758000	-0.431797000
H	4.667309000	-5.701046000	-0.452160000
C	4.830983000	-4.651728000	1.444680000
H	5.571709000	-5.359733000	1.839289000
C	5.163548000	-3.231722000	1.927575000
H	5.148175000	-3.193023000	3.025205000
H	6.178457000	-2.953728000	1.611771000
C	4.137581000	-2.245128000	1.350384000
H	4.373521000	-1.227382000	1.686278000
C	2.730187000	-2.635758000	1.825142000
H	1.983085000	-1.938087000	1.425810000
H	2.675623000	-2.582658000	2.920657000
C	2.400790000	-4.059082000	1.354030000
H	1.393268000	-4.332498000	1.689654000
C	3.427691000	-5.046042000	1.926338000
H	3.191908000	-6.069735000	1.605205000
H	3.388246000	-5.038600000	3.023964000
C	0.699249000	-2.626855000	-8.638221000
H	0.241718000	-3.109817000	-7.770515000
H	0.555908000	-3.277478000	-9.507828000
H	0.163870000	-1.689662000	-8.827283000
C	2.828080000	-1.726370000	-9.652390000
H	3.895840000	-1.535928000	-9.508471000
H	2.344668000	-0.776772000	-9.907521000
H	2.714304000	-2.393625000	-10.512501000
C	2.194629000	-2.355149000	-8.408837000
H	2.684725000	-3.321125000	-8.232784000
C	2.413724000	-1.504856000	-7.186121000
C	2.771008000	-0.167892000	-7.112027000
H	2.994261000	0.487830000	-7.940092000
C	2.821563000	0.140114000	-5.740180000
C	3.295803000	1.431779000	-5.127899000
C	2.589623000	2.641512000	-5.782919000
H	1.506743000	2.563254000	-5.618291000
H	2.747550000	2.621538000	-6.868924000
C	4.821397000	1.568107000	-5.382841000

H	5.338356000	0.711340000	-4.931832000
H	5.017836000	1.525886000	-6.462010000
C	3.060173000	1.483599000	-3.610703000
H	3.567586000	0.638622000	-3.125252000
H	1.987813000	1.396117000	-3.391153000
C	3.120861000	3.959224000	-5.200459000
H	2.601983000	4.799951000	-5.679566000
C	4.630548000	4.065615000	-5.465217000
H	5.015717000	5.015541000	-5.071378000
H	4.826178000	4.066208000	-6.546325000
C	5.352782000	2.884943000	-4.798402000
H	6.431119000	2.954260000	-4.993238000
C	5.094583000	2.912216000	-3.284507000
H	5.485409000	3.842502000	-2.850794000
H	5.625108000	2.084141000	-2.795897000
C	3.585226000	2.800263000	-3.023134000
H	3.385198000	2.798175000	-1.947090000
C	2.863952000	3.982711000	-3.686810000
H	3.218321000	4.929355000	-3.258007000
H	1.785953000	3.927225000	-3.485056000
C	-0.174085000	-6.875052000	-7.211121000
H	0.299648000	-7.530958000	-7.948579000
H	-0.854006000	-6.200676000	-7.740397000
H	-0.773886000	-7.508388000	-6.548726000
C	0.893524000	-6.101706000	-6.430180000
H	1.492579000	-5.537104000	-7.152579000
C	1.832725000	-7.068065000	-5.690696000
H	2.316465000	-7.752108000	-6.396851000
H	1.271485000	-7.668464000	-4.966474000
H	2.610860000	-6.529484000	-5.143136000
C	0.271861000	-5.122712000	-5.468125000
C	-0.936741000	-5.240649000	-4.805215000
H	-1.656840000	-6.037491000	-4.911797000
C	-1.032755000	-4.114844000	-3.972772000
C	-2.189705000	-3.815656000	-3.053602000
C	-2.009852000	-2.526927000	-2.233547000
H	-1.862568000	-1.673206000	-2.908726000
H	-1.123235000	-2.600767000	-1.583466000
C	-3.483841000	-3.680956000	-3.898563000
H	-3.370219000	-2.848413000	-4.606370000
H	-3.625506000	-4.587826000	-4.499810000
C	-2.379907000	-4.995199000	-2.066192000
H	-1.471989000	-5.108017000	-1.459635000
H	-2.503964000	-5.930352000	-2.626893000
C	-3.599337000	-4.757586000	-1.163740000
H	-3.706080000	-5.606499000	-0.475740000
C	-3.397337000	-3.461814000	-0.366018000
H	-4.256153000	-3.285823000	0.295082000
H	-2.509891000	-3.535958000	0.274249000
C	-3.234243000	-2.283249000	-1.335517000
H	-3.064098000	-1.367048000	-0.760200000
C	-4.497442000	-2.155179000	-2.198276000
H	-4.408749000	-1.301477000	-2.884188000
H	-5.368889000	-1.961404000	-1.558904000
C	-4.703899000	-3.449140000	-2.997315000
H	-5.601607000	-3.361918000	-3.623921000
C	-4.861146000	-4.633538000	-2.031763000

H	-5.743547000	-4.484985000	-1.395235000
H	-5.027323000	-5.561454000	-2.596289000
B	2.253940000	-3.434082000	-5.431992000
N	3.250800000	-3.620004000	-4.267126000
N	2.912358000	-3.304210000	-2.983552000
N	2.256071000	-1.952579000	-5.908628000
N	2.491804000	-0.940171000	-5.021363000
N	0.853409000	-3.966110000	-5.045234000
N	0.055897000	-3.344265000	-4.123309000
O	-0.420489000	0.004797000	-4.160184000
Yb	1.177255000	-1.433933000	-2.921417000
H	2.638350000	-4.095141000	-6.352303000

Int'

C	0.289614000	-0.051544000	0.519580000
C	1.143933000	2.647807000	4.233152000
H	1.449199000	3.573659000	3.733476000
H	1.445255000	1.804712000	3.606514000
C	1.663301000	2.579161000	5.663430000
H	1.735829000	1.539157000	6.001266000
H	2.650899000	3.037403000	5.764184000
C	0.567589000	3.315857000	6.436709000
H	0.690813000	4.399381000	6.333823000
H	0.550651000	3.074212000	7.503070000
C	-0.692205000	2.848163000	5.720679000
H	-1.060794000	1.898336000	6.123725000
H	-1.506967000	3.575476000	5.726862000
C	-6.121156000	-1.195836000	3.430699000
H	-6.761894000	-1.796915000	4.085622000
H	-5.807292000	-1.825525000	2.590908000
H	-5.225817000	-0.912221000	3.988980000
C	-8.154845000	-0.372637000	2.178674000
H	-8.811342000	-0.945413000	2.841563000
H	-8.710545000	0.498147000	1.817578000
H	-7.923782000	-1.008398000	1.316607000
C	-6.881411000	0.038812000	2.921408000
H	-7.177481000	0.629843000	3.797913000
C	-5.998529000	0.908301000	2.068646000
C	-5.990118000	1.066889000	0.693239000
H	-6.660581000	0.602961000	-0.014589000
C	-4.963485000	1.990313000	0.416688000
C	-4.696972000	2.660280000	-0.909268000
C	-4.376521000	1.631245000	-2.016870000
H	-3.461667000	1.086518000	-1.750930000
H	-5.184257000	0.889537000	-2.081804000
C	-3.548999000	3.682074000	-0.836103000
H	-3.758834000	4.414330000	-0.046714000
H	-2.605539000	3.181207000	-0.577918000
C	-5.992562000	3.418116000	-1.313124000
H	-6.831788000	2.712332000	-1.365079000
H	-6.239419000	4.146990000	-0.530210000
C	-5.816860000	4.124048000	-2.664168000
H	-6.748947000	4.645447000	-2.920879000
C	-5.495867000	3.078088000	-3.743002000
H	-5.381042000	3.566611000	-4.720177000
H	-6.327447000	2.365833000	-3.836761000
C	-4.201099000	2.340905000	-3.368993000

C	-3.050557000	3.353967000	-3.270291000
H	-2.107386000	2.855680000	-3.018044000
H	-2.903489000	3.853286000	-4.238050000
C	-3.374067000	4.393185000	-2.187280000
H	-2.540798000	5.100891000	-2.107645000
C	-4.664895000	5.134358000	-2.561847000
H	-4.899483000	5.896882000	-1.806789000
H	-4.535728000	5.660110000	-3.517857000
C	-4.400700000	3.042461000	7.632031000
H	-4.174753000	3.724296000	6.807917000
H	-5.123158000	3.533389000	8.293437000
H	-3.480104000	2.877523000	8.203239000
C	-5.320839000	0.783612000	8.288062000
H	-5.723372000	-0.171758000	7.938208000
H	-4.445778000	0.574219000	8.913322000
H	-6.072779000	1.257691000	8.926994000
C	-4.962397000	1.705822000	7.119420000
H	-5.884466000	1.922842000	6.566433000
C	-4.006000000	1.044009000	6.164886000
C	-3.103179000	0.021637000	6.410619000
H	-2.966980000	-0.501984000	7.343690000
C	-2.432364000	-0.202648000	5.195599000
C	-1.456741000	-1.320488000	4.905097000
C	-1.013075000	-2.000904000	6.219534000
H	-0.526519000	-1.263771000	6.873025000
H	-1.893571000	-2.375763000	6.757564000
C	-2.157577000	-2.389229000	4.027555000
H	-2.481004000	-1.925907000	3.088126000
H	-3.061489000	-2.741040000	4.542535000
C	-0.195808000	-0.834951000	4.163903000
H	0.314627000	-0.078334000	4.772300000
C	-0.060586000	-3.171536000	5.939281000
H	0.236125000	-3.627038000	6.893410000
C	-0.782628000	-4.214231000	5.072147000
H	-0.119335000	-5.068221000	4.878901000
H	-1.659878000	-4.605006000	5.605578000
C	-1.211091000	-3.565874000	3.747909000
H	-1.734256000	-4.305912000	3.128327000
C	0.031897000	-3.051067000	3.007877000
H	0.710757000	-3.885289000	2.782903000
H	-0.254182000	-2.599654000	2.050328000
C	0.751646000	-2.009092000	3.877323000
H	1.628925000	-1.631133000	3.340227000
C	1.182977000	-2.658053000	5.199940000
H	1.876840000	-3.487850000	5.008532000
H	1.720190000	-1.930322000	5.823792000
C	-7.464505000	5.767078000	5.362067000
H	-8.508416000	5.581956000	5.635361000
H	-6.899475000	5.957349000	6.279651000
H	-7.442469000	6.679270000	4.755871000
C	-6.901456000	4.570058000	4.589920000
H	-7.011580000	3.682618000	5.223769000
C	-7.705763000	4.327132000	3.302957000
H	-8.765087000	4.171231000	3.536008000
H	-7.628449000	5.191650000	2.634700000
H	-7.340322000	3.451197000	2.760583000
C	-5.436535000	4.749338000	4.287502000

C	-4.728159000	5.932360000	4.175377000
H	-5.115180000	6.924738000	4.339750000
C	-3.414959000	5.573573000	3.829232000
C	-2.283208000	6.551303000	3.577147000
C	-2.045513000	6.744962000	2.058654000
H	-1.766698000	5.788455000	1.601870000
H	-2.982006000	7.070944000	1.586432000
C	-0.959613000	6.097970000	4.228308000
H	-0.663555000	5.121464000	3.829213000
H	-1.116027000	5.972519000	5.308943000
C	-2.656981000	7.931238000	4.172081000
H	-3.582568000	8.294111000	3.707975000
H	-2.854322000	7.828068000	5.247780000
C	-1.546189000	8.961908000	3.931371000
H	-1.849062000	9.920894000	4.372795000
C	-1.335109000	9.130861000	2.419603000
H	-0.554105000	9.878890000	2.227350000
H	-2.256707000	9.502583000	1.950971000
C	-0.933975000	7.779095000	1.811499000
H	-0.784285000	7.886319000	0.729813000
C	0.370568000	7.297307000	2.464110000
H	0.685031000	6.347929000	2.015240000
H	1.172475000	8.025700000	2.281180000
C	0.154001000	7.128566000	3.975415000
H	1.082752000	6.772830000	4.442216000
C	-0.246079000	8.478351000	4.588123000
H	0.553614000	9.215344000	4.434169000
H	-0.386611000	8.379563000	5.673598000
B	-4.886707000	2.228604000	4.025193000
N	-5.010248000	1.701834000	2.571823000
N	-4.355257000	2.343948000	1.555691000
N	-3.865420000	1.397467000	4.859358000
N	-2.885967000	0.652619000	4.261413000
N	-4.566390000	3.738236000	4.028987000
N	-3.323195000	4.231750000	3.736545000
O	-0.300029000	2.638817000	4.343617000
S	-1.320747000	0.141975000	0.400837000
S	1.652723000	-0.715820000	-0.112561000
Yb	-1.995193000	2.360034000	2.502772000
H	-5.957397000	2.086329000	4.549948000
C	-0.197768000	0.023856000	-3.429010000
H	-1.009227000	-0.347176000	-2.792957000
H	0.398330000	0.733318000	-2.851150000
C	-0.710302000	0.579032000	-4.747024000
C	-0.847937000	-0.684445000	-5.597129000
H	-1.770992000	-1.217496000	-5.342634000
H	-0.857649000	-0.487056000	-6.672508000
C	0.374380000	-1.490718000	-5.175364000
H	1.255077000	-1.243892000	-5.778205000
H	0.221936000	-2.573423000	-5.198229000
C	7.332450000	-4.286491000	-5.322996000
H	7.858513000	-4.748349000	-6.165938000
H	8.031348000	-3.614380000	-4.813713000
H	6.513959000	-3.679250000	-5.718804000
C	7.974748000	-6.230790000	-3.846649000
H	8.463372000	-6.733949000	-4.687117000
H	7.628434000	-6.995998000	-3.145452000

H	8.735824000	-5.627040000	-3.340626000
C	6.818825000	-5.362581000	-4.352702000
H	6.132461000	-6.012476000	-4.906864000
C	6.057635000	-4.737269000	-3.212507000
C	6.520515000	-4.440222000	-1.942311000
H	7.497408000	-4.669383000	-1.548513000
C	5.459814000	-3.804992000	-1.278746000
C	5.492650000	-3.274161000	0.137891000
C	5.632083000	-1.731455000	0.148349000
H	4.766497000	-1.275730000	-0.351990000
H	6.521723000	-1.442356000	-0.426634000
C	4.226904000	-3.656979000	0.934776000
H	4.107663000	-4.748471000	0.931587000
H	3.334720000	-3.239035000	0.449414000
C	6.720637000	-3.861785000	0.874204000
H	7.636837000	-3.584032000	0.337930000
H	6.661728000	-4.958201000	0.865676000
C	6.807802000	-3.343441000	2.314760000
H	7.686552000	-3.787877000	2.800462000
C	6.949683000	-1.814302000	2.288592000
H	7.031993000	-1.422777000	3.311206000
H	7.871960000	-1.531011000	1.763120000
C	5.725767000	-1.204593000	1.590382000
H	5.817209000	-0.111345000	1.564345000
C	4.457730000	-1.598457000	2.361307000
H	3.578726000	-1.139828000	1.894777000
H	4.515552000	-1.220387000	3.391125000
C	4.316904000	-3.128690000	2.376345000
H	3.402191000	-3.408169000	2.913376000
C	5.537005000	-3.742178000	3.077353000
H	5.447677000	-4.836518000	3.114075000
H	5.590841000	-3.390134000	4.116154000
C	2.242286000	-4.295017000	-7.787407000
H	1.823815000	-4.694951000	-6.859876000
H	2.195683000	-5.079374000	-8.550595000
H	1.606232000	-3.466444000	-8.118005000
C	4.275865000	-3.310216000	-8.914405000
H	5.311609000	-2.978257000	-8.795731000
H	3.692953000	-2.471057000	-9.309875000
H	4.257543000	-4.105406000	-9.666131000
C	3.691297000	-3.818758000	-7.594429000
H	4.284991000	-4.684677000	-7.274382000
C	3.784387000	-2.779004000	-6.510259000
C	3.996353000	-1.413865000	-6.630275000
H	4.171295000	-0.868321000	-7.544842000
C	3.972687000	-0.901652000	-5.319567000
C	4.333890000	0.495771000	-4.880926000
C	3.788263000	1.546700000	-5.873398000
H	2.691789000	1.491829000	-5.901559000
H	4.144966000	1.322210000	-6.886813000
C	5.884497000	0.599185000	-4.869821000
H	6.287389000	-0.147916000	-4.173970000
H	6.272059000	0.349367000	-5.866184000
C	3.823990000	0.839550000	-3.467413000
H	4.226363000	0.113661000	-2.745159000
H	2.728586000	0.773432000	-3.438390000
C	4.237551000	2.958278000	-5.469040000

H	3.835202000	3.681567000	-6.190157000
C	5.772503000	3.028506000	-5.469073000
H	6.101469000	4.041643000	-5.203237000
H	6.163038000	2.819410000	-6.474721000
C	6.331590000	2.010199000	-4.464003000
H	7.428865000	2.051945000	-4.466058000
C	5.801007000	2.328723000	-3.057644000
H	6.127130000	3.330074000	-2.747507000
H	6.214114000	1.618383000	-2.328672000
C	4.266528000	2.255281000	-3.061314000
H	3.873229000	2.477046000	-2.062893000
C	3.708724000	3.275757000	-4.064054000
H	4.002068000	4.290090000	-3.765321000
H	2.612817000	3.251334000	-4.052054000
C	2.050538000	-8.461107000	-5.751477000
H	2.684126000	-9.164704000	-6.300784000
H	1.364408000	-7.991892000	-6.462840000
H	1.455629000	-9.044714000	-5.040644000
C	2.917551000	-7.422182000	-5.033662000
H	3.532239000	-6.919656000	-5.788258000
C	3.862491000	-8.101853000	-4.028985000
H	4.507500000	-8.827255000	-4.536755000
H	3.287903000	-8.635237000	-3.264148000
H	4.497297000	-7.372361000	-3.518757000
C	2.076209000	-6.379588000	-4.345677000
C	0.810067000	-6.532733000	-3.806262000
H	0.196427000	-7.419620000	-3.845624000
C	0.489801000	-5.303918000	-3.211754000
C	-0.818277000	-4.976330000	-2.536831000
C	-0.803925000	-3.625853000	-1.801209000
H	-0.563191000	-2.817568000	-2.504845000
H	-0.028548000	-3.634582000	-1.019973000
C	-1.939596000	-4.939599000	-3.609224000
H	-1.707349000	-4.162919000	-4.350275000
H	-1.958877000	-5.894834000	-4.149348000
C	-1.171667000	-6.082735000	-1.510787000
H	-0.388554000	-6.128868000	-0.742652000
H	-1.185191000	-7.060545000	-2.007930000
C	-2.538031000	-5.809392000	-0.865465000
H	-2.759388000	-6.608680000	-0.146194000
C	-2.496402000	-4.456071000	-0.143301000
H	-3.461138000	-4.252808000	0.339553000
H	-1.739169000	-4.475312000	0.650773000
C	-2.171210000	-3.346582000	-1.153227000
H	-2.128209000	-2.378353000	-0.642870000
C	-3.258159000	-3.312997000	-2.237854000
H	-3.054107000	-2.505746000	-2.954262000
H	-4.232218000	-3.091752000	-1.782563000
C	-3.304173000	-4.665143000	-2.962480000
H	-4.074461000	-4.643839000	-3.744607000
C	-3.623007000	-5.778603000	-1.952756000
H	-4.606999000	-5.604046000	-1.498018000
H	-3.675471000	-6.749363000	-2.464488000
B	3.814971000	-4.439866000	-4.485845000
N	4.771708000	-4.301957000	-3.281511000
N	4.398228000	-3.718234000	-2.100977000
N	3.637566000	-3.052518000	-5.182750000

N	3.735707000	-1.896073000	-4.455779000
N	2.475759000	-5.105882000	-4.083551000
N	1.507255000	-4.442173000	-3.381205000
O	0.645238000	-1.102948000	-3.803910000
Yb	2.322021000	-2.293067000	-2.481755000
H	4.335444000	-5.162480000	-5.283706000
C	-0.052623000	3.374793000	-0.440023000
S	0.183398000	3.680676000	1.174575000
S	0.645557000	3.640554000	-1.877600000
H	-3.976223000	1.590098000	-4.139998000
H	0.025312000	1.262820000	-5.183910000
H	-1.646567000	1.126200000	-4.624938000
H	-0.478364000	-0.358477000	3.218586000

¹TS4

C	5.464519000	0.324355000	-0.100471000
C	6.391659000	2.300130000	3.949175000
H	6.754274000	3.251580000	3.543097000
H	6.689882000	1.500757000	3.267243000
C	6.841679000	2.098512000	5.389904000
H	6.841851000	1.033977000	5.649821000
H	7.846754000	2.491223000	5.566382000
C	5.751488000	2.838353000	6.167853000
H	5.936888000	3.917903000	6.150188000
H	5.672520000	2.523801000	7.212142000
C	4.502137000	2.493169000	5.367297000
H	4.060152000	1.545098000	5.693698000
H	3.732501000	3.268051000	5.382609000
C	-1.259173000	-1.019547000	2.742647000
H	-1.977047000	-1.584877000	3.347538000
H	-1.012261000	-1.618597000	1.859510000
H	-0.343905000	-0.890293000	3.325733000
C	-3.158923000	0.133038000	1.542053000
H	-3.891079000	-0.401080000	2.156247000
H	-3.599135000	1.088043000	1.239339000
H	-2.990460000	-0.464232000	0.639072000
C	-1.857799000	0.333119000	2.322992000
H	-2.095075000	0.889309000	3.239043000
C	-0.862099000	1.145448000	1.541297000
C	-0.795750000	1.369864000	0.176427000
H	-1.497115000	1.025040000	-0.568754000
C	0.347872000	2.164763000	-0.028722000
C	0.751903000	2.836560000	-1.318403000
C	0.852196000	1.817459000	-2.476202000
H	1.629034000	1.079808000	-2.238919000
H	-0.094795000	1.270024000	-2.573763000
C	2.090896000	3.586865000	-1.205702000
H	2.036739000	4.314246000	-0.386159000
H	2.892309000	2.876280000	-0.967138000
C	-0.350853000	3.871121000	-1.676570000
H	-1.319829000	3.361478000	-1.757097000
H	-0.440803000	4.597306000	-0.858313000
C	-0.021200000	4.586042000	-2.994177000
H	-0.817983000	5.307272000	-3.220811000
C	0.072803000	3.549493000	-4.124250000
H	0.290344000	4.049384000	-5.078010000
H	-0.890200000	3.034352000	-4.244524000

C	1.179383000	2.535186000	-3.795094000
C	2.519922000	3.271436000	-3.656745000
H	3.325808000	2.561355000	-3.435422000
H	2.777611000	3.771198000	-4.600875000
C	2.422706000	4.303885000	-2.524154000
H	3.385351000	4.817567000	-2.416001000
C	1.320170000	5.320228000	-2.855371000
H	1.253916000	6.079423000	-2.064455000
H	1.560367000	5.849745000	-3.787577000
C	0.678032000	2.553863000	7.277065000
H	0.945292000	3.314103000	6.538353000
H	-0.052522000	2.989310000	7.967796000
H	1.577250000	2.304212000	7.851254000
C	-0.326765000	0.268037000	7.655776000
H	-0.738826000	-0.633100000	7.191880000
H	0.516285000	-0.031565000	8.288370000
H	-1.091699000	0.695063000	8.312251000
C	0.101853000	1.296580000	6.605420000
H	-0.792370000	1.598439000	6.046803000
C	1.076662000	0.709532000	5.620772000
C	1.932633000	-0.367525000	5.791966000
H	2.009111000	-0.991403000	6.668397000
C	2.649115000	-0.489657000	4.589059000
C	3.612346000	-1.597437000	4.227343000
C	4.024106000	-2.377217000	5.496348000
H	4.506805000	-1.695604000	6.210228000
H	3.129545000	-2.778210000	5.990343000
C	2.914337000	-2.589950000	3.262091000
H	2.618581000	-2.055648000	2.351484000
H	1.995571000	-2.966093000	3.731766000
C	4.891759000	-1.079155000	3.540684000
H	5.398171000	-0.367934000	4.204215000
C	4.966781000	-3.537802000	5.150770000
H	5.239218000	-4.064108000	6.075296000
C	4.248098000	-4.504664000	4.197957000
H	4.902934000	-5.352273000	3.954795000
H	3.355219000	-4.919558000	4.685554000
C	3.853826000	-3.755497000	2.916716000
H	3.333387000	-4.442665000	2.236871000
C	5.117006000	-3.206996000	2.236678000
H	5.789146000	-4.031845000	1.963005000
H	4.857383000	-2.678495000	1.311246000
C	5.832683000	-2.242024000	3.192622000
H	6.723194000	-1.837100000	2.698841000
C	6.230432000	-2.989774000	4.472695000
H	6.917972000	-3.812676000	4.234124000
H	6.764774000	-2.317059000	5.158002000
C	-1.819610000	5.811006000	5.331481000
H	-2.860645000	5.692378000	5.649054000
H	-1.194468000	5.879628000	6.226889000
H	-1.748589000	6.763697000	4.795460000
C	-1.403365000	4.636510000	4.440499000
H	-1.562020000	3.713969000	5.010099000
C	-2.287039000	4.570383000	3.184168000
H	-3.343521000	4.480760000	3.461088000
H	-2.168464000	5.480518000	2.586363000
H	-2.023560000	3.718678000	2.551409000

C	0.055257000	4.715651000	4.070350000
C	0.846832000	5.846679000	3.981660000
H	0.547899000	6.854789000	4.218455000
C	2.105329000	5.410539000	3.536685000
C	3.291383000	6.312698000	3.253011000
C	3.544474000	6.430776000	1.730185000
H	3.764376000	5.442354000	1.309888000
H	2.630437000	6.791509000	1.239984000
C	4.584370000	5.808165000	3.928692000
H	4.817031000	4.798166000	3.572491000
H	4.418073000	5.734990000	5.012690000
C	2.999227000	7.734830000	3.789685000
H	2.093817000	8.129083000	3.310977000
H	2.798963000	7.686752000	4.868596000
C	4.169745000	8.687036000	3.511342000
H	3.923857000	9.679749000	3.911362000
C	4.393850000	8.781234000	1.994676000
H	5.217709000	9.473756000	1.775394000
H	3.496835000	9.186601000	1.506840000
C	4.716545000	7.384584000	1.444728000
H	4.875816000	7.437169000	0.360362000
C	5.988538000	6.855927000	2.124520000
H	6.251330000	5.875026000	1.711802000
H	6.831484000	7.529341000	1.917572000
C	5.758302000	6.759055000	3.640130000
H	6.663312000	6.369077000	4.125656000
C	5.437165000	8.154607000	4.194517000
H	6.279833000	8.835643000	4.014811000
H	5.287791000	8.108813000	5.282167000
B	0.366702000	2.186835000	3.594467000
N	0.201286000	1.784180000	2.107015000
N	0.959322000	2.387107000	1.140695000
N	1.288280000	1.195538000	4.368382000
N	2.263984000	0.475539000	3.735610000
N	0.827951000	3.658054000	3.704174000
N	2.088151000	4.073718000	3.368293000
O	4.946163000	2.339869000	3.997864000
S	3.793792000	0.227611000	-0.101865000
S	6.778496000	-0.520149000	-0.701639000
Yb	3.291842000	2.111544000	2.094861000
H	-0.714094000	2.115678000	4.108722000
C	4.910091000	-0.037528000	-4.285624000
H	4.108454000	-0.457523000	-3.666322000
H	5.403699000	0.755307000	-3.719110000
C	4.401364000	0.373943000	-5.657775000
C	4.426527000	-0.955335000	-6.415934000
H	3.542638000	-1.551897000	-6.164210000
H	4.453757000	-0.836176000	-7.502515000
C	5.693724000	-1.615139000	-5.881202000
H	6.574519000	-1.361706000	-6.480164000
H	5.623977000	-2.703410000	-5.800386000
C	12.629606000	-4.286803000	-5.537181000
H	13.164546000	-4.851986000	-6.308530000
H	13.317485000	-3.540773000	-5.124623000
H	11.803794000	-3.750997000	-6.012981000
C	13.295318000	-6.000692000	-3.807899000
H	13.796178000	-6.603949000	-4.571986000

H	12.956759000	-6.670920000	-3.012084000
H	14.044410000	-5.323148000	-3.384044000
C	12.128496000	-5.226699000	-4.428854000
H	11.453110000	-5.956621000	-4.888942000
C	11.355359000	-4.463099000	-3.384707000
C	11.814995000	-3.979996000	-2.172680000
H	12.799843000	-4.125291000	-1.760119000
C	10.742098000	-3.282935000	-1.595698000
C	10.773417000	-2.579227000	-0.254399000
C	10.633193000	-1.046010000	-0.409660000
H	9.670722000	-0.799356000	-0.875768000
H	11.422352000	-0.674379000	-1.077137000
C	9.652611000	-3.085489000	0.682573000
H	9.737828000	-4.174444000	0.796307000
H	8.671339000	-2.885386000	0.234107000
C	12.133287000	-2.858640000	0.428396000
H	12.946310000	-2.499344000	-0.216066000
H	12.268625000	-3.941960000	0.546090000
C	12.225441000	-2.170985000	1.795474000
H	13.202001000	-2.397405000	2.243767000
C	12.080328000	-0.653675000	1.607486000
H	12.158526000	-0.141782000	2.576070000
H	12.896561000	-0.273130000	0.978086000
C	10.720967000	-0.352701000	0.961023000
H	10.605449000	0.729111000	0.818869000
C	9.599223000	-0.874499000	1.871830000
H	8.624094000	-0.636335000	1.431685000
H	9.652049000	-0.375220000	2.849466000
C	9.746266000	-2.392976000	2.052733000
H	8.939772000	-2.767928000	2.695167000
C	11.103718000	-2.698765000	2.700888000
H	11.220554000	-3.780759000	2.851970000
H	11.162389000	-2.229335000	3.692128000
C	7.643078000	-4.714865000	-8.010068000
H	7.217794000	-5.011994000	-7.047633000
H	7.636549000	-5.588484000	-8.670906000
H	6.988852000	-3.954525000	-8.451084000
C	9.672657000	-3.816820000	-9.214983000
H	10.695859000	-3.440995000	-9.119860000
H	9.076207000	-3.053018000	-9.726226000
H	9.694621000	-4.701354000	-9.859249000
C	9.072197000	-4.170632000	-7.852451000
H	9.682979000	-4.969427000	-7.412237000
C	9.109592000	-2.998481000	-6.909313000
C	9.300679000	-1.654822000	-7.195523000
H	9.495911000	-1.223090000	-8.165718000
C	9.223625000	-0.983037000	-5.960623000
C	9.496686000	0.475831000	-5.692749000
C	8.682066000	1.380933000	-6.645001000
H	7.610170000	1.204780000	-6.485624000
H	8.897337000	1.113539000	-7.687939000
C	11.005826000	0.746306000	-5.944212000
H	11.601067000	0.104591000	-5.281876000
H	11.260846000	0.463867000	-6.973993000
C	9.174791000	0.871267000	-4.240168000
H	9.753347000	0.241525000	-3.550903000
H	8.107217000	0.708212000	-4.032438000

C	9.016686000	2.860733000	-6.401678000
H	8.422800000	3.479765000	-7.086883000
C	10.513220000	3.098306000	-6.657137000
H	10.755845000	4.158409000	-6.505181000
H	10.764395000	2.859847000	-7.699792000
C	11.340064000	2.225215000	-5.700953000
H	12.410407000	2.384952000	-5.886439000
C	11.003879000	2.590178000	-4.247832000
H	11.255259000	3.641253000	-4.053910000
H	11.606660000	1.984710000	-3.557746000
C	9.507785000	2.351413000	-3.994369000
H	9.256439000	2.602615000	-2.957849000
C	8.682796000	3.226896000	-4.949342000
H	8.897096000	4.287744000	-4.766524000
H	7.611783000	3.084321000	-4.760170000
C	7.581703000	-8.630015000	-5.303985000
H	8.271783000	-9.389867000	-5.684479000
H	6.928999000	-8.319672000	-6.125540000
H	6.959602000	-9.108106000	-4.539591000
C	8.365502000	-7.446767000	-4.727751000
H	9.010534000	-7.053858000	-5.521356000
C	9.267057000	-7.901730000	-3.568370000
H	9.963728000	-8.678142000	-3.903319000
H	8.662884000	-8.315748000	-2.753906000
H	9.847324000	-7.068628000	-3.162486000
C	7.446671000	-6.340835000	-4.279676000
C	6.153451000	-6.457027000	-3.800412000
H	5.571552000	-7.363097000	-3.728220000
C	5.751510000	-5.161407000	-3.444892000
C	4.373924000	-4.792890000	-2.950105000
C	4.250577000	-3.326110000	-2.508884000
H	4.530369000	-2.668871000	-3.340644000
H	4.940431000	-3.118036000	-1.677214000
C	3.361509000	-5.042933000	-4.101514000
H	3.629589000	-4.413507000	-4.961060000
H	3.439993000	-6.084558000	-4.438051000
C	3.975608000	-5.695492000	-1.756398000
H	4.678975000	-5.534649000	-0.929110000
H	4.057610000	-6.751930000	-2.041474000
C	2.540126000	-5.388867000	-1.302452000
H	2.286955000	-6.040455000	-0.455726000
C	2.442125000	-3.917989000	-0.875149000
H	1.424533000	-3.689584000	-0.531655000
H	3.113996000	-3.720957000	-0.031720000
C	2.813054000	-3.013041000	-2.057594000
H	2.764337000	-1.964559000	-1.742754000
C	1.836967000	-3.268809000	-3.214826000
H	2.071501000	-2.612501000	-4.064608000
H	0.812767000	-3.026407000	-2.901980000
C	1.927821000	-4.739079000	-3.646326000
H	1.238870000	-4.927164000	-4.480589000
C	1.566787000	-5.649274000	-2.462262000
H	0.535332000	-5.456321000	-2.138830000
H	1.613774000	-6.703253000	-2.769003000
B	9.114927000	-4.383462000	-4.684796000
N	10.059351000	-4.071137000	-3.504649000
N	9.673893000	-3.338090000	-2.414243000

N	8.923752000	-3.104462000	-5.561973000
N	8.976903000	-1.865067000	-4.986339000
N	7.785454000	-5.024393000	-4.212273000
N	6.751116000	-4.295289000	-3.688784000
O	5.889745000	-1.074832000	-4.550739000
Yb	7.530355000	-2.041123000	-2.983166000
H	9.657917000	-5.193832000	-5.376821000
C	5.845204000	2.541737000	-0.661537000
S	5.602656000	3.312470000	0.771128000
S	6.327816000	2.797868000	-2.170923000
H	1.242692000	1.790749000	-4.601283000
H	5.083522000	1.096253000	-6.119405000
H	3.408287000	0.826796000	-5.611413000
H	4.631947000	-0.546835000	2.617547000

⁰TS4

C	4.993726000	0.406276000	0.019642000
C	6.644284000	1.717415000	2.880482000
H	7.016553000	2.649546000	2.437090000
H	6.750643000	0.918889000	2.143778000
C	7.304818000	1.454957000	4.225928000
H	7.221548000	0.396533000	4.493734000
H	8.364230000	1.725957000	4.229218000
C	6.453050000	2.311294000	5.164343000
H	6.763234000	3.360892000	5.107177000
H	6.510190000	1.999916000	6.211272000
C	5.054212000	2.122660000	4.586452000
H	4.551983000	1.253822000	5.023081000
H	4.404267000	2.994319000	4.691789000
C	-1.391426000	-0.566965000	3.985572000
H	-1.969801000	-0.860080000	4.869304000
H	-1.488798000	-1.360934000	3.237067000
H	-0.338520000	-0.501946000	4.271221000
C	-3.398295000	0.672744000	3.085644000
H	-3.975351000	0.427249000	3.983275000
H	-3.779783000	1.614875000	2.680500000
H	-3.590193000	-0.114666000	2.348324000
C	-1.907321000	0.767008000	3.422471000
H	-1.786309000	1.526615000	4.204351000
C	-1.099404000	1.203822000	2.230166000
C	-1.385807000	1.044737000	0.886843000
H	-2.278398000	0.608272000	0.463941000
C	-0.296890000	1.602353000	0.191865000
C	-0.257017000	1.782371000	-1.308068000
C	-0.368242000	0.416074000	-2.025638000
H	0.486344000	-0.210188000	-1.741077000
H	-1.272843000	-0.106850000	-1.689555000
C	1.014891000	2.489780000	-1.795136000
H	1.099495000	3.462309000	-1.294220000
H	1.891127000	1.896386000	-1.509913000
C	-1.476726000	2.646419000	-1.729285000
H	-2.404887000	2.168098000	-1.392222000
H	-1.420841000	3.618451000	-1.222207000
C	-1.513352000	2.838862000	-3.252013000
H	-2.384535000	3.453061000	-3.516638000
C	-1.622297000	1.466986000	-3.934818000
H	-1.667921000	1.589601000	-5.025649000

H	-2.551449000	0.966620000	-3.629903000
C	-0.408666000	0.607514000	-3.549492000
C	0.878456000	1.310832000	-4.004936000
H	1.748084000	0.693063000	-3.744046000
H	0.877122000	1.430323000	-5.097711000
C	0.984034000	2.681271000	-3.318841000
H	1.908820000	3.183934000	-3.633032000
C	-0.226877000	3.540436000	-3.710968000
H	-0.151352000	4.532564000	-3.246224000
H	-0.247188000	3.696715000	-4.798473000
C	1.945081000	3.265879000	6.845725000
H	2.017214000	3.841416000	5.919401000
H	1.475362000	3.899406000	7.606186000
H	2.961419000	3.033094000	7.182920000
C	1.002875000	1.209013000	7.965680000
H	0.408829000	0.297924000	7.845510000
H	1.985454000	0.924703000	8.358921000
H	0.515305000	1.834967000	8.719748000
C	1.133839000	1.975605000	6.647752000
H	0.125960000	2.269307000	6.325985000
C	1.719854000	1.112922000	5.562295000
C	2.337018000	-0.124041000	5.669608000
H	2.480090000	-0.693569000	6.574272000
C	2.697005000	-0.493618000	4.359745000
C	3.292924000	-1.812943000	3.919337000
C	3.360001000	-2.783067000	5.121398000
H	3.993343000	-2.353492000	5.909797000
H	2.355909000	-2.908471000	5.548095000
C	2.400683000	-2.458180000	2.830781000
H	2.336845000	-1.788199000	1.965974000
H	1.381493000	-2.574730000	3.222113000
C	4.721827000	-1.656711000	3.352099000
H	5.368489000	-1.202663000	4.114894000
C	3.920645000	-4.147747000	4.698652000
H	3.951917000	-4.808403000	5.575449000
C	3.016672000	-4.761552000	3.619691000
H	3.399431000	-5.747363000	3.322255000
H	2.005515000	-4.917746000	4.019908000
C	2.966796000	-3.821291000	2.406684000
H	2.316572000	-4.251389000	1.633827000
C	4.383803000	-3.632408000	1.844815000
H	4.793288000	-4.599240000	1.519994000
H	4.359274000	-2.973737000	0.967806000
C	5.285337000	-3.021255000	2.926952000
H	6.293318000	-2.876075000	2.520639000
C	5.338704000	-3.962427000	4.138829000
H	5.759830000	-4.934106000	3.846428000
H	5.997868000	-3.548111000	4.914338000
C	-1.085083000	6.498054000	4.253050000
H	-2.154871000	6.555828000	4.479410000
H	-0.530872000	6.596996000	5.191432000
H	-0.838515000	7.359262000	3.622276000
C	-0.764705000	5.177755000	3.545475000
H	-1.089365000	4.358919000	4.196967000
C	-1.545814000	5.062610000	2.225757000
H	-2.623420000	5.139783000	2.409820000
H	-1.260090000	5.869344000	1.541607000

H	-1.349638000	4.110684000	1.726039000
C	0.713367000	5.023189000	3.307019000
C	1.647618000	6.014758000	3.072425000
H	1.471724000	7.079967000	3.079050000
C	2.868580000	5.355095000	2.856758000
C	4.182980000	6.086546000	2.675370000
C	4.123400000	6.977680000	1.409395000
H	3.967284000	6.344495000	0.527624000
H	3.259293000	7.651300000	1.473680000
C	5.404808000	5.161807000	2.572275000
H	5.288828000	4.478321000	1.726570000
H	5.465880000	4.542700000	3.472654000
C	4.402845000	7.014548000	3.901443000
H	3.545411000	7.688498000	4.015949000
H	4.445676000	6.403613000	4.813010000
C	5.691763000	7.836365000	3.748613000
H	5.812959000	8.480856000	4.629482000
C	5.598708000	8.701772000	2.482560000
H	6.507962000	9.308108000	2.371959000
H	4.755936000	9.401567000	2.564857000
C	5.414517000	7.795087000	1.256085000
H	5.344057000	8.410933000	0.349738000
C	6.611958000	6.841330000	1.140788000
H	6.503949000	6.201421000	0.255935000
H	7.541174000	7.413020000	1.011233000
C	6.697941000	5.978327000	2.408494000
H	7.547046000	5.287363000	2.323261000
C	6.891798000	6.886190000	3.631352000
H	7.823388000	7.460179000	3.534485000
H	6.983235000	6.280751000	4.543768000
B	0.746377000	2.455020000	3.561399000
N	0.108146000	1.827245000	2.306905000
N	0.622342000	2.055046000	1.060642000
N	1.724128000	1.451180000	4.243144000
N	2.340344000	0.478222000	3.504557000
N	1.367658000	3.832566000	3.232169000
N	2.689512000	4.021438000	2.929418000
O	5.239044000	1.870651000	3.173134000
S	3.479859000	-0.207115000	-0.433790000
S	6.503950000	-0.291452000	-0.407095000
Yb	3.342283000	1.770164000	1.542276000
H	-0.131072000	2.652099000	4.358608000
C	5.178447000	0.622905000	-3.805963000
H	4.375720000	0.239254000	-3.166978000
H	5.767673000	1.337151000	-3.226415000
C	4.657652000	1.174268000	-5.125251000
C	4.597081000	-0.081399000	-5.997267000
H	3.696493000	-0.660696000	-5.766016000
H	4.597034000	0.133267000	-7.069425000
C	5.848070000	-0.833533000	-5.562219000
H	6.733628000	-0.520507000	-6.125592000
H	5.757864000	-1.921433000	-5.628294000
C	12.754984000	-3.547134000	-5.127237000
H	13.355610000	-3.998406000	-5.924954000
H	13.380598000	-2.815503000	-4.604577000
H	11.922802000	-3.007524000	-5.587323000
C	13.441430000	-5.402603000	-3.560273000

H	14.006889000	-5.892962000	-4.359167000
H	13.107691000	-6.171147000	-2.856716000
H	14.132729000	-4.737156000	-3.031698000
C	12.260318000	-4.625695000	-4.149985000
H	11.644620000	-5.333350000	-4.716957000
C	11.402076000	-4.024509000	-3.067472000
C	11.774702000	-3.660714000	-1.784797000
H	12.746390000	-3.795696000	-1.338410000
C	10.631207000	-3.106118000	-1.189698000
C	10.530128000	-2.599391000	0.231015000
C	10.195246000	-1.091548000	0.281461000
H	9.229784000	-0.896457000	-0.202713000
H	10.957233000	-0.530407000	-0.276196000
C	9.448900000	-3.377698000	1.017187000
H	9.675095000	-4.451473000	0.978722000
H	8.471354000	-3.240749000	0.537231000
C	11.885457000	-2.805732000	0.946985000
H	12.671941000	-2.263685000	0.405066000
H	12.153136000	-3.870330000	0.924507000
C	11.827894000	-2.317982000	2.399692000
H	12.805847000	-2.481926000	2.871295000
C	11.487508000	-0.820530000	2.418909000
H	11.454615000	-0.452993000	3.453454000
H	12.270203000	-0.249559000	1.900995000
C	10.129303000	-0.603261000	1.737498000
H	9.873737000	0.463882000	1.741187000
C	9.048881000	-1.393569000	2.491135000
H	8.072345000	-1.219950000	2.023098000
H	8.984554000	-1.040237000	3.528671000
C	9.390972000	-2.889931000	2.472595000
H	8.616096000	-3.452869000	3.008457000
C	10.749505000	-3.109510000	3.153320000
H	11.003582000	-4.178248000	3.160884000
H	10.702758000	-2.784711000	4.201405000
C	7.753815000	-3.994710000	-7.772255000
H	7.328627000	-4.360699000	-6.834134000
H	7.749343000	-4.818238000	-8.494434000
H	7.099018000	-3.205505000	-8.158284000
C	9.778886000	-2.997609000	-8.905788000
H	10.803788000	-2.634408000	-8.783500000
H	9.182850000	-2.191916000	-9.348834000
H	9.795084000	-3.825640000	-9.621221000
C	9.182225000	-3.461882000	-7.575354000
H	9.795243000	-4.292539000	-7.201773000
C	9.221374000	-2.370754000	-6.539937000
C	9.448194000	-1.013872000	-6.707082000
H	9.672935000	-0.507225000	-7.633740000
C	9.359792000	-0.447246000	-5.420096000
C	9.656275000	0.983000000	-5.042269000
C	8.813966000	1.963833000	-5.890129000
H	7.748737000	1.780827000	-5.699960000
H	8.984699000	1.774783000	-6.957929000
C	11.156652000	1.262928000	-5.330431000
H	11.771168000	0.571262000	-4.740056000
H	11.371302000	1.056224000	-6.386708000
C	9.393573000	1.270221000	-3.552062000
H	9.983824000	0.582254000	-2.933754000

H	8.332975000	1.095840000	-3.321252000
C	9.170089000	3.418548000	-5.551450000
H	8.555320000	4.091373000	-6.163502000
C	10.657563000	3.664781000	-5.848434000
H	10.917309000	4.709173000	-5.630599000
H	10.862985000	3.501149000	-6.915124000
C	11.513865000	2.717470000	-4.994423000
H	12.577266000	2.884290000	-5.210317000
C	11.239109000	2.975717000	-3.505973000
H	11.505635000	4.008275000	-3.244125000
H	11.863145000	2.317305000	-2.887063000
C	9.752399000	2.725890000	-3.212949000
H	9.553932000	2.902541000	-2.149483000
C	8.896968000	3.677433000	-4.062238000
H	9.129295000	4.720392000	-3.810081000
H	7.832803000	3.527916000	-3.837434000
C	8.012942000	-8.261682000	-5.090619000
H	8.787625000	-8.980468000	-5.376545000
H	7.441946000	-8.000131000	-5.986573000
H	7.337424000	-8.770635000	-4.394535000
C	8.651776000	-7.027187000	-4.447027000
H	9.361812000	-6.603369000	-5.166016000
C	9.436128000	-7.416546000	-3.182786000
H	10.203487000	-8.160863000	-3.422309000
H	8.764273000	-7.850838000	-2.434583000
H	9.925939000	-6.549926000	-2.730882000
C	7.623853000	-5.972833000	-4.133959000
C	6.289456000	-6.154189000	-3.815443000
H	5.753368000	-7.090754000	-3.792707000
C	5.771456000	-4.875652000	-3.561988000
C	4.314348000	-4.580482000	-3.301218000
C	4.017091000	-3.094180000	-3.049044000
H	4.379132000	-2.494462000	-3.891946000
H	4.540799000	-2.740095000	-2.148227000
C	3.511241000	-5.032767000	-4.552928000
H	3.862776000	-4.471403000	-5.429248000
H	3.714729000	-6.091616000	-4.755783000
C	3.805221000	-5.391951000	-2.084841000
H	4.358829000	-5.086932000	-1.187855000
H	4.008188000	-6.459699000	-2.237642000
C	2.298446000	-5.169154000	-1.881216000
H	1.966419000	-5.751994000	-1.012090000
C	2.027341000	-3.677408000	-1.642128000
H	0.954472000	-3.509402000	-1.479146000
H	2.546255000	-3.328271000	-0.742007000
C	2.508153000	-2.870358000	-2.855130000
H	2.336700000	-1.804521000	-2.668963000
C	1.742762000	-3.324096000	-4.105728000
H	2.058329000	-2.741274000	-4.982498000
H	0.667567000	-3.144344000	-3.973564000
C	2.006569000	-4.816406000	-4.348324000
H	1.470625000	-5.149677000	-5.247051000
C	1.536412000	-5.630804000	-3.133156000
H	0.456243000	-5.499023000	-2.986181000
H	1.706952000	-6.701872000	-3.309338000
B	9.203436000	-3.932433000	-4.445282000
N	10.090795000	-3.699176000	-3.207412000

N	9.608219000	-3.123949000	-2.064394000
N	9.007318000	-2.585422000	-5.209573000
N	9.073805000	-1.400017000	-4.527337000
N	7.876166000	-4.637887000	-4.069011000
N	6.745453000	-3.956866000	-3.699040000
O	6.046529000	-0.483899000	-4.171215000
Yb	7.455936000	-1.806527000	-2.651301000
H	9.792475000	-4.666947000	-5.185904000
C	5.489335000	3.216272000	-0.582249000
S	3.978541000	3.683854000	-0.733761000
S	7.049129000	3.106948000	-0.606248000
H	-0.483254000	-0.374629000	-4.034965000
H	5.361164000	1.900242000	-5.547730000
H	3.689937000	1.667271000	-5.009257000
H	4.713284000	-0.979364000	2.491030000

Int5

C	-0.565141000	-0.626826000	0.474944000
C	1.139197000	1.417963000	3.385627000
H	1.530935000	2.077911000	2.604148000
H	1.095414000	0.401063000	2.987965000
C	1.922323000	1.527108000	4.689437000
H	1.841921000	0.599063000	5.266228000
H	2.983397000	1.727058000	4.516764000
C	1.196797000	2.664691000	5.410882000
H	1.526934000	3.635122000	5.025261000
H	1.348076000	2.657893000	6.494005000
C	-0.253248000	2.399937000	5.030344000
H	-0.719838000	1.667639000	5.698745000
H	-0.878883000	3.294192000	4.992525000
C	-7.006624000	0.174971000	4.930713000
H	-7.635997000	0.043415000	5.818176000
H	-7.106409000	-0.720023000	4.307072000
H	-5.964974000	0.242538000	5.254510000
C	-8.913938000	1.328551000	3.746310000
H	-9.542512000	1.228828000	4.637203000
H	-9.241659000	2.215256000	3.194996000
H	-9.096743000	0.450799000	3.116482000
C	-7.439586000	1.424857000	4.147173000
H	-7.326964000	2.289846000	4.812889000
C	-6.555316000	1.648183000	2.949914000
C	-6.814329000	1.379297000	1.617121000
H	-7.735790000	0.999495000	1.202013000
C	-5.644834000	1.731093000	0.919470000
C	-5.496649000	1.752423000	-0.580971000
C	-5.829941000	0.362970000	-1.173656000
H	-5.115879000	-0.374386000	-0.786521000
H	-6.829276000	0.048543000	-0.845713000
C	-4.089592000	2.162982000	-1.045636000
H	-3.838208000	3.149814000	-0.636373000
H	-3.345824000	1.448842000	-0.669983000
C	-6.511832000	2.780143000	-1.150776000
H	-7.525782000	2.517716000	-0.822918000
H	-6.291194000	3.771583000	-0.733945000
C	-6.449385000	2.819270000	-2.684322000
H	-7.177027000	3.552918000	-3.056594000
C	-6.785668000	1.427932000	-3.242250000

H	-6.761937000	1.444715000	-4.340695000
H	-7.804643000	1.139513000	-2.949796000
C	-5.772803000	0.404268000	-2.707418000
C	-4.358294000	0.809226000	-3.143839000
H	-3.634441000	0.071639000	-2.774131000
H	-4.293280000	0.816721000	-4.241708000
C	-4.024664000	2.200931000	-2.581063000
H	-3.009081000	2.492226000	-2.878524000
C	-5.034711000	3.221769000	-3.125142000
H	-4.794957000	4.226061000	-2.751352000
H	-4.978315000	3.265546000	-4.221879000
C	-3.153094000	4.060849000	7.364035000
H	-3.006432000	4.495737000	6.371870000
H	-3.535440000	4.844773000	8.027284000
H	-2.176300000	3.743780000	7.746447000
C	-4.366268000	2.314797000	8.725351000
H	-5.063023000	1.471265000	8.710919000
H	-3.430754000	1.974071000	9.183129000
H	-4.784262000	3.091404000	9.373959000
C	-4.126399000	2.871615000	7.319714000
H	-5.085290000	3.243982000	6.936960000
C	-3.647248000	1.802133000	6.375579000
C	-3.075641000	0.574765000	6.670163000
H	-2.905526000	0.165822000	7.653587000
C	-2.801285000	-0.033916000	5.430971000
C	-2.302878000	-1.448075000	5.217098000
C	-2.060746000	-2.134333000	6.581220000
H	-1.305052000	-1.574335000	7.149583000
H	-2.986339000	-2.116733000	7.171798000
C	-3.373124000	-2.266960000	4.452358000
H	-3.557497000	-1.798733000	3.479513000
H	-4.317521000	-2.238114000	5.012644000
C	-0.985636000	-1.501466000	4.413526000
H	-0.213612000	-0.924745000	4.940339000
C	-1.598744000	-3.586380000	6.394350000
H	-1.436501000	-4.039126000	7.381867000
C	-2.679416000	-4.371965000	5.636485000
H	-2.367810000	-5.418212000	5.512353000
H	-3.612920000	-4.382594000	6.215726000
C	-2.910934000	-3.720277000	4.265396000
H	-3.686408000	-4.273204000	3.718934000
C	-1.602228000	-3.738944000	3.461786000
H	-1.271807000	-4.775113000	3.302334000
H	-1.765551000	-3.285978000	2.476409000
C	-0.523480000	-2.955063000	4.224483000
H	0.407927000	-2.955047000	3.644536000
C	-0.288726000	-3.607438000	5.593537000
H	0.060037000	-4.641702000	5.467308000
H	0.496772000	-3.069612000	6.142798000
C	-5.758965000	7.219048000	5.019707000
H	-6.713870000	7.430845000	5.511805000
H	-4.956259000	7.388513000	5.743807000
H	-5.641847000	7.945455000	4.208042000
C	-5.746640000	5.782557000	4.488294000
H	-5.935822000	5.111789000	5.334079000
C	-6.874249000	5.575017000	3.464248000
H	-7.846991000	5.812146000	3.909808000

H	-6.728326000	6.230006000	2.598371000
H	-6.903475000	4.544100000	3.101908000
C	-4.407399000	5.424680000	3.897912000
C	-3.457622000	6.279141000	3.366216000
H	-3.510386000	7.355490000	3.340042000
C	-2.416519000	5.462353000	2.897175000
C	-1.139804000	5.957556000	2.248230000
C	-1.146602000	5.713461000	0.719896000
H	-1.242581000	4.640872000	0.517064000
H	-2.024984000	6.203969000	0.279147000
C	0.104849000	5.271847000	2.852068000
H	0.039532000	4.188918000	2.698595000
H	0.117577000	5.448344000	3.936675000
C	-1.003230000	7.482330000	2.476550000
H	-1.865848000	7.999096000	2.036633000
H	-1.014531000	7.696145000	3.553722000
C	0.283702000	8.026835000	1.843146000
H	0.344023000	9.107303000	2.030766000
C	0.251089000	7.765712000	0.329928000
H	1.158891000	8.164241000	-0.143366000
H	-0.602283000	8.288879000	-0.123041000
C	0.143981000	6.254330000	0.080588000
H	0.116023000	6.056333000	-0.998631000
C	1.361934000	5.551444000	0.700191000
H	1.310540000	4.473704000	0.506454000
H	2.285320000	5.927118000	0.237272000
C	1.392297000	5.815686000	2.212784000
H	2.257258000	5.304694000	2.657559000
C	1.498600000	7.325375000	2.466870000
H	2.427885000	7.719204000	2.033082000
H	1.537360000	7.529345000	3.545943000
B	-4.631755000	2.862418000	4.215162000
N	-5.287040000	2.138450000	3.019990000
N	-4.715097000	2.167954000	1.779324000
N	-3.700050000	1.904129000	5.018702000
N	-3.162667000	0.790868000	4.433017000
N	-3.931621000	4.159392000	3.751487000
N	-2.715084000	4.168514000	3.127175000
O	-0.205590000	1.844381000	3.697816000
S	-2.245331000	-0.811617000	0.776721000
S	0.683358000	-1.954337000	0.597461000
Yb	-2.215219000	1.741166000	2.186974000
H	-5.511759000	3.188007000	4.962886000
C	-0.419002000	0.096667000	-3.212813000
H	-1.237252000	-0.453484000	-2.735032000
H	-0.012068000	0.803653000	-2.486483000
C	-0.849174000	0.724513000	-4.528198000
C	-0.693309000	-0.440954000	-5.505807000
H	-1.546009000	-1.124047000	-5.422924000
H	-0.611025000	-0.126473000	-6.549759000
C	0.582547000	-1.105623000	-5.008003000
H	1.476126000	-0.658377000	-5.456423000
H	0.611651000	-2.187544000	-5.161019000
C	7.739502000	-2.429378000	-4.612264000
H	8.441334000	-2.527092000	-5.447943000
H	8.207257000	-1.797952000	-3.849136000
H	6.845882000	-1.912946000	-4.972643000

C	8.671511000	-4.538516000	-3.584261000
H	9.346625000	-4.673851000	-4.435159000
H	8.447441000	-5.524584000	-3.166316000
H	9.213717000	-3.963650000	-2.825516000
C	7.399882000	-3.811840000	-4.031688000
H	6.939074000	-4.404643000	-4.830408000
C	6.406208000	-3.692941000	-2.905988000
C	6.650242000	-3.709600000	-1.543543000
H	7.603974000	-3.868295000	-1.065373000
C	5.406713000	-3.509866000	-0.924210000
C	5.157534000	-3.495985000	0.565663000
C	5.492543000	-2.105395000	1.160863000
H	4.855259000	-1.342864000	0.692873000
H	6.530392000	-1.845146000	0.914983000
C	3.701382000	-3.845078000	0.915877000
H	3.441451000	-4.823362000	0.492041000
H	3.023194000	-3.115083000	0.451793000
C	6.073321000	-4.542148000	1.251147000
H	7.123964000	-4.316702000	1.032248000
H	5.866183000	-5.536387000	0.834685000
C	5.863734000	-4.543045000	2.771925000
H	6.525404000	-5.294284000	3.222638000
C	6.204645000	-3.152608000	3.329848000
H	6.079492000	-3.141232000	4.420700000
H	7.257250000	-2.912390000	3.126640000
C	5.285736000	-2.104926000	2.683542000
H	5.526148000	-1.108642000	3.076826000
C	3.823259000	-2.447661000	3.001050000
H	3.154230000	-1.693476000	2.569248000
H	3.660408000	-2.436954000	4.086896000
C	3.485868000	-3.836696000	2.437140000
H	2.436521000	-4.074350000	2.649165000
C	4.400800000	-4.885210000	3.086596000
H	4.158523000	-5.888069000	2.710079000
H	4.239565000	-4.903426000	4.172505000
C	2.996116000	-3.005217000	-7.824109000
H	2.527737000	-3.605325000	-7.039396000
H	3.135867000	-3.642039000	-8.704321000
H	2.304028000	-2.201007000	-8.097612000
C	5.010969000	-1.638681000	-8.494244000
H	5.973915000	-1.223292000	-8.182487000
H	4.377642000	-0.811404000	-8.833396000
H	5.184428000	-2.291896000	-9.355081000
C	4.342398000	-2.423674000	-7.362907000
H	4.996831000	-3.265791000	-7.104460000
C	4.177603000	-1.581652000	-6.126530000
C	4.181060000	-0.200694000	-6.010529000
H	4.348088000	0.512881000	-6.803092000
C	3.966694000	0.074159000	-4.647515000
C	4.043729000	1.430804000	-3.993271000
C	3.217177000	2.474101000	-4.780005000
H	2.161728000	2.172458000	-4.787105000
H	3.546828000	2.501516000	-5.826566000
C	5.529759000	1.883335000	-4.005069000
H	6.132410000	1.148544000	-3.455752000
H	5.901305000	1.891422000	-5.037886000
C	3.558271000	1.421225000	-2.534732000

H	4.137237000	0.686688000	-1.958763000
H	2.504532000	1.114337000	-2.498608000
C	3.365099000	3.867362000	-4.150929000
H	2.767447000	4.585395000	-4.727477000
C	4.843118000	4.287403000	-4.177640000
H	4.955922000	5.292344000	-3.749951000
H	5.204558000	4.339336000	-5.213893000
C	5.678449000	3.276105000	-3.377659000
H	6.736463000	3.568597000	-3.401846000
C	5.183044000	3.234804000	-1.924317000
H	5.300179000	4.220671000	-1.455360000
H	5.788318000	2.528675000	-1.339839000
C	3.705694000	2.814214000	-1.902318000
H	3.340711000	2.775214000	-0.869188000
C	2.870581000	3.827666000	-2.697994000
H	2.956586000	4.822671000	-2.242902000
H	1.809877000	3.550755000	-2.656040000
C	3.310561000	-7.466948000	-6.557027000
H	4.097070000	-7.953655000	-7.142499000
H	2.601523000	-7.008059000	-7.252618000
H	2.783683000	-8.251181000	-6.002954000
C	3.924314000	-6.431505000	-5.610319000
H	4.485944000	-5.713923000	-6.218921000
C	4.911892000	-7.100140000	-4.640022000
H	5.707685000	-7.611516000	-5.192566000
H	4.396593000	-7.842943000	-4.021517000
H	5.372586000	-6.369867000	-3.969303000
C	2.863255000	-5.675323000	-4.854755000
C	1.584309000	-6.095419000	-4.532786000
H	1.119186000	-7.026193000	-4.819883000
C	1.019885000	-5.067914000	-3.762053000
C	-0.373914000	-5.077061000	-3.185381000
C	-0.653552000	-3.866934000	-2.283082000
H	-0.515904000	-2.936935000	-2.851027000
H	0.060140000	-3.857321000	-1.447421000
C	-1.414664000	-5.082002000	-4.334357000
H	-1.284724000	-4.178999000	-4.946237000
H	-1.229837000	-5.939426000	-4.994133000
C	-0.578507000	-6.363667000	-2.345097000
H	0.155702000	-6.384594000	-1.528963000
H	-0.385012000	-7.246924000	-2.966905000
C	-2.006399000	-6.423351000	-1.783047000
H	-2.120349000	-7.343820000	-1.195563000
C	-2.255901000	-5.199841000	-0.889857000
H	-3.268135000	-5.237666000	-0.467070000
H	-1.558980000	-5.198542000	-0.041534000
C	-2.081919000	-3.918536000	-1.717843000
H	-2.248121000	-3.041923000	-1.080439000
C	-3.089516000	-3.919125000	-2.876042000
H	-2.993569000	-2.994699000	-3.461961000
H	-4.113545000	-3.937361000	-2.481238000
C	-2.843217000	-5.141912000	-3.772414000
H	-3.556560000	-5.143831000	-4.607149000
C	-3.012423000	-6.425437000	-2.943931000
H	-4.036833000	-6.488888000	-2.554227000
H	-2.856524000	-7.308568000	-3.578703000
B	4.286299000	-3.541719000	-4.400960000

N	5.070689000	-3.495202000	-3.071165000
N	4.451633000	-3.358147000	-1.858696000
N	3.964813000	-2.091713000	-4.881034000
N	3.818652000	-1.075452000	-3.973974000
N	3.034490000	-4.443444000	-4.301731000
N	1.906449000	-4.066701000	-3.624339000
O	0.622760000	-0.853495000	-3.578650000
Yb	2.291828000	-2.027484000	-2.230798000
H	5.002775000	-4.029838000	-5.225756000
C	0.202478000	0.471729000	0.205019000
S	-0.175085000	2.139057000	0.054037000
S	1.896558000	-0.250740000	0.181996000
H	-6.010137000	-0.591890000	-3.104116000
H	-0.176975000	1.546094000	-4.799080000
H	-1.866213000	1.117304000	-4.481498000
H	-1.137807000	-1.039798000	3.431835000

4B

C	6.074976000	-0.421815000	0.139475000
C	8.840299000	0.427190000	3.333283000
H	9.360795000	1.036384000	2.588137000
H	8.333978000	-0.389514000	2.815928000
C	9.753327000	-0.025861000	4.464409000
H	9.372563000	-0.942962000	4.926328000
H	10.770340000	-0.220048000	4.114493000
C	9.661883000	1.144368000	5.445832000
H	10.305538000	1.968136000	5.119706000
H	9.940824000	0.876328000	6.468565000
C	8.195234000	1.535109000	5.334799000
H	7.561046000	0.930258000	5.992180000
H	7.999299000	2.593453000	5.518794000
C	1.109840000	1.854185000	6.160170000
H	0.564672000	1.815772000	7.109844000
H	0.619331000	1.170929000	5.458687000
H	2.124579000	1.486269000	6.331846000
C	-0.318316000	3.803162000	5.426728000
H	-0.841497000	3.798493000	6.388142000
H	-0.333943000	4.824584000	5.034588000
H	-0.887821000	3.166929000	4.740399000
C	1.111969000	3.286766000	5.602417000
H	1.614450000	3.929092000	6.336836000
C	1.889792000	3.366477000	4.316267000
C	1.419378000	3.467834000	3.017268000
H	0.388027000	3.551397000	2.710364000
C	2.556220000	3.477160000	2.191259000
C	2.576563000	3.726556000	0.703883000
C	1.956019000	2.541349000	-0.072906000
H	2.539750000	1.633606000	0.123038000
H	0.936325000	2.356805000	0.291254000
C	4.002210000	3.973488000	0.180417000
H	4.459943000	4.803523000	0.733581000
H	4.625446000	3.084186000	0.344485000
C	1.730534000	4.994831000	0.410753000
H	0.706117000	4.851517000	0.776771000
H	2.148764000	5.846134000	0.963951000
C	1.703823000	5.298372000	-1.094238000
H	1.095277000	6.195960000	-1.267724000

C	1.090491000	4.105567000	-1.843183000
H	1.052950000	4.316285000	-2.920819000
H	0.055020000	3.944448000	-1.513336000
C	1.933173000	2.848819000	-1.578443000
H	1.495962000	1.993307000	-2.110807000
C	3.368840000	3.087675000	-2.070064000
H	3.978791000	2.195337000	-1.886393000
H	3.372780000	3.274971000	-3.152654000
C	3.978260000	4.282812000	-1.323376000
H	5.007412000	4.446036000	-1.665606000
C	3.136601000	5.538194000	-1.589715000
H	3.573988000	6.404488000	-1.075428000
H	3.132851000	5.771070000	-2.663306000
C	6.380531000	3.451235000	8.404050000
H	6.577081000	4.010420000	7.485511000
H	6.386524000	4.157753000	9.241230000
H	7.202731000	2.743164000	8.556258000
C	4.748825000	1.988215000	9.656393000
H	3.789743000	1.462552000	9.628620000
H	5.530910000	1.256430000	9.887148000
H	4.719755000	2.707400000	10.480986000
C	5.035316000	2.710027000	8.337105000
H	4.250209000	3.462124000	8.187468000
C	4.986340000	1.764021000	7.167441000
C	5.084604000	0.381836000	7.164481000
H	5.181948000	-0.255068000	8.029051000
C	4.987386000	-0.017703000	5.819418000
C	4.899080000	-1.442683000	5.314280000
C	4.916871000	-2.425942000	6.507307000
H	5.853673000	-2.309801000	7.070104000
H	4.095230000	-2.185100000	7.195121000
C	3.566396000	-1.642132000	4.549039000
H	3.530916000	-0.959877000	3.693610000
H	2.729635000	-1.381304000	5.211224000
C	6.066476000	-1.814902000	4.373884000
H	6.069363000	-1.144128000	3.507691000
H	7.017775000	-1.682886000	4.907611000
C	4.780308000	-3.878246000	6.027422000
H	4.796376000	-4.543889000	6.900896000
C	3.451734000	-4.043589000	5.273264000
H	3.335385000	-5.083537000	4.939610000
H	2.608964000	-3.825569000	5.943757000
C	3.432958000	-3.094362000	4.067476000
H	2.484665000	-3.201837000	3.525201000
C	4.602592000	-3.431069000	3.130865000
H	4.507601000	-4.464611000	2.770507000
H	4.589129000	-2.776920000	2.251664000
C	5.927707000	-3.266872000	3.890067000
H	6.763633000	-3.495316000	3.217949000
C	5.951549000	-4.218047000	5.093446000
H	5.874369000	-5.259716000	4.754144000
H	6.903768000	-4.127244000	5.634778000
C	5.135150000	7.709302000	7.018251000
H	4.437622000	8.147417000	7.739302000
H	6.040459000	7.411875000	7.555967000
H	5.406337000	8.496855000	6.306922000
C	4.481158000	6.519095000	6.309771000

H	4.172096000	5.801496000	7.078037000
C	3.221764000	6.965831000	5.549629000
H	2.507102000	7.437252000	6.233266000
H	3.481958000	7.694748000	4.774556000
H	2.726504000	6.122262000	5.061458000
C	5.449848000	5.829018000	5.384488000
C	6.557399000	6.372475000	4.757209000
H	6.931076000	7.375784000	4.879660000
C	7.096772000	5.355440000	3.955843000
C	8.323998000	5.496175000	3.076098000
C	7.937514000	5.584583000	1.578970000
H	7.407169000	4.675534000	1.270956000
H	7.244155000	6.424054000	1.434319000
C	9.303847000	4.319399000	3.266611000
H	8.806674000	3.376892000	3.012098000
H	9.588569000	4.260551000	4.326600000
C	9.068766000	6.801709000	3.444015000
H	8.401764000	7.660440000	3.295562000
H	9.340792000	6.783226000	4.507944000
C	10.324074000	6.988641000	2.580666000
H	10.823795000	7.920409000	2.877207000
C	9.909753000	7.069264000	1.103858000
H	10.793647000	7.219658000	0.469616000
H	9.251107000	7.934337000	0.945223000
C	9.192844000	5.770637000	0.709120000
H	8.888406000	5.818226000	-0.343848000
C	10.144234000	4.582080000	0.914459000
H	9.654567000	3.651686000	0.606275000
H	11.036328000	4.705899000	0.285587000
C	10.555428000	4.505112000	2.392508000
H	11.226514000	3.648869000	2.542752000
C	11.273375000	5.801090000	2.793087000
H	12.182863000	5.930512000	2.191338000
H	11.588910000	5.754996000	3.844747000
B	4.261280000	3.523258000	5.392997000
N	3.247435000	3.316256000	4.247495000
N	3.659988000	3.353258000	2.944340000
N	4.841736000	2.158296000	5.873428000
N	4.863035000	1.071574000	5.037732000
N	5.351124000	4.538040000	4.974023000
N	6.353297000	4.236721000	4.089009000
O	7.826708000	1.254087000	3.963415000
S	4.828241000	0.045878000	1.254063000
S	5.883522000	-1.973739000	-0.619004000
Yb	5.792876000	2.052867000	2.892751000
H	3.671571000	3.997640000	6.321223000
C	7.195925000	0.421918000	-0.139580000
S	8.442686000	-0.045785000	-1.254153000
S	7.387385000	1.973846000	0.618905000
C	4.430872000	-0.426596000	-3.333427000
H	3.910241000	-1.035609000	-2.588227000
H	4.937382000	0.390036000	-2.816148000
C	3.517937000	0.026558000	-4.464580000
H	3.898927000	0.943508000	-4.926611000
H	2.500979000	0.221042000	-4.114671000
C	3.609073000	-1.143810000	-5.445871000
H	2.965219000	-1.967380000	-5.119636000

H	3.330170000	-0.875818000	-6.468626000
C	5.075628000	-1.534911000	-5.334825000
H	5.709955000	-0.930337000	-5.992328000
H	5.271273000	-2.593339000	-5.518657000
C	12.161269000	-1.855039000	-6.160470000
H	12.706443000	-1.816855000	-7.110150000
H	12.651953000	-1.171836000	-5.459057000
H	11.146622000	-1.486886000	-6.332179000
C	13.588950000	-3.804296000	-5.426867000
H	14.112112000	-3.799842000	-6.388292000
H	13.604331000	-4.825686000	-5.034634000
H	14.158621000	-3.168139000	-4.740606000
C	12.158791000	-3.287566000	-5.602578000
H	11.656136000	-3.929841000	-6.336925000
C	11.380981000	-3.366962000	-4.316402000
C	11.851409000	-3.468272000	-3.017403000
H	12.882750000	-3.552016000	-2.710518000
C	10.714586000	-3.477350000	-2.191368000
C	10.694220000	-3.726671000	-0.703978000
C	11.315009000	-2.541553000	0.072750000
H	10.731458000	-1.633701000	-0.123225000
H	12.334738000	-2.357235000	-0.291427000
C	9.268531000	-3.973305000	-0.180480000
H	8.810621000	-4.803264000	-0.733612000
H	8.645472000	-3.083881000	-0.344560000
C	11.540007000	-4.995094000	-0.410802000
H	12.564449000	-4.851992000	-0.776833000
H	11.121608000	-5.846343000	-0.963955000
C	11.566671000	-5.298577000	1.094202000
H	12.175049000	-6.196273000	1.267720000
C	12.180240000	-4.105859000	1.843092000
H	12.217745000	-4.316545000	2.920736000
H	13.215742000	-3.944957000	1.513237000
C	11.337804000	-2.848959000	1.578301000
H	11.775190000	-1.993508000	2.110619000
C	9.902092000	-3.087504000	2.069943000
H	9.292313000	-2.195060000	1.886221000
H	9.898124000	-3.274736000	3.152543000
C	9.292434000	-4.282564000	1.323325000
H	8.263252000	-4.445572000	1.665571000
C	10.133853000	-5.538098000	1.589710000
H	9.696288000	-6.404328000	1.075467000
H	10.137578000	-5.770927000	2.663312000
C	6.890105000	-3.451015000	-8.404052000
H	6.693552000	-4.010190000	-7.485509000
H	6.883995000	-4.157520000	-9.241243000
H	6.067966000	-2.742861000	-8.556202000
C	8.521870000	-1.988125000	-9.656466000
H	9.481004000	-1.462554000	-9.628746000
H	7.739839000	-1.256261000	-9.887155000
H	8.550817000	-2.707296000	-10.481076000
C	8.235395000	-2.709937000	-8.337177000
H	9.020443000	-3.462110000	-8.187605000
C	8.284530000	-1.763961000	-7.167495000
C	8.186416000	-0.381764000	-7.164494000
H	8.089092000	0.255172000	-8.029044000
C	8.283770000	0.017726000	-5.819425000

C	8.372261000	1.442668000	-5.314209000
C	8.354523000	2.426014000	-6.507166000
H	7.417673000	2.310026000	-7.069913000
H	9.176096000	2.185125000	-7.195048000
C	9.704994000	1.641913000	-4.549005000
H	9.740436000	0.959587000	-3.693629000
H	10.541707000	1.381046000	-5.211238000
C	7.204942000	1.814939000	-4.373735000
H	7.202022000	1.144095000	-3.507595000
H	6.253606000	1.683065000	-4.907430000
C	8.491267000	3.878267000	-6.027177000
H	8.475238000	4.543981000	-6.900598000
C	9.819886000	4.043408000	-5.273056000
H	9.936365000	5.083318000	-4.939327000
H	10.662609000	3.825342000	-5.943594000
C	9.838609000	3.094087000	-4.067337000
H	10.786937000	3.201421000	-3.525097000
C	8.669052000	3.430844000	-3.130651000
H	8.764175000	4.464345000	-2.770211000
H	8.682485000	2.776615000	-2.251506000
C	7.343889000	3.266859000	-3.889817000
H	6.508010000	3.495342000	-3.217654000
C	7.320101000	4.218127000	-5.093127000
H	7.397405000	5.259762000	-4.753751000
H	6.367850000	4.127465000	-5.634425000
C	8.135241000	-7.709296000	-7.018296000
H	8.832723000	-8.147454000	-7.739367000
H	7.229923000	-7.411840000	-7.555981000
H	7.864047000	-8.496828000	-6.306947000
C	8.789316000	-6.519101000	-6.309868000
H	9.098376000	-5.801535000	-7.078165000
C	10.048732000	-6.965866000	-5.549781000
H	10.763325000	-7.437360000	-6.233440000
H	9.788548000	-7.694729000	-4.774654000
H	10.544072000	-6.122299000	-5.061686000
C	7.820702000	-5.828957000	-5.384557000
C	6.713144000	-6.372351000	-4.757239000
H	6.339432000	-7.375652000	-4.879643000
C	6.173847000	-5.355280000	-3.955868000
C	4.946678000	-5.495976000	-3.076039000
C	5.333268000	-5.584389000	-1.578942000
H	5.863658000	-4.675358000	-1.270963000
H	6.026618000	-6.423877000	-1.434338000
C	3.966849000	-4.319168000	-3.266486000
H	4.464077000	-3.376681000	-3.012005000
H	3.682059000	-4.260316000	-4.326457000
C	4.201847000	-6.801487000	-3.443904000
H	4.868837000	-7.660237000	-3.295499000
H	3.929747000	-6.782998000	-4.507814000
C	2.946600000	-6.988387000	-2.580462000
H	2.446831000	-7.920141000	-2.876969000
C	3.361024000	-7.069018000	-1.103682000
H	2.477168000	-7.219386000	-0.469381000
H	4.019659000	-7.934108000	-0.945089000
C	4.077994000	-5.770411000	-0.708996000
H	4.382505000	-5.818004000	0.343950000
C	3.126620000	-4.581827000	-0.914274000

H	3.616339000	-3.651447000	-0.606127000
H	2.234566000	-4.705618000	-0.285340000
C	2.715326000	-4.504852000	-2.392293000
H	2.044245000	-3.648597000	-2.542489000
C	1.997315000	-5.800811000	-2.792817000
H	1.087869000	-5.930209000	-2.190999000
H	1.681703000	-5.754711000	-3.844453000
B	9.009452000	-3.523315000	-5.393087000
N	10.023352000	-3.316440000	-4.247607000
N	9.610822000	-3.353335000	-2.944441000
N	8.429134000	-2.158286000	-5.873496000
N	8.407995000	-1.071587000	-5.037780000

References

- [1] X. Shi, P. Deng, T. Rajeshkumar, L. Zhao, L. Maron and J. Cheng, *Chem. Commun.*, 2021, **57**, 10047-10050.
- [2] SMART Software Users Guide, Version 4.21; Bruker AXS, Inc.: Madison, WI, 1997.
- [3] SAINT, Version 6.45; Bruker AXS, Inc.: Madison, WI, 2003.
- [4] G. M. Sheldrick, SADABS, Version 2.10; Bruker AXS, Inc.: Madison, WI, 2003.
- [5] G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3–8.
- [6] L. Palatinus and G. Chapuis, *J. Appl. Cryst.*, 2007, **40**, 786–790.
- [7] L. Palatinus, S. J. Prathapa and S. van Smaalen, *J. Appl. Cryst.*, 2012, **45**, 575–580.
- [8] A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, *J. Appl. Cryst.*, 1999, **32**, 115–119.
- [9] L. J. Farrugia, *J. Appl. Cryst.*, 2012, **45**, 849–854.
- [10] P. Van der. Sluis and A. L. Spek, *Acta Cryst.*, 1990, **A46**, 194–201.
- [11] A. L. Spek, *Acta Cryst.*, 2009, **D65**, 148–155.
- [12] A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652.
- [13] (a) D. Andrae, U. Häussermann, M. Dolg, H. Stoll and H. Preuss, *Theor. Chim. Acta*, 1990, **77**, 123-141; (b) J. M. L. Martin and A. Sundermann, *J. Chem. Phys.*, 2001, **114**, 3408-3420.
- [14] R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724-728.
- [15] W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257–2261.
- [16] P. C. Hariharan and J. A. Pople, *Theor. Chem. Acc.*, **1973**, 28, 213–222.
- [17] Gaussian 09, Revision D.01: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheesman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, M. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian Inc., 2009, Wallingford CT.