

Electronic Supporting Information
for

Cooperative Metal-Ligand Hydroamination Catalysis Supported by C-H Activation in Cyclam Zr(IV) Complexes

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Synthesis and characterization of compounds 1 and 2

Compounds 1,8-diallyl-1,4,8,11-tetraazacyclotetradecane, **1**, and 1,8-bis(2-methylallyl)-1,4,8,11-tetraazacyclotetradecane, **2**, were prepared according to previously described procedures¹ upon basic hydrolyses of the corresponding 1,8-R-4,11-diazoniatricyclo[9.3.1.1^{4,8}]hexadecane-1,8-dium dichloride salts (R = allyl, **1a**; R = 2-methylallyl, **2a**). Compounds **1** and **2** were obtained in high yields as beige oil and a white solid, respectively. In the ¹H NMR spectra, the macrocycle germinal protons are equivalent, giving raise to the emergence of only five signals integrating to four protons each in agreement with a C_{2v} symmetry in solution. The methylene protons of the allyl or methallyl pendant arms show up as singlets in accordance with allowed nitrogen inversion as observed in other *trans*-disubstituted cyclams displaying benzyl groups as pendant arms.¹ The ¹³C{¹H} NMR spectra

of compounds **1** and **2** display five different resonances for the macrocycle and a set of resonances corresponding to the allyl or methallyl moieties. Selected chemical shifts observed in ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for the CH_2 groups of the macrocyclic pendant arms of dichlorido (**5** and **6**) and dialkyl (**8** - **11**) complexes are presented in Table SI1.

Table SI1 – Selected chemical shifts (ppm) observed in ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for the CH_2 groups of the macrocyclic pendant arms of dichlorido (**5** and **6**) and dialkyl (**8** - **11**) complexes.

Compound	NCH_2R		NCH_2R
$(\text{All}_2\text{Cyclam})\text{ZrCl}_2$, 5	4.05	3.90	56.4
	4.03	3.87	
$(\text{All}_2\text{Cyclam})\text{ZrMe}_2$, 8	4.06	3.67	56.5
	4.01	3.62	
$(\text{All}_2\text{Cyclam})\text{Zr}(\text{CH}_2\text{Ph})_2$, 9	3.46	3.15-3.03	59.8
	3.41		
$(^{\text{Me}}\text{All}_2\text{Cyclam})\text{ZrCl}_2$, 6	4.03	3.75	58.2
$(^{\text{Me}}\text{All}_2\text{Cyclam})\text{ZrMe}_2$, 10	4.12	3.52	57.5
$(^{\text{Me}}\text{All}_2\text{Cyclam})\text{Zr}(\text{CH}_2\text{Ph})_2$, 11	3.68	3.04-2.80	61.7

Crystals of **1** and **2** suitable for X-ray diffraction were obtained from concentrated chloroform solutions at -20°C . Crystallographic and experimental details of data collection and crystal structure determination are presented in Table SI2. An ORTEP depiction of the molecular structures of **1** and **2** are shown in Figure SI1 and SI2, respectively.

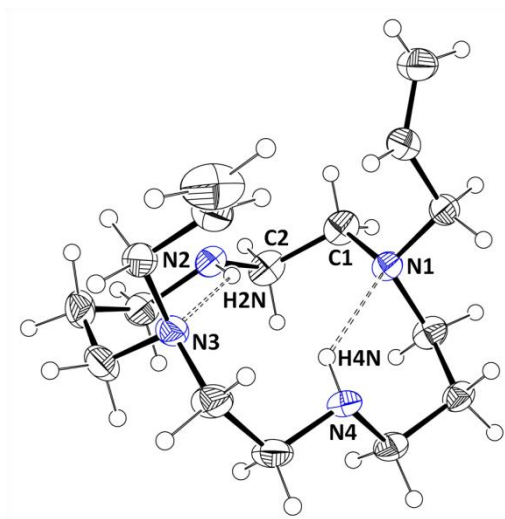


Figure SI1 – ORTEP diagram of 1,8-diallyl-1,4,8,11-tetraazacyclotetradecane, **1**, showing thermal ellipsoids at 40% probability level. Dashed lines represent hydrogen bonds.

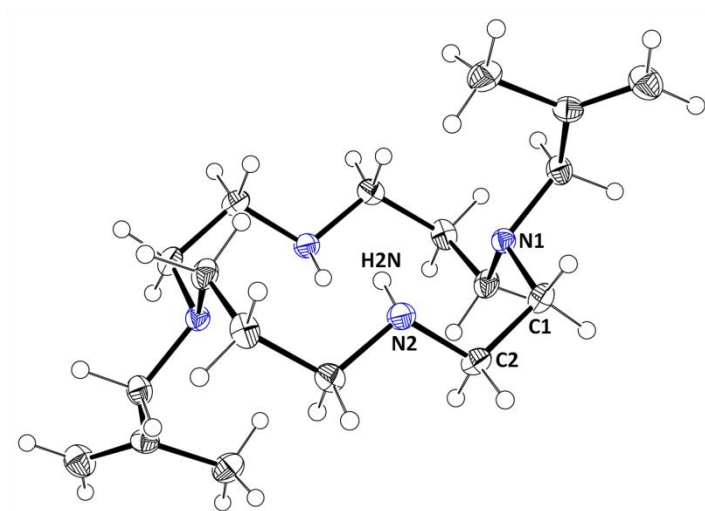


Figure SI2 – ORTEP diagram of 1,8-bis(2-methylallyl)-1,4,8,11-tetraazacyclotetradecane, **2**, showing thermal ellipsoids at 40% probability level.

The solid state molecular structure of **1** shows the two allyl pendant arms pointing the same side of the macrocyclic ring. These structural feature of the macrocycle is determined by the intramolecular hydrogen bonds N(2)-H(2N)⋯N(3) and N(4)-H(4N)⋯N(1) with bond lengths of 0.84(1) and 0.86(1) Å, respectively. Such interactions define two 6-member heterocycles and force both N_{Bn} atoms to adopt a tetrahedral geometry with (*R,R*) configuration. On the other hand, in **2**, the two methallyl pendant arms are located at opposite faces of the cyclam ring

hampering the formation of intramolecular hydrogen bonds as observed in compound **1**. The overall distances and angles are similar in both compounds and fit the usual values reported in the literature.²

Table SI2 - Crystal data and structure refinement for compounds **1** and **2**

Compound	1	2
Empirical formula	C16 H32 N4	C18 H36 N4
Formula weight	280.46	308.51
Temperature (K)	150(2)	150(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	P -1	P -1
Unit Cell Dimensions:		
<i>a</i> (Å)	9.9859(6)	6.7142(6)
<i>b</i> (Å)	10.0495(6)	9.4260(8)
<i>c</i> (Å)	10.0957(7)	15.522(1)
α (°)	106.935(3)	82.613(5)
β (°)	106.963(4)	84.559(6)
γ (°)	97.278(3)	78.693(5)
Volume (Å ³)	901.9(1)	952.85(13)
<i>Z</i>	2	2
Calculated density (g m ⁻³)	1.033	1.075
Absorption coefficient (mm ⁻¹)	0.063	0.065
<i>F</i> (000)	312	344
Crystal size (mm)	0.20 x 0.10 x 0.10	0.30 x 0.20 x 0.20
Theta range for data collection (°)	2.25 – 32.67	2.45 – 26.43
Limiting indices	-10 ≤ <i>h</i> ≤ 15, -15 ≤ <i>k</i> ≤ 15, -15 ≤ <i>l</i> ≤ 15	-8 ≤ <i>h</i> ≤ 8, -11 ≤ <i>k</i> ≤ 11, -19 ≤ <i>l</i> ≤ 16
Reflections collected/unique [<i>R</i> _{int}]	21539/6489 [0.0346]	8353/3865 [0.0296]
Completeness to θ (%)	98.2 (θ = 32.67)	98.6 (θ = 26.43)
Refinement method	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²

Data/restraints/parameters	6489/0/213	3865/0/209
Goodness-of-fit on F^2	1.112	1.031
Final R indices [$I > 2\sigma(I)$] ^[a]	$R_1 = 0.0519$, $wR_2 = 0.1433$	$R_1 = 0.0480$, $wR_2 = 0.1144$
R indices (all data) ^[a]	$R_1 = 0.0904$, $wR_2 = 0.1563$	$R_1 = 0.0812$, $wR_2 = 0.1240$
Absorption correction	Multi-scan	Multi-scan
Largest diff. peak/hole ($e \text{ \AA}^{-3}$)	0.249 and -0.160	0.192 and -0.194

^[a] $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; $wR_2 = \{\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]\}^{1/2}$

1,8-allyl-4,11-diazoniatricyclo[9.3.1.1^{4,8}]hexadecane-1,8-diium

dichloride (1a): 1,4,8,11-tetraazatricyclo[9.3.1.14,8]hexadecane (3.00 g, 13.4 mmol) was dissolved in acetonitrile and two equiv. of allyl chloride (2.40 mL, 29.4 mmol) were rapidly added. The solution was stirred at room temperature and the white precipitate formed was then filtered, washed with a small quantity of CH₃CN and dried under reduced pressure. The compound was obtained as a white powder in 41% yield (2.05 g, 5.43 mmol). ¹H NMR (D₂O/(CD₃)₂CO, 300.1 MHz, 296 K): δ (ppm) 6.05 (m, 2H, CH₂CHCH₂N), 5.78-5.72 (m, 4H, CH₂CHCH₂N), 5.37 (d, $J_{A-B} = 10$ Hz, 2H, NCH₂N), 4.40 (m, 2H, [C2]CH₂N), 4.21 (d, $J_{A-B} = 14$ Hz, 1H, CH₂CHCH₂N), 4.16 (d, $J_{A-B} = 14$ Hz, 1H, CH₂CHCH₂N), 3.97 (d, $J_{A-B} = 14$ Hz, 1H, CH₂CHCH₂N), 3.92 (d, $J_{A-B} = 14$ Hz, 1H, CH₂CHCH₂N), 3.60 (m, 2H, [C3]CH₂N), 3.52 (d, $J_{A-B} = 10$ Hz, 2H, NCH₂N), 3.42-3.29 (overlapping, 4H total, 2H, [C3]CH₂N and 2H, [C2]CH₂N), 3.15 (m, 2H, [C3]CH₂N), 3.02 (m, 2H, [C2]CH₂N), 2.86 (m, 2H, [C2]CH₂N), 2.60 (m, 2H, [C3]CH₂N), 2.43 (m, 2H, CH₂CH₂CH₂), 1.91 (m, 2H, CH₂CH₂CH₂). ¹³C{¹H} NMR (D₂O/(CD₃)₂CO, 75.5 MHz, 296 K): δ (ppm) 129.0 (CH₂CHCH₂N), 123.0 (CH₂CHCH₂N), 76.5 (NCH₂N), 61.6 (CH₂CHCH₂N), 59.9 ([C3]CH₂N), 51.1 ([C3]CH₂N), 47.0 ([C2]CH₂N), 46.9 ([C2]CH₂N), 19.4 (CH₂CH₂CH₂). Anal. calcd for C₁₈H₃₄Cl₂N₄.(H₂O)₂: C, 52.29; H, 9.26; N, 13.55. Found: C, 52.13; H, 9.08; N, 13.56. FT-IR (KBr, cm⁻¹): 1608 ($\nu_{C=C}$)

1,8-bis(2-methylallyl)-4,11-diazoniatricyclo[9.3.1.1^{4,8}]hexadecane-1,8-diium dichloride

(**2a**): 1,4,8,11-tetraazatricyclo[9.3.1.1^{4,8}]hexadecane (4.00 g, 17.8 mmol) was dissolved in acetonitrile and 2.3 equiv. of methallyl chloride (4.00 mL, 41.1 mmol) along with a slightly excess of NaI were rapidly added. The solution was stirred for one week at room temperature and the white precipitate formed was then filtered, washed with a small quantity of CH₃CN and dried under reduced pressure. The compound was obtained as a white powder in 34% yield (2.48 g, 6.12 mmol). ¹H NMR (D₂O/(CD₃)₂CO, 400.1 MHz, 296 K): δ (ppm) 5.72 (s, 2H, CH₂C(Me)CH₂N), 5.56-5.52 (overlapping, 4H total, 2H, CH₂C(Me)CH₂N and 2H, NCH₂N), 4.64 (m, 2H, [C2]CH₂N), 4.35 (d, *J*_{A-B} = 13 Hz, 2H, CH₂C(Me)CH₂N), 4.08 (d, *J*_{A-B} = 13 Hz, 2H, CH₂C(Me)CH₂N), 3.74-3.72 (overlapping, 4H total, 2H, NCH₂N and 2H, [C2]CH₂N), 3.61-3.54 (overlapping, 4H total, 2H, [C3]CH₂N and 2H, [C2]CH₂N), 3.32 (m, 2H, [C3]CH₂N), 3.22 (m, 2H, [C2]CH₂N), 3.08 (m, 2H, [C3]CH₂N), 2.75 (m, 2H, [C3]CH₂N), 2.62 (m, 2H, CH₂CH₂CH₂), 2.13 (s, 6H, CH₂C(Me)CH₂N), 2.05 (m, 2H, CH₂CH₂CH₂). ¹³C{¹H} NMR (D₂O/(CD₃)₂CO, 100.6 MHz, 296 K): δ (ppm) 133.6 (CH₂C(Me)CH₂N), 129.0 (CH₂C(Me)CH₂N), 78.4 (NCH₂N), 66.0 (CH₂C(Me)CH₂N), 61.7 ([C2]CH₂N), 52.6 ([C3]CH₂N), 49.1 ([C2]CH₂N), 48.9 ([C3]CH₂N), 24.9 (CH₂C(Me)CH₂N), 21.0 (CH₂CH₂CH₂). Anal. calcd for C₂₀H₃₈Cl₂N₄·(H₂O)₆: C, 46.78; H, 9.81; N, 10.91. Found: C, 46.92; H, 9.28; N, 11.21. FT-IR (KBr, cm⁻¹): 1624 (ν_{C=C}).

1,8-diallyl-1,4,8,11-tetraazacyclotetradecane (1): Compound **1a** (1.50 g, 3.97 mmol) was hydrolyzed in an aqueous NaOH solution (3 M) and the product was extracted with small portions of CHCl₃. The organic phases were collected and dried with MgSO₄ anhydrous. The compound was obtained as beige oil in 88% yield (0.98 g, 3.49 mmol). ¹H NMR (CDCl₃, 300.1 MHz, 296 K): δ (ppm) 5.75 (m, 2H, CH₂CHCH₂N), 5.07-5.01 (m, 4H, CH₂CHCH₂N), 3.00 (d, ³*J*_{H-H} = 7 Hz, 4H, CH₂CHCH₂N), 2.85 (br, 2H, NH), 2.57 (m, 4H, [C3]CH₂N), 2.51 (m, 4H, [C2]CH₂N), 2.41-2.37 (overlapping, 8H total, 4H, [C3]CH₂N and 4H, [C2]CH₂N), 1.62 (m,

4H, CH₂CH₂CH₂). ¹³C{¹H} NMR (CDCl₃, 75.5 MHz, 296 K): δ (ppm) 134.7 (CH₂CHCH₂N), 117.8 (CH₂CHCH₂N), 56.5 (CH₂CHCH₂N), 54.0 ([C3]CH₂N or [C2]CH₂N), 53.1 ([C3]CH₂N or [C2]CH₂N), 50.7 ([C3]CH₂N), 47.9 ([C2]CH₂N), 25.9 (CH₂CH₂CH₂). FT-IR (KBr, cm⁻¹): 3292 (ν_{N-H}), 1643 (ν_{C=C}).

1,8-bis(2-methylallyl)-1,4,8,11-tetraazacyclotetradecane (2): Compound **2a** (2.48 g, 6.12 mmol) was hydrolyzed in an aqueous NaOH solution (3 M) and the product was extracted with small portions of CHCl₃. The organic phases were collected and dried with MgSO₄ anhydrous. The compound was obtained as a white solid in 68% yield (1.29 g, 4.18 mmol). ¹H NMR (CDCl₃, 300.1 MHz, 296 K): δ (ppm) 4.83 (s, 4H, CH₂C(Me)CH₂N), 2.91 (s, 4H, CH₂C(Me)CH₂N), 2.70-2.62 (overlapping, 8H total, [C3]CH₂N and [C2]CH₂N), 2.50-2.42 (overlapping, 8H total, [C3]CH₂N and [C2]CH₂N), 1.73-1.71 (overlapping, 10H total, 6H, CH₂C(Me)CH₂N and 4H, CH₂CH₂CH₂). ¹³C{¹H} NMR (CDCl₃, 75.5 MHz, 296 K): δ (ppm) 143.0 (CH₂C(Me)CH₂N), 113.9 (CH₂C(Me)CH₂N), 60.7 (CH₂C(Me)CH₂N), 54.2 ([C3]CH₂N or [C2]CH₂N), 50.8 ([C3]CH₂N or [C2]CH₂N), 48.8 ([C3]CH₂N or [C2]CH₂N), 47.8 ([C3]CH₂N or [C2]CH₂N), 26.1 (CH₂C(Me)CH₂N), 21.8 (CH₂CH₂CH₂). Anal. calcd for C₁₈H₃₆N₄: C, 70.08; H, 11.76; N, 18.16. Found: C, 69.30; H, 10.92; N, 18.29. FT-IR (KBr, cm⁻¹): 3240 (ν_{N-H}), 1641 (ν_{C=C}).

Crystallographic Studies

Crystals of (All₂Cyclam)Zr(NMe₂)₂, **4**, (All₂Cyclam)ZrCl₂, **5**, (All₂Cyclam)ZrMe₂, **8**, ((CH=C(Me)CH₂)₂Cyclam)Zr, **15** and (Bn₂Cyclam)Zr(O^tBu)₂, **17**, suitable for X-ray diffraction were obtained from concentrated solutions of toluene (**4**, **8**, **15** and **17**) or 1,2-dichlorobenzene (**5**) at -20 °C. Complexes **4** and **17** crystallize with two molecules in the asymmetric unit. All compounds reveal distorted trigonal prismatic coordination geometries

of the zirconium with the four nitrogen atoms of the macrocycle defining the rectangular face of the prism and the NMe₂ (in **4**), Cl (in **5**), Me (in **8**) or O^tBu (in **17**) ligands occupying the other vertices of the trigonal faces. ORTEP depictions of the molecular structures of **4**, **5**, **8**, **15** and **17** are shown in Figures 2a-b and 3a-c, respectively. Relevant distances and angles are presented in Table SI3.

Table SI3 - Selected bond lengths (Å) and angles (°) for compounds **4**, **5**, **8**, **15**, **17**, **21** and **22**

	Ligand Set			Substituents	
	M-N _{amine}	M-N _{amido}	M-[N ₄ Plane]	M-X	
4a	2.737(2)	2.079(2)	1.265(1)	2.086(2)	2.098(2)
	2.775(2)	2.095(2)			
4b	2.733(2)	2.085(2)	1.248(1)	2.098(2)	2.090(2)
	2.738(2)	2.091(2)			
5	2.431(1)	2.054(1)	1.0600(9)	2.5078(4)	
8	2.503(2)	2.086(3)	1.060(3)	2.318(3)	
15	2.45(2)	2.11(2)	0.926(8)	2.31(2)	2.29(2)
	2.46(2)	2.10(2)			
17a	2.540(3)	2.098(3)	1.167(2)	2.011(3)	1.998(3)
	2.539(3)	2.106(3)			
17b	2.505(4)	2.110(3)	1.134(2)	2.000(3)	2.001(3)
	2.489(4)	2.110(4)			
21	2.550(2)	2.102(2)	1.196(1)	2.193(2)	2.198(2)
	2.557(2)	2.104(2)			

22	2.564(3)	2.075(3)	1.207(2)	2.240(3)	2.275(4)
	2.562(4)	2.089(3)		2.274(4)	2.245(4)
	N _{amine} -M-N _{amine}	N _{amido} -M-N _{amido}	X-M-X		
4a	114.73(6)	120.05(8)	90.55(8)		
4b	115.56(6)	120.18(8)	89.65(8)		
5	129.76(6)	116.77(7)	84.47(2)		
8	128.2(1)	120.4(1)	80.3(2)		
15	146.8(5)	113.4(6)	80.6(6)		
17a	123.9(1)	114.3(1)	95.4(1)		
17b	127.0(1)	113.6(2)	94.9(1)		
21	122.99(6)	112.19(8)	75.23(7)	104.96(7)	
22	122.4(1)	111.2(1)	80.2(1)	102.2(1)	
			78.7(1)	82.8(1)	

In complexes **5** and **8**, the distances between the planes defined by the nitrogen atoms (1.0600(9) Å in **5** and 1.060(3) Å in **8**) and the zirconium and the bonding lengths Zr-N_{amido} and Zr-N_{amine} are very similar and within the values determined for related complexes.^{1a, 3} Conversely, in **4**, the Zr-N_{amine} distances ranging from 2.733(2) and 2.775(2) Å are longer than the typical values observed in other trigonal prismatic complexes supported by cyclam ligands.^{1a, 3, 4} Despite being closer to the ones observed in complexes of the type (Bn₂Cyclam)Zr(NHR)₂ (R = ^tBu, NH^{2,6}-MePh),⁵ which are best described as double-capped tetrahedral, they reveal coordination to the metal center. Such Zr-N_{amine} elongation might be responsible for the longer distances between the zirconium to the mean planes defined by the four nitrogen atoms (1.265(1) and 1.248(1) Å). The Zr-N_{amido} bond lengths are within the

usual values and no significant differences exist between the Zr-N_{amido} distances for the ligand frame and for the NMe₂ moieties. The N-Zr-N angle defined by the two *cis* NMe₂ ligands is slightly larger than the C-Zr-C angle but much wider than the Cl-Zr-Cl angle. These values are still in agreement with observations made for other compounds presenting adjacent amido, chloro, alkoxido or methyl ligands.^{1a, 3, 4, 5} In **15** the coordination geometry of zirconium is best described as distorted trigonal prismatic with the four nitrogen atoms of the macrocycle defining the rectangular face of the prism and the two carbon atoms of the pending arms that undergone the C-H activation reaction occupying the other vertices of the trigonal faces. The C-H activation reactions are responsible for the formation of two 5-membered metallacycles with internal angles of 70.3(6)° and 70.0(6)°. These values are lower than the ones observed in other complexes displaying the same $\kappa_2(\text{C,N})\text{-CH=CHCH}_2\text{N}$ fragment⁶ but the Zr-C and the Zr-N bond lengths are very similar to the values determined for related Zr(IV) complexes.^{3c, 7} In **17** the zirconium is coordinated to the four nitrogen atoms of the macrocycle and to the oxygen atoms of the *tert*-butoxido ligands. The metal coordination geometry is trigonal prismatic with the four nitrogen atoms of the macrocycle defining one rectangular face. The metal is located above this plane with distances of 1.167(2) Å (in **17a**) and 1.134(2) Å (in **17b**). The N-Zr-N angles inside the five member metallacycles defined by the metal and the [C2] chains are narrower than N-Zr-N angles inside the six member metallacycles. The Zr-N bond lengths, ranging from 2.098(3) to 2.110(4) Å for Zr-N_{amido} and from 2.489(4) to 2.540(3) Å for Zr-N_{amine} are within the values usually observed.^{3a, 5, 8} Both O^tBu ligands occupy adjacent positions in the metal coordination sphere with Zr-O distances that compare with values reported for this type of bonds in Zr(IV) complexes.⁹ The O(1)-Zr(1)-O(2) angles range of 95.4(1)° (in **17a**) and 94.9(1)° (in **17b**) and are slightly wider than the X-Zr-X angles in the dichlorido and the dialkyl complexes supported by the same ancillary ligand.^{3a, 5} The Zr-O-C angles ranging from 149.9(3)° and

160.5(2)° may reflect π -donation from the oxygen to the zirconium. It is interesting to observe that the bulky O^tBu ligand forces the widening of the O-Zr-O angle as reported by Rothwell.¹⁰

Crystals of (Bn₂Cyclam)Zr(NHNCPh₂)₂, **21**, and (Bn₂Cyclam)Zr(C₃H₃N₂)₂, **22**, suitable for X-ray diffraction were obtained in the NMR tube solutions. ORTEP depictions of the molecular structures of **21** and **22** along with relevant distances and angles are shown in Figures 3b and 3c, respectively. Relevant distances and angles are presented in Table SI3. The solid-state molecular structures of **21** and **22** show the expected coordination of the zirconium to the four nitrogen atoms of the macrocycle and the metal center perched on the macrocyclic cavity with distances of 1.196(1) and 1.207(2) Å in **21** and **22**, respectively, as observed in all cyclam based zirconium complexes reported to date.^{3a, 5, 8b} In **21** the geometry around the metal center is square antiprismatic with two η^2 -benzophenone hydrazone ligands. The bonding distances between the zirconium and the nitrogen atoms of benzophenone hydrazone ranges from 2.193(2) and 2.306(2) Å. In comparison with Zr-NHR bonds supported by the Bn₂Cyclam ligand (*ca.* 2.07 Å) the Zr-N distances in **21** are slightly elongated, while they are shortened in comparison to Zr-N(sp³) (*ca.* 2.5 Å) and Zr-N(sp²) (*ca.* 2.4 Å) bond lengths. The Zr-N distances observed reveal that the charge is delocalized between the two nitrogen atoms of the NHNCPh₂ ligand. In accordance, the N(5)-N(6) and N(7)-N(8) bond lengths of 1.330(3) and 1.336(3) Å, respectively, are between the expected values for N-N single and double bonds. The increase of the metal coordination number to eight does not cause significant changes in the Zr-N_{amido} or the Zr-N_{amine} bond lengths.^{3a, 5, 8a-b} The N_{amido}-Zr-N_{amido} and N_{amine}-Zr-N_{amine} angles within the macrocycle (112.19(8)° and 122.99(6)°, respectively) are also in the expected values for this type of compounds. In complex **22**, the pyrazole ligands are coordinated to the metal center by both nitrogen atoms with distances in the range 2.240(4) to 2.275(4) Å. The distances inside the pyrazole rings are

compatible with aromatic systems and the geometry of the complex may be taken as trigonal prismatic if the medium point of the N-N bond is considered. The distances between the middle of the N-N bonds of pyrazole rings and the metal center are 2.155(4) and 2.161(4) Å and the angle defined by them is 85.7(2)°. The coordination parameters involving the ancillary ligand are similar to other (Bn₂Cyclam)ZrX₂ complexes described.^{3a, 5, 8a-b}

Table SI4 - Crystal data and structure refinement for complexes **4**, **5**, **8**, **15**, **17**, **21** and **22**.

Compound	4	5	8	15	17	21	22
Empirical formula	C20 H42 N6 Zr	C16 H30 Cl2 N4 Zr	C18 H36 N4 Zr	C18 H32 N4 Zr	C32 H52 N4 O2 Zr	C50 H56 N8 Zr	C30 H40 N8 Zr
Formula weight	457.81	440.56	399.73	395.69	616.00	860.25	603.92
Temperature (K)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.7173	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Triclinic
Space group	P2 ₁ /c	C2/c	C2/c	P2 ₁ /c	P-1	P2 ₁ /n	P-1
Unit Cell Dimensions:							
<i>a</i> (Å)	17.2002(9)	19.9786(5)	13.323(4)	10.004(1)	13.763(5)	16.8912(7)	11.044(8)
<i>b</i> (Å)	15.5560(9)	7.4030(2)	7.694(3)	15.835(2)	15.282(5)	15.5512(7)	12.40(1)
<i>c</i> (Å)	17.293(1)	13.5330(4)	19.512(9)	12.182(2)	17.682(5)	20.3066(9)	15.35(1)
α(°)	90	90	90	90	96.190(5)	90	84.82(4)
β(°)	90.710(3)	107.540(2)	106.30(2)	102.597(6)	109.084(6)	93.021(2)	77.98(3)
γ(°)	90	90	90	90	92.802(5)	90	74.91(4)
Volume (Å ³)	4626.7(4)	1908.49(9)	1920(1)	1883.5(4)	3480(2)	5326.7(4)	1984(3)
Z	8	4	4	4	4	4	2
Calculated density (g m ⁻³)	1.314	1.533	1.383	1.395	1.176	1.073	1.012
Absorption coefficient (mm ⁻¹)	0.492	0.861	0.579	0.589	0.346	0.243	0.302
<i>F</i> (000)	1952	912	848	832	1312	1808	632
Crystal size (mm)	0.20 x 0.20 x 0.40	0.08 x 0.10 x 0.20	0.04 x 0.14 x 0.20	0.04 x 0.18 x 0.40	0.05 x 0.10 x 0.20	0.08 x 0.10 x 0.10	0.02 x 0.08 x 0.20
Theta range for data collection (°)	1.76 – 25.77	3.19 – 28.69	3.12 – 27.36	2.57 – 25.34	1.35 – 28.56	2.73 – 25.39	1.36 – 25.52

Limiting indices	-21≤ <i>h</i> ≤21, -18≤ <i>k</i> ≤18, -21≤ <i>l</i> ≤21	-24≤ <i>h</i> ≤26, -9≤ <i>k</i> ≤9, 18≤ <i>l</i> ≤18	-17≤ <i>h</i> ≤13, -8≤ <i>k</i> ≤9, -24≤ <i>l</i> ≤24	-12≤ <i>h</i> ≤12, -19≤ <i>k</i> ≤19, -14≤ <i>l</i> ≤14	-18≤ <i>h</i> ≤18, -20≤ <i>k</i> ≤20, 23≤ <i>l</i> ≤23	-17≤ <i>h</i> ≤20, -17≤ <i>k</i> ≤18, -24≤ <i>l</i> ≤24	-13≤ <i>h</i> ≤13, -11≤ <i>k</i> ≤15, -18≤ <i>l</i> ≤18
Reflections collected/unique [<i>R</i> _{int}]	54737/8808 [0.0790]	11484/2452 [0.0311]	6814/2090 [0.0533]	75268/3436 [0.1820]	48026/17330 [0.1066]	55663/9772 [0.0617]	27145/7154 [0.1215]
Completeness to θ (%)	99.3 (θ = 25.77)	99.8 (θ = 28.69)	96.5 (θ = 27.36)	98.9 (θ = 25.39)	97.7 (θ = 28.56)	99.8 (θ = 25.39)	96.6 (θ = 25.52)
Refinement method	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²
Data/restraints/parameters	8808/0/495	2452/0/105	2090/0/106	3436/6/211	17330/0/703	9772/0/540	7154/0/352
Goodness-of-fit on <i>F</i> ²	0.999	1.069	1.112	1.091	0.835	1.043	0.871
Final <i>R</i> indices [<i>I</i> >2σ(<i>I</i>)] ^[a]	<i>R</i> ₁ = 0.0336, <i>wR</i> ₂ = 0.0718	<i>R</i> ₁ = 0.0224, <i>wR</i> ₂ = 0.0565	<i>R</i> ₁ = 0.0377, <i>wR</i> ₂ = 0.0870	<i>R</i> ₁ = 0.1378, <i>wR</i> ₂ = 0.3928	<i>R</i> ₁ = 0.0621, <i>wR</i> ₂ = 0.1064	<i>R</i> ₁ = 0.0402, <i>wR</i> ₂ = 0.1009	<i>R</i> ₁ = 0.0517, <i>wR</i> ₂ = 0.1099
<i>R</i> indices (all data) ^[a]	<i>R</i> ₁ = 0.0603, <i>wR</i> ₂ = 0.0787	<i>R</i> ₁ = 0.0268, <i>wR</i> ₂ = 0.0580	<i>R</i> ₁ = 0.0514, <i>wR</i> ₂ = 0.0997	<i>R</i> ₁ = 0.1521, <i>wR</i> ₂ = 0.3999	<i>R</i> ₁ = 0.1585, <i>wR</i> ₂ = 0.1279	<i>R</i> ₁ = 0.0586, <i>wR</i> ₂ = 0.1065	<i>R</i> ₁ = 0.0845, <i>wR</i> ₂ = 0.1163
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Largest diff. peak/hole (e Å ⁻³)	0.342 and -0.380	0.379 and -0.283	1.067 and -0.972	4.739 and -2.946	1.023 and -0.524	0.289 and -0.283	0.412 and -0.807

^[a] $R_1 = \Sigma ||F_0| - |F_c|| / \Sigma |F_0|$; $wR_2 = \{\Sigma[w(F^2_0 - F^2_c)^2] / \Sigma[w(F^2_0)^2]\}^{1/2}$

Catalytic Studies

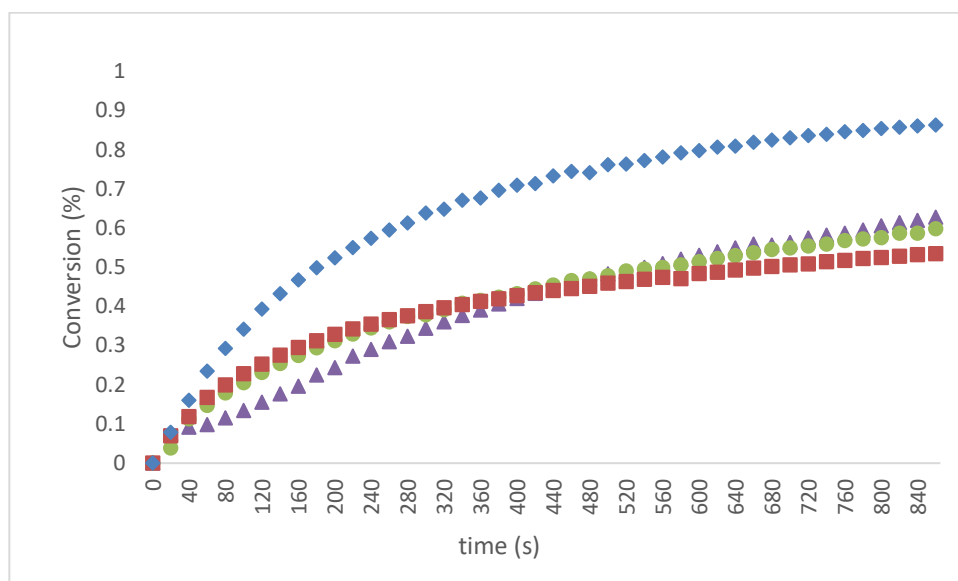
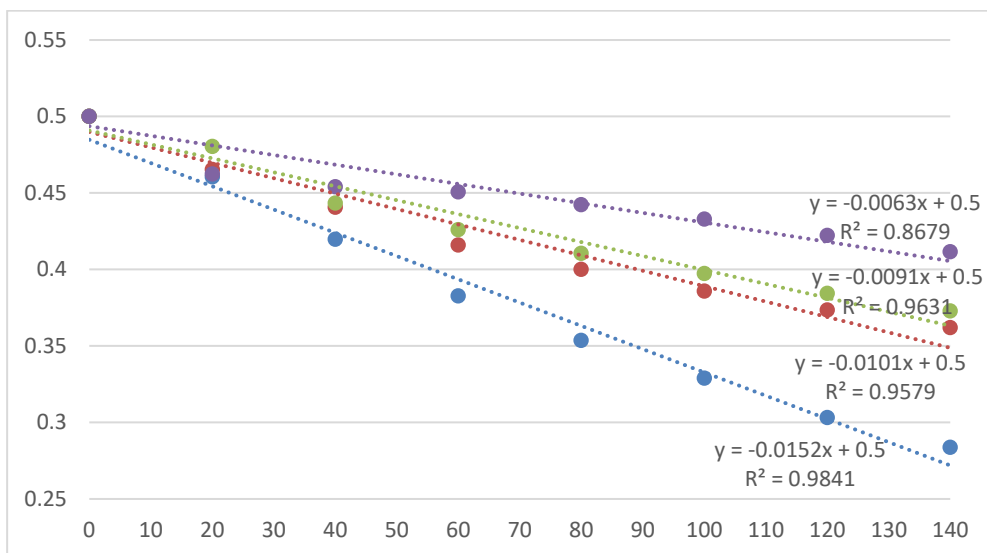


Figure SI3 – Representative kinetic plot for the intramolecular hydroamination of 2,2-diphenyl-pent-4-enylamine catalyzed by **4** (▲), **14** (■), **15** (◆) and **16** (●). Typical reaction conditions: 10% catalyst in toluene- d_8 at 95°C.



DFT Calculations

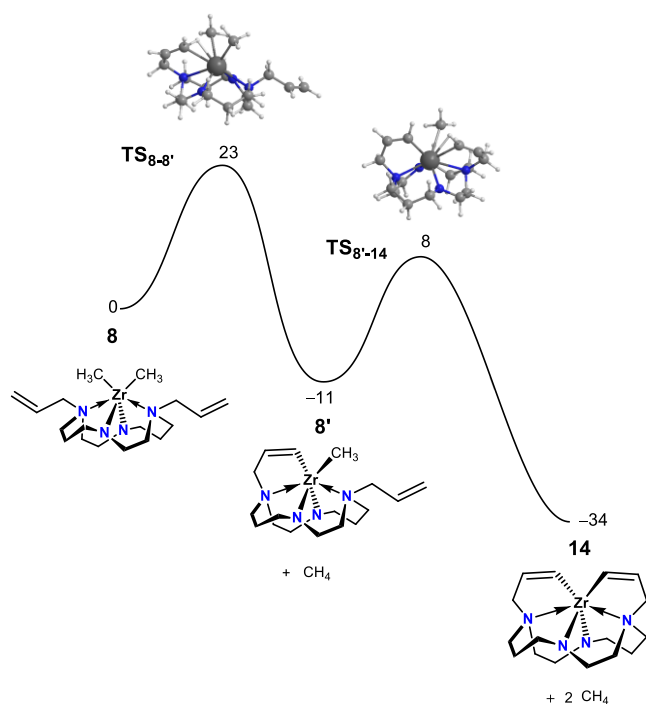


Figure SI5 - Free energy profile (kcal/mol) for the C-H activation of the allyl arm in **8** and formation of **14**.

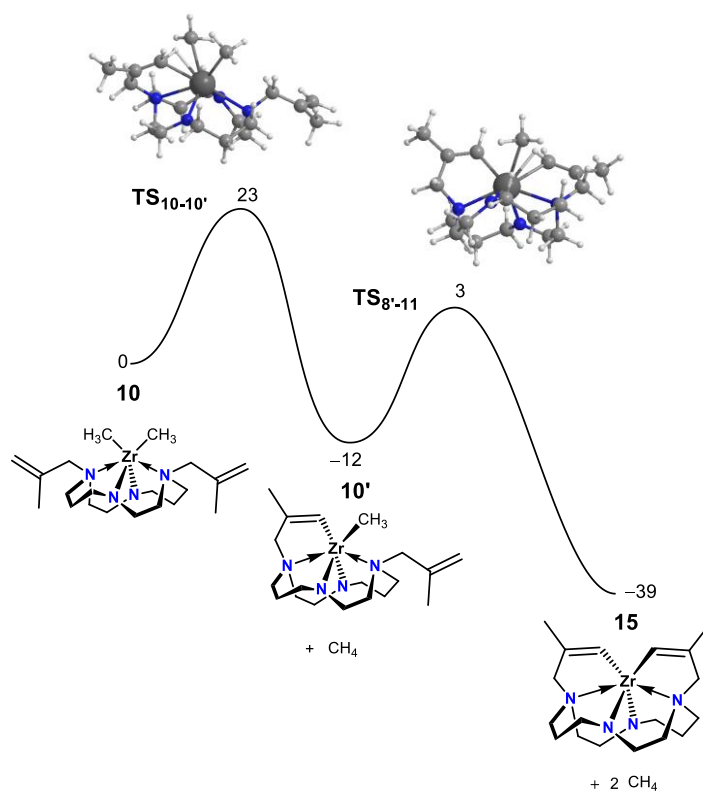


Figure SI6 - Free energy profile (kcal/mol) for the C-H activation of the 2-methylallyl arm in **10** and formation of **15**.

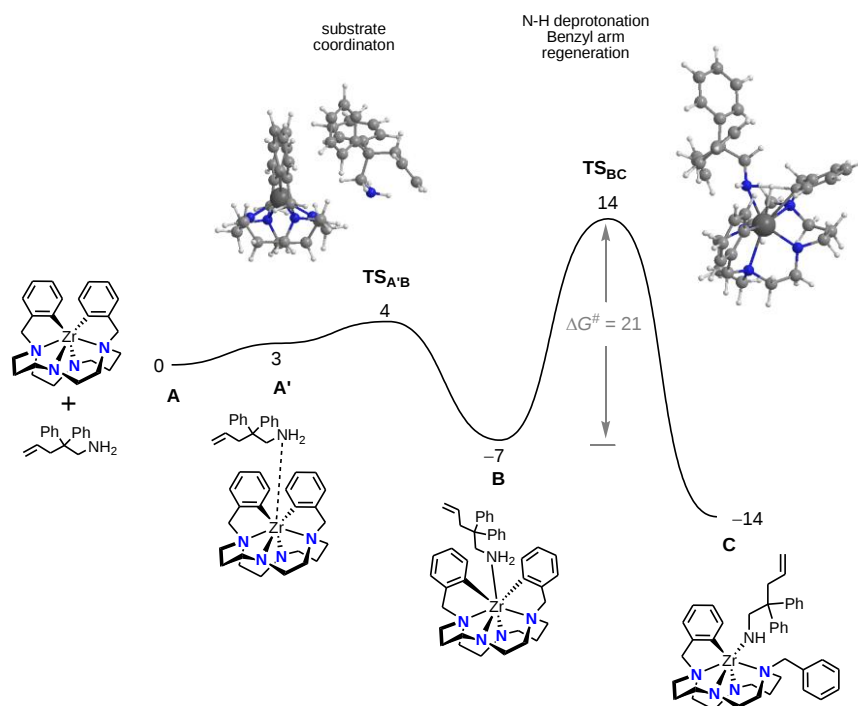


Figure SI7 - Free energy profile for the formation of amido intermediate **C**, from **16** and 2,2-diphenyl-pent-4-enylamine. Free energy values (kcal/mol) relative to the separated reagents: **16** + 2,2-diphenyl-pent-4-enylamine (**A**).

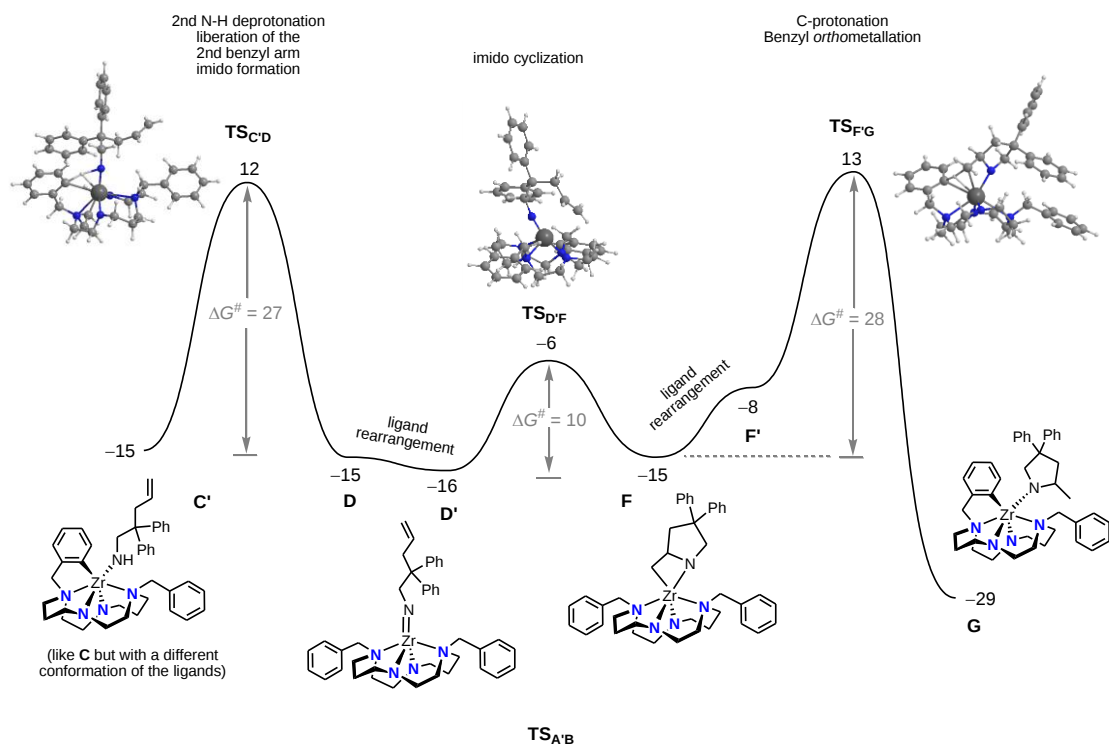


Figure SI8 - Free energy profile for the formation of cyclic amido intermediate **G** by the imido route (*via* intermediate **D**). Free energy values (kcal/mol) relative to the separated reagents: **16** + 2,2-diphenyl-pent-4-enylamine (**A**).

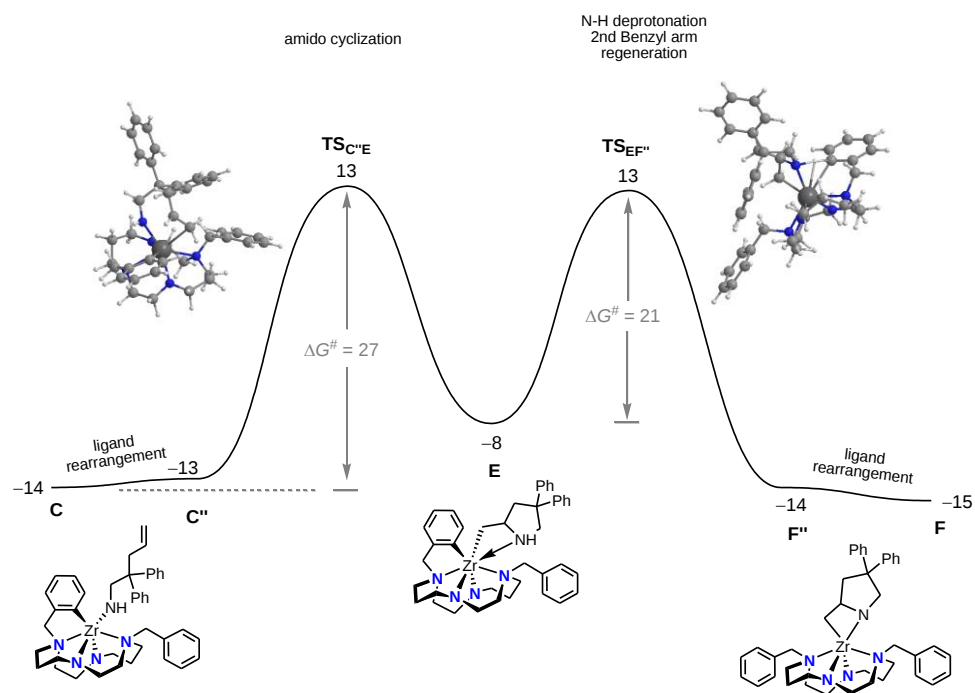


Figure SI9 - Free energy profile for the formation of intermediate **F** from **C** by the amido route (*via* intermediate **E**). Free energy values (kcal/mol) relative to the separated reagents: **16** + 2,2-diphenyl-pent-4-enylamine (**A**).

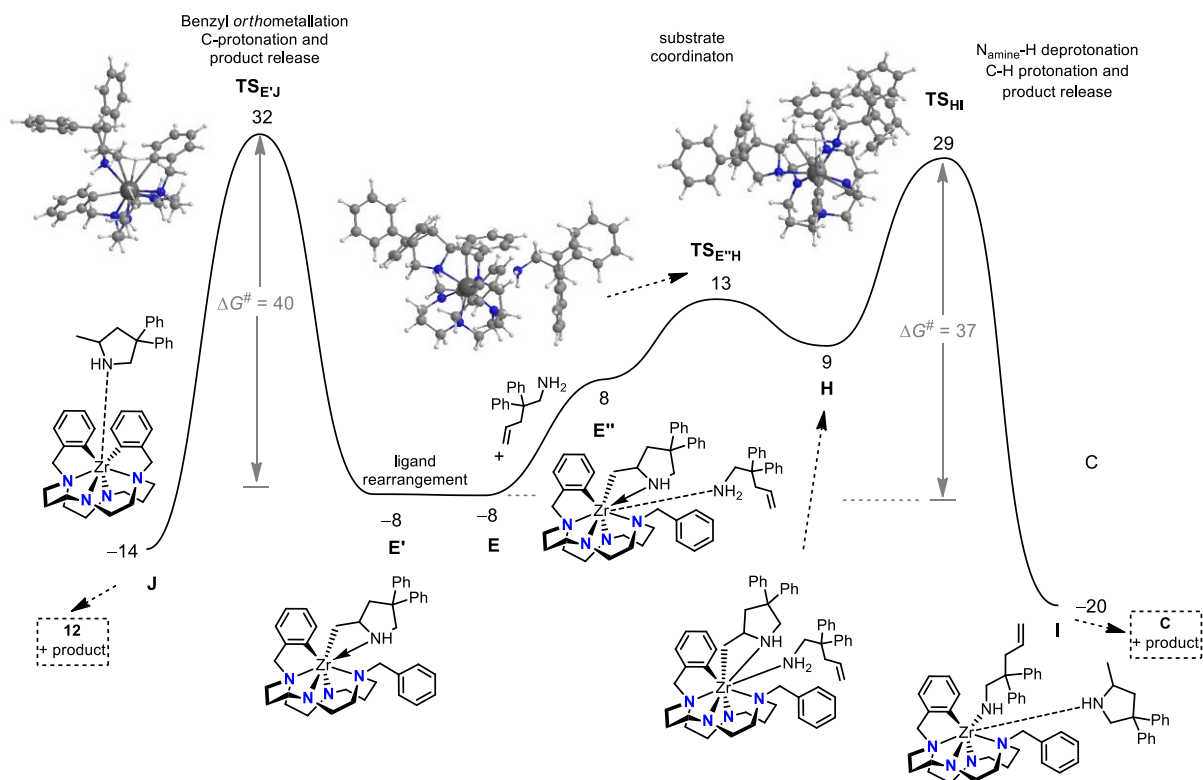


Figure SI10 - Free energy profile for product release from intermediate **E**. Right side: C-protonation by a new substrate molecule. Left side: C-protonation by the benzyl arm with *orthometallation*. Free energy values (kcal/mol) relative to the separated reagents: **16** + 2,2-diphenyl-pent-4-enylamine (**A**).

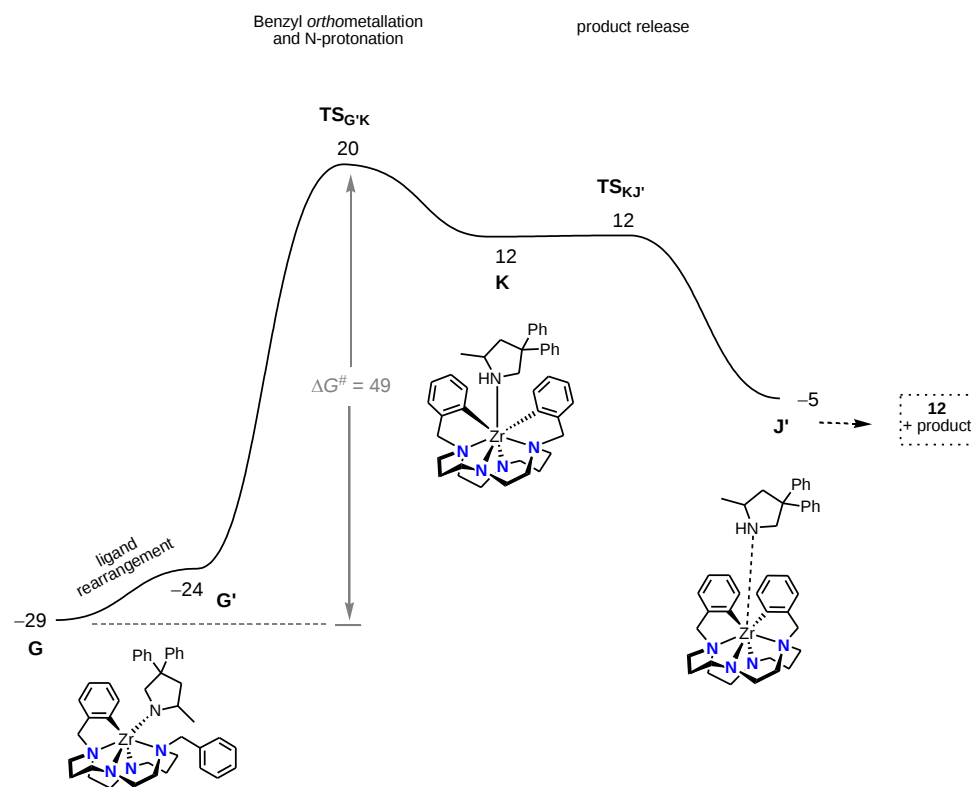


Figure SI11 - Free energy profile for product release from intermediate **G** with N-protonation by the benzyl arm with *orthometallation*. Free energy values (kcal/mol) relative to the separated reagents: **16** + 2,2-diphenyl-pent-4-enylamine (**A**).

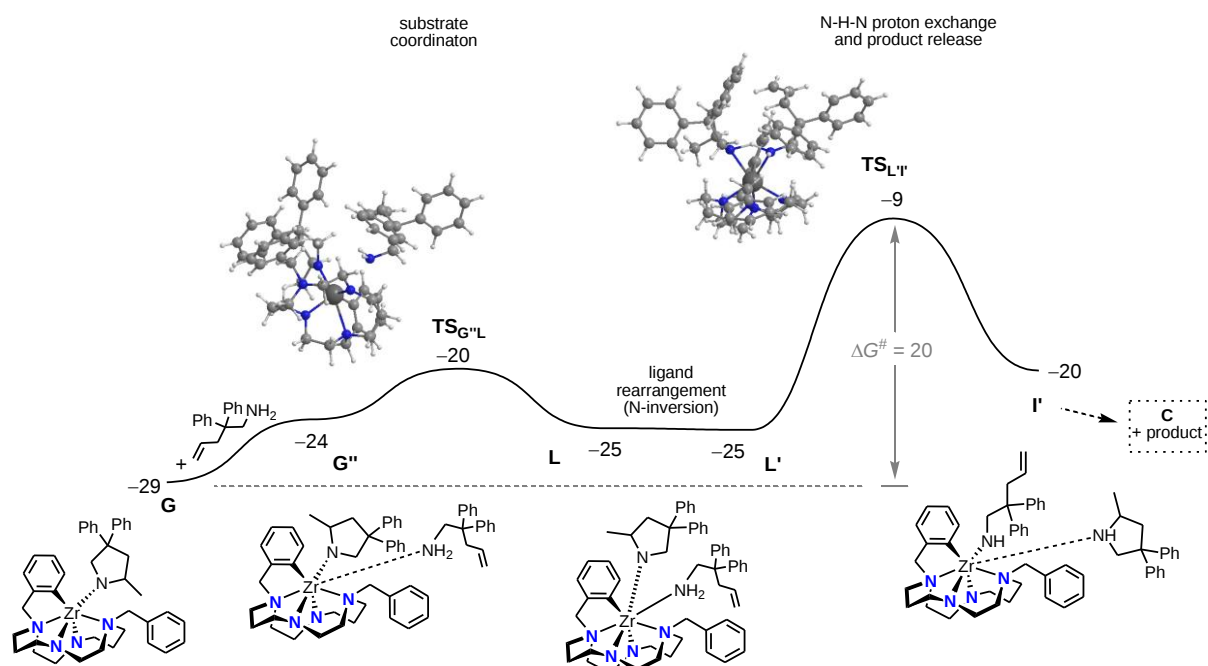


Figure SI12 - Free energy profile for product release from intermediate **G** with N-protonation by a new substrate molecule. Free energy values (kcal/mol) relative to the separated reagents: **16** + 2,2-diphenyl-pent-4-enylamine (**A**).

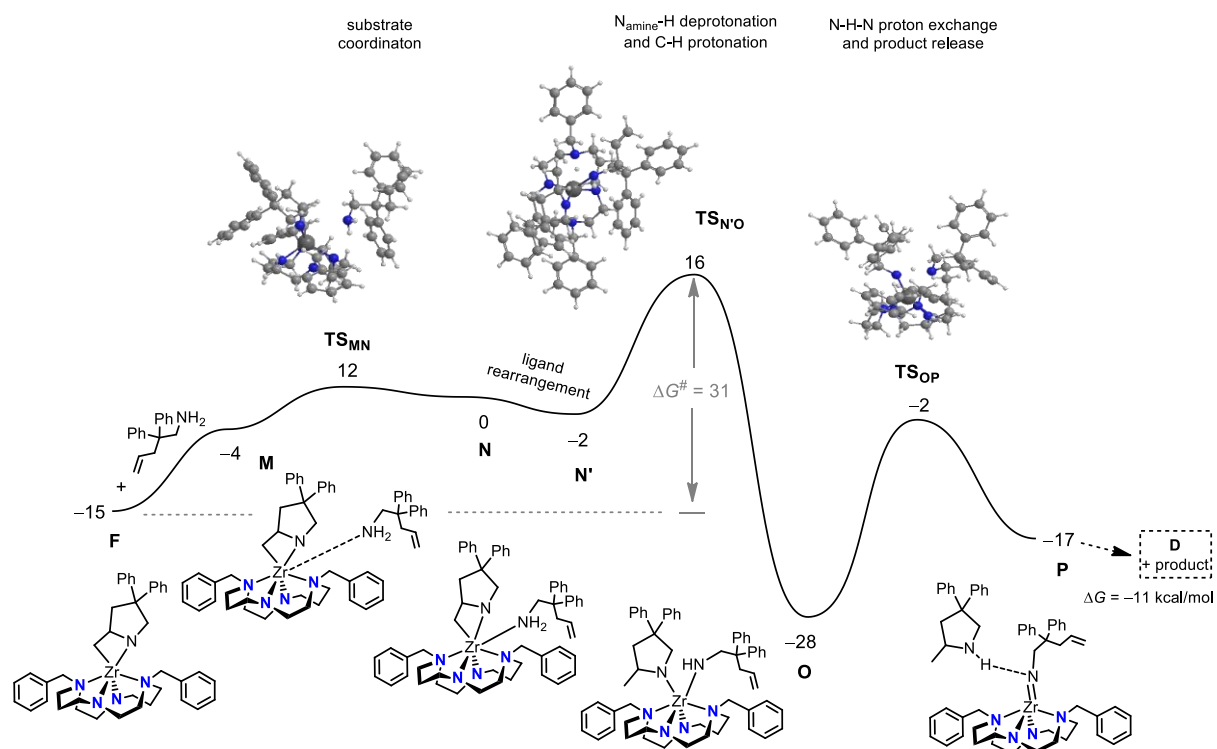


Figure SI13 - Free energy profile for protonation of the amido/alkyl ligand in **F** by means of new substrate molecule closing the cycle to **D**. Free energy values (kcal/mol) relative to the separated reagents: **16** + 2,2-diphenyl-pent-4-enylamine (**A**).

Table SI5 - Atomic coordinates of the optimized species

CH₄				C	6.053924	-0.489794	1.383159
C	0.229416	0.011028	-0.810406	H	6.221443	0.490292	0.915298
H	0.568730	-1.026364	-0.835992	H	5.876810	-1.208235	0.559357
H	1.070923	0.662430	-0.565492	C	7.325985	-0.862078	2.126850
H	-0.550078	0.122165	-0.053990	H	8.111506	-0.947710	1.361114
H	-0.171795	0.287100	-1.788006	H	7.250119	-1.857789	2.588088
				C	7.740440	0.166591	3.179738
				H	8.797805	-0.006951	3.450411
8				H	7.714584	1.166601	2.718515
Zr	5.292414	1.109111	4.681926	C	3.756479	0.191586	1.298313
N	4.706464	-0.057514	2.461194	H	3.339486	-0.607264	0.658355
N	7.077631	0.027339	4.471532	H	4.245129	0.901807	0.614830
C	5.832174	-0.321475	1.537766	C	7.437975	-0.814196	5.327745
H	6.071349	0.634282	1.049954	H	8.340715	-0.407181	5.828967
H	5.498461	-1.011296	0.742037	H	7.777265	-1.752443	4.843719
C	7.111161	-0.879281	2.149621	C	6.395048	-1.210159	6.355209
H	7.804160	-1.035759	1.309710	H	5.697883	-1.918780	5.897117
H	6.942204	-1.877078	2.581755	H	6.865139	-1.697545	7.227198
C	7.768354	0.026052	3.191658	C	2.993065	1.599814	3.157844
H	8.817199	-0.289947	3.333147	H	4.247338	2.126052	3.100731
H	7.819219	1.049981	2.789581	H	2.211628	2.160167	3.677431
C	3.662738	0.746544	1.771513	C	2.681860	0.917462	2.051394
H	4.151020	1.673362	1.444756	H	1.674414	0.872904	1.627708
H	2.913754	1.035260	2.520237	C	4.376224	2.636310	5.796973
C	7.501213	-1.047368	5.335570	H	3.760360	3.347698	5.230063
H	8.478745	-0.827407	5.811856	H	5.268867	3.191435	6.123846
H	7.659135	-1.991468	4.778156	H	3.802214	2.377642	6.703460
C	6.447348	-1.318196	6.393604	N	5.601897	-0.038103	6.774695
H	5.624423	-1.890727	5.946072	N	3.637158	-0.854609	4.745058
H	6.864211	-1.923477	7.218038	C	4.508716	-0.421662	7.695583
C	1.683264	-0.152644	0.550284	H	4.003670	0.511383	7.986492
H	1.024935	0.120701	1.375127	H	4.937719	-0.853496	8.616286
H	1.214792	-0.604699	-0.320395	C	3.469250	-1.390801	7.153038
C	2.992076	0.077976	0.610252	H	2.735390	-1.533350	7.960048
H	3.619298	-0.195926	-0.240633	H	3.911049	-2.379654	6.964857
C	4.953324	2.834140	6.153459	C	2.752658	-0.915799	5.894996
H	4.214980	3.502707	5.681149	H	1.913093	-1.600393	5.689550
H	5.867333	3.435501	6.285061	H	2.277571	0.064729	6.104100
H	4.571075	2.597898	7.158739	C	6.473630	0.971914	7.434649
N	5.878359	-0.057523	6.902654	H	5.814605	1.787761	7.756742
N	3.507193	0.027343	4.892314	H	7.141468	1.390100	6.670357
C	4.752647	-0.321485	7.826078	C	3.250811	-1.673321	3.631628
H	4.513472	0.634271	8.313893	H	2.326377	-1.310642	3.130406
H	5.086356	-1.011309	8.621806	H	3.036650	-2.713589	3.946071
C	3.473659	-0.879287	7.214219	C	4.389604	-1.724078	2.633311
H	2.780659	-1.035767	8.054130	H	5.250047	-2.194641	3.124746
H	3.642614	-1.877082	6.782081	H	4.123986	-2.340750	1.753832
C	2.816469	0.026053	6.172187	C	8.600106	0.597977	8.679791
H	1.767623	-0.289943	6.030696	H	9.176581	1.040256	7.867222
H	2.765606	1.049980	6.574268	H	9.156835	0.277828	9.556884
C	6.922077	0.746538	7.592343	C	7.277747	0.478582	8.599546
H	6.433792	1.673364	7.919072	H	6.734323	0.042809	9.440494
H	7.671080	1.035239	6.843632	C	5.600375	2.700918	2.984001
C	3.083609	-1.047359	4.028272	H	6.488049	2.742836	3.631986
H	2.106079	-0.827394	3.551983	H	5.162260	3.706261	2.998402
H	2.925681	-1.991460	4.585683	H	5.924176	2.481402	1.959489
C	4.137476	-1.318189	2.970241				
H	4.960401	-1.890720	3.417774	8'			
H	3.720614	-1.923468	2.145805	Zr	4.517955	0.532210	4.302669
C	8.901515	-0.152621	8.813654	N	4.357984	-0.879641	2.265443
H	9.559873	0.120719	7.988832	N	6.578133	0.196231	4.110253
H	9.369959	-0.604660	9.684356	C	5.491666	-0.822441	1.311523
C	7.592704	0.077990	8.753636	H	5.389368	0.128992	0.774414
H	6.965454	-0.195902	9.604504	H	5.353728	-1.631687	0.569958
C	5.631511	2.834147	3.210401	C	6.893490	-0.886943	1.897515
H	6.369853	3.502711	3.682718	H	7.584857	-0.901256	1.041976
H	4.717503	3.435508	3.078799	H	7.064300	-1.830874	2.437556
H	6.013765	2.597910	2.205122	C	7.221098	0.293103	2.811354
				H	8.316281	0.369545	2.938909
TS_{8-8'}				H	6.918048	1.225694	2.307017
Zr	4.895334	0.812344	4.501005	C	3.151802	-0.392067	1.558576
N	4.807114	-0.377151	2.179001	H	2.266651	-0.801077	2.065238
N	6.910106	0.132902	4.366179	H	3.132076	-0.795642	0.528135

C	7.366257	-0.540243	5.068751	N	5.669716	-0.078139	6.724549
H	8.192144	0.081359	5.473918	N	4.385828	-1.198224	4.147572
H	7.862155	-1.418718	4.610983	C	4.233907	-0.032193	7.092791
C	6.489679	-1.057949	6.194247	H	3.879672	0.984900	6.880012
H	5.919615	-1.922891	5.830211	H	4.151678	-0.174178	8.187802
H	7.104674	-1.394456	7.048070	C	3.303731	-1.000497	6.376815
C	3.796492	1.791317	2.531658	H	2.312966	-0.861905	6.835206
H	6.456710	3.619799	4.046545	H	3.580273	-2.048498	6.564679
H	3.692586	2.881969	2.489334	C	3.209378	-0.760680	4.870422
C	3.123852	1.111819	1.586572	H	2.312540	-1.276669	4.485880
H	2.505256	1.578211	0.809342	H	3.024112	0.313530	4.700115
C	3.658628	2.297099	5.491296	C	6.349591	1.080937	7.356870
H	2.695758	2.573978	5.034852	H	6.551364	0.852233	8.418981
H	4.298303	3.192935	5.427589	H	5.639909	1.921403	7.357313
H	3.464271	2.115908	6.561151	C	4.188961	-2.492021	3.531916
N	5.508037	-0.043357	6.619047	H	3.502031	-2.423633	2.662211
N	3.312140	-1.107363	4.744605	H	3.700327	-3.208638	4.222868
C	4.579131	-0.592898	7.629096	C	5.512934	-3.116679	3.122228
H	3.988596	0.255720	8.004317	H	5.973523	-3.574410	4.004712
H	5.154586	-0.986018	8.486451	H	5.364091	-3.908071	2.364298
C	3.612714	-1.671125	7.153931	C	7.657213	1.445335	5.302665
H	3.026362	-1.963765	8.037489	H	6.450437	1.660858	4.728265
H	4.149820	-2.577774	6.838297	H	8.556673	1.792787	4.788285
C	2.669023	-1.215922	6.042944	C	7.597630	1.508192	6.637456
H	1.816999	-1.914461	5.979237	H	8.412661	1.883285	7.263280
H	2.229807	-0.246434	6.332247				
C	6.185309	1.164527	7.154281				
H	5.390022	1.854059	7.466984				
H	6.708030	1.655517	6.324954				
C	3.184083	-2.289267	3.928826				
H	2.150471	-2.404885	3.543419				
H	3.381731	-3.216287	4.503397				
C	4.185322	-2.245271	2.783365				
H	5.166659	-2.573716	3.152206				
H	3.891814	-2.935084	1.969860				
C	8.411916	1.330220	8.250368				
H	8.822309	1.822311	7.367356				
H	9.083508	1.198236	9.094886				
C	7.142306	0.934265	8.283955				
H	6.755329	0.457595	9.187261				
C	7.471764	3.602013	4.455300				
H	7.844616	2.573798	4.412773				
H	7.447858	3.946220	5.493328				
H	8.117975	4.259063	3.868645				

TS⁸⁻¹⁴

Zr	6.304439	-0.300639	4.234354	N	2.953781	3.329718	2.393920
N	6.464240	-2.107194	2.624004	N	1.217625	2.754546	0.729786
N	7.624086	-1.581891	5.277155	N	4.643027	2.788665	4.119453
C	7.802473	-2.709107	2.404460	N	3.828322	1.992081	0.997511
H	8.396453	-1.945875	1.884917	N	1.975427	2.222057	3.918895
H	7.678293	-3.557756	1.706405	C	5.486320	4.989817	3.424144
C	8.562071	-3.167888	3.636517	C	0.217484	3.822951	0.459802
H	9.514806	-3.579383	3.271679	H	-0.780313	3.470984	0.764492
H	8.044132	-3.994584	4.142802	H	0.139956	3.978719	-0.629420
C	8.839467	-2.065312	4.647909	C	5.731217	3.791893	4.277131
H	9.524425	-2.464963	5.414405	H	5.824137	4.058565	5.343403
H	9.406791	-1.253049	4.148183	H	6.694964	3.325575	4.019573
C	6.029248	-1.520929	1.331096	C	0.570298	5.081275	1.177165
H	4.933308	-1.445027	1.339266	C	0.550044	1.518565	1.186648
H	6.288576	-2.210264	0.506112	H	1.294741	0.711600	1.218458
C	7.659774	-1.574384	6.712110	H	-0.208657	1.229071	0.436771
H	8.354218	-0.809895	7.125677	C	3.838021	2.763626	5.357003
H	8.007073	-2.545642	7.114865	H	3.554003	3.806451	5.561357
C	6.261962	-1.336622	7.238753	H	4.447773	2.407829	6.207387
H	5.631537	-2.167096	6.898044	C	2.008931	2.525942	-0.496547
H	6.242593	-1.322734	8.344680	H	2.376991	3.511817	-0.816521
C	7.019967	0.548034	2.238484	H	1.364318	2.128894	-1.301658
H	7.426576	1.546334	2.038107	C	0.827842	1.356017	3.743811
C	6.641535	-0.158789	1.161139	H	0.197997	1.391398	4.654595
H	6.717096	0.195907	0.125702	H	1.156011	0.294984	3.660478
C	5.093821	1.919203	4.184251	C	5.204595	1.460232	3.801454
H	4.443776	1.439932	3.439095	C	-0.082339	1.668280	2.566352
H	5.472075	2.837963	3.719533	H	-0.493135	2.679880	2.690802
H	4.485502	2.202926	5.052111	H	-0.935885	0.979835	2.626382
				C	3.180986	1.613703	-0.230655
				H	2.844242	0.554674	-0.200712
				H	3.868995	1.665750	-1.097349
				C	2.593619	1.927311	5.184696
				H	2.842297	0.847304	5.271076
				H	1.915216	2.130218	6.036553
				C	5.836661	1.410665	2.414295
				C	4.897500	1.054059	1.272653
				C	4.472973	5.017103	2.546985
				H	4.392982	5.934575	1.950903
				C	1.585861	5.115511	2.051619
				H	1.749718	6.083590	2.541047
				H	5.524300	0.937112	0.366765
				H	4.478391	0.040774	1.467771
				H	6.328700	2.366853	2.187129
				H	6.629696	0.651165	2.428895
				H	4.399455	0.715065	3.860375
				H	5.945017	1.195462	4.578232
				H	-0.074133	5.939098	0.944708
				H	6.206694	5.806618	3.562260

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Zr	5.290609	1.016406	4.680421
N	4.695955	-0.139030	2.460038
N	7.069849	-0.078547	4.467573
C	5.825964	-0.383663	1.537022
H	6.074662	0.585372	1.080767
H	5.484873	-1.046543	0.721247
C	7.101094	-0.963475	2.136008
H	7.791574	-1.106706	1.291668
H	6.928585	-1.969007	2.547494
C	7.768658	-0.082511	3.192103
H	8.809315	-0.423053	3.337829
H	7.845545	0.943609	2.799893
C	3.641189	0.665003	1.776999
H	4.085379	1.648122	1.579495
H	2.842813	0.821874	2.511361
C	7.473392	-1.165150	5.324325
H	8.471196	-0.976891	5.773625
H	7.589393	-2.115423	4.766085
C	6.429992	-1.401854	6.401641
H	5.590668	-1.957346	5.964248
H	6.836222	-2.012645	7.226470
C	2.041250	-0.753261	0.505005
H	1.565502	-1.070544	1.431773
H	1.622666	-1.149001	-0.418881
C	3.070645	0.097241	0.493961
C	4.890635	2.744685	6.132735
H	4.095989	3.344999	5.658274
H	5.760335	3.414149	6.225556
H	4.545333	2.511961	7.151847
N	5.887384	-0.128582	6.906320
N	3.513451	-0.080823	4.898299
C	4.757801	-0.371644	7.830271
H	4.507416	0.598675	8.282881
H	5.099938	-1.030841	8.648568
C	3.483655	-0.955839	7.233505
H	2.793358	-1.096868	8.078363
H	3.657810	-1.962686	6.825976
C	2.814878	-0.080100	6.173858
H	1.774511	-0.422246	6.029831
H	2.737281	0.947656	6.561590
C	6.940564	0.680238	7.586213
H	6.494686	1.663437	7.779524
H	7.738948	0.835341	6.851481
C	3.111869	-1.171833	4.046266
H	2.113871	-0.987189	3.595902
H	2.997424	-2.119889	4.608584
C	4.156088	-1.411212	2.970337
H	4.996609	-1.962409	3.410849
H	3.751695	-2.026792	2.148160
C	8.544208	-0.728144	8.864193
H	9.021181	-1.047171	7.938657
H	8.963729	-1.119336	9.789586
C	7.512056	0.119063	8.871763
C	5.687707	2.738903	3.220419
H	6.481248	3.342299	3.692857
H	4.817110	3.406741	3.124387
H	6.033939	2.502522	2.202454
C	3.656120	0.591908	-0.795421
H	4.727388	0.370689	-0.881505
H	3.149327	0.153900	-1.661476
H	3.562347	1.684365	-0.863592
C	6.924635	0.616547	10.159182
H	5.854101	0.392192	10.246026
H	7.432770	0.183466	11.026922
H	7.014857	1.709556	10.223322

TS_{10-10'}

Zr	4.857374	0.783054	4.533866
N	4.787771	-0.370872	2.183659
N	6.864531	0.083867	4.406041
C	6.042725	-0.467851	1.399094
H	6.216140	0.523378	0.957225
H	5.873744	-1.166526	0.556646
C	7.304826	-0.862471	2.148590

H	8.099256	-0.931311	1.390377
H	7.220416	-1.869493	2.582981
C	7.711683	0.136401	3.232707
H	8.763203	-0.055541	3.514305
H	7.703786	1.147328	2.795877
C	3.742488	0.205168	1.307149
H	3.301694	-0.594964	0.681269
H	4.229076	0.896538	0.602346
C	7.375356	-0.886292	5.353260
H	8.292532	-0.507388	5.847884
H	7.686681	-1.827584	4.855179
C	6.336321	-1.272732	6.391312
H	5.633740	-1.981068	5.940569
H	6.815272	-1.762666	7.257784
C	3.011605	1.617637	3.164293
H	4.275475	2.124774	3.128036
H	2.243519	2.211263	3.670848
C	2.671959	0.964455	2.044254
C	4.316555	2.580002	5.859282
H	3.716797	3.303687	5.290511
H	5.201130	3.125560	6.220721
H	3.718295	2.304275	6.744820
N	5.547444	-0.103107	6.820122
N	3.604132	-0.889950	4.734234
C	4.427029	-0.490868	7.707829
H	3.929876	0.443503	8.008075
H	4.822025	-0.949859	8.627083
C	3.382982	-1.435995	7.130178
H	2.634278	-1.576852	7.924030
H	3.814105	-2.429054	6.938672
C	2.695410	-0.942011	5.865141
H	1.849355	-1.612442	5.639620
H	2.230619	0.044420	6.071411
C	6.415738	0.914598	7.478812
H	5.741047	1.686010	7.873448
H	7.007155	1.391396	6.688257
C	3.221062	-1.685940	3.603999
H	2.301612	-1.309889	3.103626
H	2.997250	-2.730887	3.896345
C	4.369021	-1.724228	2.616359
H	5.223493	-2.200344	3.112410
H	4.113269	-2.330412	1.726672
C	8.674461	0.603878	8.404040
H	9.094583	0.969165	7.468583
H	9.379711	0.369240	9.199554
C	7.357266	0.467851	8.576115
C	5.630489	2.699178	3.079905
H	6.481899	2.727502	3.776018
H	5.191477	3.704334	3.091341
H	6.012030	2.502542	2.070889
C	1.322790	0.969237	1.395725
H	1.376010	1.360502	0.368840
H	0.914414	-0.048950	1.316159
H	0.612648	1.584215	1.956413
C	6.806792	-0.008514	9.889879
H	6.444972	-1.044245	9.839173
H	7.574360	0.026437	10.670207
H	5.958245	0.607174	10.216391

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Zr	4.418056	0.433463	4.415697
N	4.254913	-0.943553	2.348666
N	6.478011	0.122017	4.183148
C	5.369144	-0.843972	1.376757
H	5.241301	0.118440	0.864356
H	5.231989	-1.637769	0.618353
C	6.781682	-0.896884	1.937531
H	7.459085	-0.874185	1.071082
H	6.979208	-1.851299	2.449072
C	7.098953	0.264887	2.877556
H	8.193993	0.362437	2.991166
H	6.768955	1.203217	2.401444
C	3.030095	-0.465013	1.677612
H	2.157398	-0.898322	2.186892
H	2.996815	-0.843209	0.635789
C	7.305098	-0.607410	5.114257

H	8.123994	0.029411	5.507030	H	4.445282	1.432241	3.456009
H	7.809964	-1.467777	4.632035	H	5.463052	2.837965	3.740727
C	6.474564	-1.161543	6.258881	H	4.474015	2.195554	5.068959
H	5.922508	-2.041848	5.903423	N	5.695344	-0.090546	6.729480
H	7.128624	-1.488622	7.087977	N	4.407257	-1.199380	4.144407
C	3.638146	1.698595	2.688557	C	4.259843	-0.056498	7.100547
H	6.309431	3.699284	3.871165	H	3.899836	0.961117	6.896206
H	3.504612	2.788999	2.681203	H	4.180172	-0.206455	8.194660
C	2.956145	1.042674	1.728610	C	3.333298	-1.023498	6.379293
C	3.536537	2.130138	5.685354	H	2.343365	-0.894112	6.842401
H	2.556364	2.387189	5.254066	H	3.616612	-2.071351	6.557740
H	4.143035	3.049546	5.638933	C	3.231660	-0.773451	4.874933
H	3.368944	1.909369	6.752078	H	2.335693	-1.291959	4.491509
N	5.477443	-0.185120	6.725369	H	3.038690	0.300894	4.713610
N	3.247770	-1.236276	4.829026	C	6.369414	1.065559	7.364942
C	4.556597	-0.781196	7.716855	H	6.580952	0.830328	8.425900
H	3.961495	0.047906	8.127289	H	5.657637	1.904720	7.379238
H	5.130907	-1.206548	8.556114	C	4.209375	-2.481669	3.506282
C	3.594202	-1.851714	7.214550	H	3.524106	-2.398683	2.636070
H	3.026733	-2.180056	8.098170	H	3.718231	-3.209049	4.184205
H	4.136242	-2.741920	6.861975	C	5.532600	-3.102274	3.088636
C	2.627306	-1.375477	6.134510	H	5.993157	-3.569515	3.965996
H	1.776008	-2.075177	6.070369	H	5.382724	-3.885165	2.321915
H	2.192580	-0.412722	6.451567	C	7.651830	1.448849	5.314293
C	6.127284	1.046256	7.248371	H	6.438914	1.662408	4.755615
H	5.320834	1.670915	7.656942	H	8.535985	1.826094	4.790281
H	6.526884	1.589560	6.383837	C	7.618906	1.523420	6.653088
C	3.135294	-2.408769	3.998987	C	6.757630	0.354377	-0.271364
H	2.099371	-2.542728	3.625499	H	7.392391	-0.311243	-0.875845
H	3.361510	-3.339419	4.556941	H	5.770132	0.358571	-0.756428
C	4.120264	-2.322225	2.842253	H	7.167080	1.367638	-0.328966
H	5.113422	-2.632240	3.194858	C	8.690204	2.089706	7.532020
H	3.833444	-3.004260	2.019784	H	8.310651	2.930612	8.131306
C	8.450198	1.357702	7.998692	H	9.055480	1.340829	8.250100
H	8.697833	1.776176	7.024192	H	9.540609	2.448642	6.944662
H	9.245979	1.342492	8.741599				
C	7.225245	0.905241	8.278241				
C	7.251973	3.590514	4.416072				
H	7.495229	2.524821	4.480729				
H	7.134916	4.003329	5.422238				
H	8.046113	4.126717	3.891171				
C	2.060910	1.648160	0.688122				
H	2.419869	1.425159	-0.328258				
H	1.040989	1.239499	0.748123				
H	1.996918	2.734668	0.801285				
C	6.902080	0.358628	9.638568				
H	6.799057	-0.734787	9.631500				
H	7.690874	0.604737	10.357142				
H	5.953772	0.761080	10.018685				

TS_{10⁻¹⁵}

Zr	6.326429	-0.297065	4.234271				
N	6.484411	-2.087652	2.602016				
N	7.639736	-1.602015	5.262473				
C	7.822193	-2.685688	2.373987				
H	8.416741	-1.914217	1.866689				
H	7.698978	-3.524154	1.663240				
C	8.581312	-3.161791	3.599545				
H	9.535007	-3.566496	3.229554				
H	8.063480	-3.996854	4.091951				
C	8.856289	-2.075830	4.629553				
H	9.537380	-2.491668	5.391351				
H	9.428571	-1.256698	4.145901				
C	6.051140	-1.482982	1.321736				
H	4.955386	-1.396400	1.327867				
H	6.304450	-2.162457	0.483932				
C	7.688499	-1.584230	6.697016				
H	8.385545	-0.816887	7.100186				
H	8.042104	-2.551817	7.103922				
C	6.295082	-1.348648	7.235607				
H	5.664282	-2.180031	6.898275				
H	6.284969	-1.336963	8.341801				
C	7.042144	0.559853	2.252355				
H	7.450359	1.563212	2.068921				
C	6.669439	-0.116966	1.149696				
C	5.088412	1.916698	4.203628				

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Zr	2.910994	3.362635	2.489748
N	1.120731	2.837024	0.860982
N	4.672594	2.748995	4.122386
N	3.759806	2.107065	0.996651
N	1.996133	2.165437	3.991209
C	5.456313	5.020573	3.545111
C	0.109320	3.906389	0.671664
H	-0.878490	3.540820	0.997041
H	-0.011627	4.108184	-0.407711
C	5.742381	3.762096	4.301950
H	5.876967	3.963990	5.379783
H	6.708126	3.341408	3.977033
C	0.462710	5.152156	1.421032
C	0.474126	1.580195	1.290211
H	1.222332	0.776359	1.264553
H	-0.308278	1.317481	0.554865
C	3.915709	2.628813	5.384481
H	3.626773	3.650665	5.670689
H	4.562549	2.224085	6.184269
C	6.443857	6.123792	3.792625
H	6.208776	7.007041	3.191044
H	7.470527	5.809566	3.550281
H	6.457432	6.425236	4.850688
C	1.868383	2.662889	-0.400621
H	2.213075	3.664115	-0.697628
H	1.199028	2.286207	-1.195537
C	0.837784	1.312685	3.825456
H	0.242007	1.313400	4.759817
H	1.156341	0.254429	3.687172
C	5.247655	1.454575	3.703240
C	-0.112190	1.673381	2.694894
H	-0.516473	2.679539	2.873562
H	-0.964726	0.983775	2.756012
C	3.060444	1.758195	-0.212023
H	2.737119	0.694302	-0.199596
H	3.708284	1.844353	-1.106767
C	-0.460780	6.306791	1.161364
H	-0.181695	7.179214	1.759932
H	-1.504791	6.050674	1.398153

H	-0.450773	6.602331	0.101582
C	2.675759	1.788921	5.202927
H	2.941536	0.709168	5.198953
H	2.033779	1.918066	6.096592
C	5.836839	1.505375	2.297393
C	4.866735	1.190054	1.170361
C	4.401110	5.059940	2.713217
H	4.276441	6.013179	2.180348
C	1.515921	5.138432	2.256338
H	1.691644	6.087085	2.782921
H	5.460826	1.148093	0.235881
H	4.486980	0.153485	1.318333
H	6.293528	2.487706	2.111934
H	6.650593	0.770251	2.239675
H	4.455800	0.693727	3.735435
H	6.014724	1.154096	4.440225

Amine substrate: 2,2-diphenyl-pent-4-enylamine

N	2.186716	-1.091781	-2.420751
C	1.843601	-0.511939	-1.139498
H	2.377107	-0.367556	-3.105789
H	2.642436	0.193856	-0.876733
C	0.474996	0.218147	-1.049522
H	1.863915	-1.307665	-0.381145
C	0.480143	1.403585	-2.043288
C	1.510465	2.442644	-1.739696
H	0.648167	1.027380	-3.062269
C	2.469943	2.815629	-2.582029
H	-0.518389	1.867201	-2.041642
C	-0.613155	-0.801807	-1.388956
H	1.450268	2.911356	-0.754913
H	3.195700	3.582767	-2.325467
C	-1.327100	-0.799978	-2.588103
H	2.560520	2.372308	-3.574217
C	-2.271942	-1.787070	-2.865113
C	-2.516727	-2.800919	-1.950545
H	-1.162878	-0.019712	-3.326758
C	-1.810524	-2.819209	-0.750415
H	-2.817071	-1.756635	-3.805953
C	-0.874589	-1.832817	-0.477147
H	-3.253375	-3.570995	-2.166267
C	0.216938	0.772425	0.352332
H	-1.992673	-3.604979	-0.020798
C	-1.033169	1.337768	0.632186
H	-0.340822	-1.847064	0.472483
H	-1.804600	1.321139	-0.137492
C	-1.312129	1.896616	1.870804
C	-0.343054	1.897309	2.870658
H	-2.292326	2.329092	2.058873
C	0.898117	1.332465	2.613233
H	-0.557847	2.331955	3.843969
C	1.176309	0.777388	1.365374
H	1.663463	1.320685	3.386056
H	2.159220	0.346188	1.195221
H	1.422647	-1.659677	-2.777583

Product: 2-methyl-4,4-diphenylpyrrolidine

N	1.608757	-1.482092	-1.412329
C	1.931841	-0.857384	-0.138135
H	1.035318	-2.300103	-1.220937
H	2.750385	-0.136095	-0.291161
C	0.660139	-0.092085	0.296591
H	2.273727	-1.600920	0.591902
C	0.290873	0.524011	-1.067515
C	0.786763	-0.485391	-2.132802
H	-0.771615	0.775979	-1.161443
C	1.607388	0.191791	-3.215176
H	0.842952	1.469244	-1.169179
C	-0.361371	-1.104842	0.809968
H	-0.060577	-1.004904	-2.603562
H	1.032249	0.979954	-3.716938
C	-1.485063	-1.503897	0.086079
H	1.941092	-0.532477	-3.964720
C	-2.367787	-2.454600	0.595885

C	-2.140887	-3.026758	1.839330
H	-1.689406	-1.069503	-0.890704
C	-1.020706	-2.642163	-2.572421
H	-3.238741	-2.744181	0.011924
C	-0.146344	-1.694785	2.061549
H	-2.831698	-3.765638	2.238276
C	0.880573	0.980897	1.346579
H	-0.832027	-3.079721	3.550201
C	-0.184437	1.820626	1.690270
H	0.719195	-1.387713	2.648462
H	-1.153012	1.670531	1.213269
C	-0.029835	2.824282	2.635432
C	1.198043	3.006172	3.266991
H	-0.871921	3.465866	2.885208
C	2.260219	2.172566	2.945614
H	1.321823	3.790497	4.009918
C	2.102017	1.167430	1.993459
H	3.222279	2.299140	3.437335
H	2.946994	0.522087	1.761750
H	2.500701	0.654782	-2.775813

16

Zr	0.713337	-0.291872	0.223041
N	2.445584	1.533517	0.577774
N	1.509663	0.229983	-1.643991
N	1.894449	-1.293469	1.633807
N	1.152859	-2.641075	-0.638445
C	3.749674	0.894676	0.852586
H	4.553619	1.651040	0.776902
H	3.923911	0.175346	0.042828
C	2.529013	1.218995	-1.868255
H	2.360296	1.764910	-2.815144
H	3.546055	0.781388	-1.961204
C	1.289207	-0.654831	-2.772474
H	1.400894	-0.097959	-3.719217
H	0.243499	-0.992022	-2.760499
C	2.570982	-0.520969	2.658400
H	2.812912	-1.165313	3.521633
H	1.877055	0.234609	3.051373
C	2.479143	2.212936	-0.731762
H	3.326830	2.921691	-0.769436
H	1.547866	2.790597	-0.810705
C	2.067217	2.517927	1.610409
H	2.382514	3.529418	1.299032
H	2.643347	2.308916	2.521757
C	2.363215	-2.612641	-1.484706
H	2.706654	-3.647314	-1.672769
H	3.148464	-2.127922	-0.890965
C	0.599658	2.471402	1.949582
C	1.419083	-3.395981	0.601783
H	1.800560	-4.404393	0.356537
H	0.453648	-3.513069	1.113149
C	-1.299630	-2.549112	-0.997681
C	3.859564	0.166467	2.193261
H	4.196444	0.851288	2.984518
H	4.663804	-0.575453	2.084067
C	-0.005565	-3.251032	-1.319350
H	-0.055607	-4.328921	-1.083839
H	0.159198	-3.203730	-2.403916
C	2.217887	-1.872886	-2.815718
H	1.867476	-2.553361	-3.604900
H	3.228559	-1.564825	-3.120101
C	2.363197	-2.647798	1.514047
H	2.375354	-3.158959	2.494671
H	3.406095	-2.715503	1.137145
C	-0.179676	1.348241	1.595439
C	0.091403	3.515287	2.727381
H	0.722582	4.375044	2.960594
C	-1.982551	2.332482	2.954463
H	-2.988762	2.255700	3.363401
C	-1.284959	-1.240517	-0.465624
C	-1.202332	3.452821	3.225886
H	-1.594956	4.265811	3.833645
C	-1.473334	1.314897	2.153527
H	-2.114589	0.454095	1.960855
C	-2.486209	-3.192822	-1.357437

H	-2.454027	-4.212843	-1.745228
C	-3.703304	-2.534490	-1.244857
H	-4.626167	-3.038381	-1.525902
C	-3.726721	-1.220825	-0.785796
H	-4.670891	-0.682561	-0.719541
C	-2.539774	-0.602266	-0.405404
H	-2.597315	0.427132	-0.050727

A'

Zr	0.622037	-3.610228	-0.340628
N	2.146053	2.072707	-2.470482
C	1.349824	2.514408	-1.341037
H	2.367808	2.854537	-3.078715
H	1.845514	3.402940	-0.929514
C	-0.143036	2.846323	-1.624200
N	2.423391	-1.825989	-0.190863
N	1.087038	-2.992584	-2.279501
H	1.380434	1.739434	-0.557365
C	-0.215148	4.012962	-2.641103
N	2.032960	-4.690403	0.762091
C	0.359816	5.296784	-2.136240
H	0.318225	3.733753	-3.560083
N	0.929405	-5.905654	-1.441644
C	1.395186	5.921669	-2.692153
H	-1.269551	4.161218	-2.921886
C	-0.782456	1.572813	-2.181027
C	3.752146	-2.467748	-0.188266
H	-0.112552	5.728267	-1.251149
H	1.783291	6.857762	-2.298684
C	-0.946604	1.335345	-3.549409
H	4.532528	-1.701934	-0.354896
H	1.889801	5.524203	-3.579365
C	-1.419617	0.108877	-4.019060
H	3.779303	-3.133775	-1.060082
C	-1.742319	-0.906340	-3.128265
C	2.039950	-1.971508	-2.627721
H	-0.712323	2.110935	-4.275148
C	-1.599645	-0.677771	-1.762614
H	-1.535824	-0.043667	-5.090337
H	1.672403	-1.355209	-3.472159
C	-1.125928	0.541096	-1.297153
H	3.012193	-2.388474	-2.967037
H	-2.106919	-1.869063	-3.482487
C	0.642186	-3.786855	-3.406756
C	-0.865391	3.283204	-0.348026
H	-1.853710	-1.456974	-1.047208
C	-2.262742	3.367966	-0.352732
H	0.561865	-3.152392	-4.307238
H	-1.016244	0.689406	-0.222849
H	-2.807770	3.071439	-1.248417
H	-0.381150	-4.140813	-3.214870
C	-2.966320	3.793365	0.765733
C	-2.285351	4.156348	1.924973
H	-4.052564	3.840249	0.732511
C	-0.898711	4.086547	1.945642
C	2.870248	-3.971007	1.703053
H	-2.833606	4.489594	2.803208
C	-0.197492	3.654366	0.821112
H	3.231011	-4.656361	2.490142
H	-0.349815	4.366663	2.842669
H	2.254895	-3.227604	2.228209
H	0.887413	3.610958	0.874455
C	2.221896	-1.060942	-1.438364
H	3.040445	-0.334536	-1.587789
H	1.292743	-0.488847	-1.306234
C	2.239594	-0.898946	0.938952
H	2.629460	0.101857	0.675586
C	2.855132	-1.241994	1.780835
H	1.953060	-5.802050	-2.501551
H	2.259676	-6.816724	-2.819009
H	2.836365	-5.339305	-2.044145
C	0.803989	-0.843410	1.385633
C	1.434080	-6.729637	-0.326689
H	1.785903	-7.706556	-0.707017
H	0.583007	-6.911495	0.343961
C	-1.549433	-5.865292	-1.320783

C	4.078600	-3.271304	1.071561
H	4.549072	-2.631292	1.831585
H	4.844259	-4.010235	0.796015
C	-0.326888	-6.499907	-1.930111
H	-0.314692	-7.592636	-1.768612
H	-0.375670	-6.374973	-3.019795
C	1.542826	-4.983704	-3.726467
H	1.040433	-5.616931	-4.471554
H	2.470171	-4.640967	-4.207235
C	2.511718	-6.009469	0.447824
H	2.727379	-6.587648	1.365712
H	3.464659	-6.002719	-0.122874
C	-0.029426	-1.971521	1.192474
H	1.635091	1.391040	-3.027813
C	0.370738	0.299052	2.062197
H	1.034513	1.161789	2.151946
C	-1.719078	-0.775391	2.531961
H	-2.704111	-0.770799	2.995876
C	-1.473305	-4.592768	-0.707225
C	-0.903015	0.347939	2.617465
H	-1.249079	1.252078	3.115427
C	-1.277554	-1.901694	1.839792
H	-1.944572	-2.762868	1.804288
C	-2.760415	-6.538706	-1.503580
H	-2.762268	-7.528256	-1.964906
C	-3.959077	-5.951527	-1.124986
H	-4.900138	-6.478414	-1.270469
C	-3.938464	-4.675777	-0.571282
H	-4.869132	-4.185855	-0.289581
C	-2.721808	-4.030642	-0.370380
H	-2.760711	-3.035898	0.073631

TS_{A'B}

Zr	0.779832	-3.645391	-0.455470
N	1.196043	1.416509	-2.978902
C	0.895447	2.097140	-1.733156
H	1.378117	2.086718	-3.719681
H	1.712841	2.805655	-1.543552
C	-0.463516	2.843844	-1.655145
N	2.518720	-1.837158	-0.093190
N	1.559056	-3.113114	-2.321800
H	0.915832	1.359381	-0.916379
C	-0.445366	4.030685	-2.648073
N	1.977124	-4.659427	0.934777
C	0.578611	5.072495	-2.333975
H	-0.261747	3.653792	-3.664789
N	1.234647	-5.988782	-1.346734
C	1.582380	5.401769	-3.143373
H	-1.446389	4.489493	-2.659812
C	-1.553590	1.829725	-2.005398
C	3.831055	-2.471020	0.138441
H	0.478616	5.577205	-1.370491
H	2.306247	6.169698	-2.882681
C	-2.230681	1.812417	-3.226961
H	4.628687	-1.708409	0.059634
H	1.711740	4.918855	-4.112900
C	-3.163198	0.816524	-3.518605
H	3.991594	-3.173844	-0.688298
C	-3.439713	-0.179905	-2.592110
C	2.546999	-2.089173	-2.549024
H	-2.045141	2.580782	-3.973783
C	-2.778336	-0.168144	-1.366718
H	-3.673993	0.827465	-4.479299
H	2.330822	-1.510588	-3.465568
C	-1.842334	0.816189	-1.083212
H	3.568644	-2.502710	-2.687192
H	-4.162982	-0.961269	-2.816497
C	1.349213	-3.989599	-3.458484
C	-0.710491	3.393765	-0.249298
H	-2.989175	-0.922168	-0.611018
C	-1.989292	3.852000	0.089457
H	1.453481	-3.420906	-4.398621
H	-1.341383	0.807638	-0.115201
H	-2.792216	3.767533	-0.642538
H	0.308639	-4.342961	-3.450735
C	-2.258928	4.382297	1.344033

C	-1.249094	4.470946	2.298983	H	2.864890	2.064593	-3.822059
H	-3.264733	4.723658	1.579325	C	-3.150571	0.890186	-2.438604
C	0.026907	4.026817	1.978186	H	4.870854	-1.968669	1.042718
C	2.676544	-3.895473	1.950527	H	1.561756	0.848121	-4.325324
H	-1.457109	4.883522	3.283580	C	-4.412277	0.315673	-2.289502
C	0.292348	3.496067	0.716900	H	4.138209	-3.191218	-0.007723
H	2.925127	-4.544361	2.808520	C	-4.877186	-0.037313	-1.030172
H	0.828230	4.089382	2.712095	C	3.747339	-1.671856	-2.078185
H	1.995998	-3.134439	2.356520	H	-2.812820	1.152428	-3.438439
H	1.302546	3.155613	0.500378	C	-4.073892	0.196419	0.084574
C	2.502215	-1.129215	-1.387843	H	-5.026837	0.137383	-3.169006
H	3.317448	-0.384626	-1.433626	H	4.053900	-1.048903	-2.941690
H	1.555303	-0.576952	-1.439487	C	-2.822831	0.777595	-0.065586
C	2.166888	-0.871916	0.962196	H	4.569412	-2.408616	-1.947868
H	2.527426	0.136804	0.686622	H	-5.859183	-0.491081	-0.914168
H	2.715135	-1.134016	1.876677	C	2.190610	-2.718496	-3.629699
C	2.446128	-5.946786	-2.190378	C	-0.855062	3.000461	-0.630566
H	2.793019	-6.978435	-2.389242	H	-4.419974	-0.078175	1.078862
H	3.228965	-5.465915	-1.590983	C	-1.719514	4.045458	-0.978321
C	0.693373	-0.870922	1.270262	H	2.555251	-1.980231	-4.370799
C	1.500073	-6.754315	-0.113630	H	-2.214610	0.958674	0.820913
H	1.882896	-7.760233	-0.367313	H	-2.437465	3.896046	-1.784591
H	0.534234	-6.877182	0.395807	H	1.096413	-2.754065	-3.784153
C	-1.216526	-5.915190	-1.707660	C	-1.699284	5.255132	-0.299529
C	3.965059	-3.220642	1.465913	C	-0.812494	5.448359	0.756912
H	4.328228	-2.550437	2.258239	H	-2.383360	6.048976	-0.591290
H	4.755705	-3.972771	1.331479	C	0.040257	4.416942	1.124823
C	0.083868	-6.600251	-2.037343	C	2.161055	-4.058298	1.892802
H	0.043506	-7.681800	-1.816497	H	-0.795065	6.393940	1.293774
H	0.248797	-6.536338	-3.120972	C	0.020470	3.204123	0.437659
C	2.296814	-5.192534	-3.513061	H	2.284719	-5.013051	2.431790
H	1.960752	-5.868479	-4.312439	H	0.730032	4.548426	1.955603
H	3.303607	-4.863921	-3.808375	H	1.374583	-3.515034	2.427593
C	2.443497	-6.013572	0.804297	H	0.691961	2.412028	0.761852
H	2.455757	-6.531824	1.781241	C	3.639633	-0.772326	-0.864194
H	3.486183	-6.079360	0.426609	H	4.623310	-0.372820	-0.551885
C	-0.106768	-1.983471	0.921902	H	3.001127	0.078401	-1.142625
H	0.402060	0.850080	-3.271365	C	2.535321	-0.525540	1.286362
C	0.193669	0.212255	1.998509	H	2.480951	0.472093	0.822503
H	0.839706	1.064789	2.217425	H	3.297383	-0.429889	2.081096
C	-1.923967	-0.893487	2.184633	C	2.552510	-5.108782	-2.853890
H	-2.949228	-0.922932	2.550708	H	2.673724	-6.134831	-3.250274
C	-1.214941	-4.618184	-1.147172	H	3.332688	-4.969318	-2.096488
C	-1.121931	0.215008	2.443752	C	1.181598	-0.872454	1.853577
H	-1.513236	1.073656	2.987317	C	1.199648	-6.021927	-1.086585
C	-1.415704	-1.958326	1.442966	H	1.473964	-7.011957	-1.497252
H	-2.077692	-2.806309	1.261670	H	0.158319	-6.070140	-0.742901
C	-2.395254	-6.562078	-2.087678	C	-1.141059	-4.581183	-2.554508
H	-2.350041	-7.572965	-2.497604	C	3.477912	-3.261495	2.025050
C	-3.620037	-5.919342	-1.968473	H	3.409611	-2.596905	2.898447
H	-4.535983	-6.425909	-2.266769	H	4.316518	-3.940841	2.238380
C	-3.657878	-4.617346	-1.478763	C	0.123297	-5.218039	-3.067069
H	-4.606913	-4.087873	-1.403584	H	-0.012390	-6.299964	-3.256998
C	-2.477774	-3.998996	-1.078106	H	0.376838	-4.777221	-4.040148
H	-2.546011	-2.979575	-0.701851	C	2.765363	-4.094046	-3.971717
B				H	2.336339	-4.447279	-4.920687
Zr	1.028703	-2.811653	-0.811048	H	3.848806	-4.019573	-4.142967
N	0.050784	-0.625150	-1.586436	C	2.068073	-5.644018	0.087958
C	0.048976	0.647696	-0.864407	H	1.881823	-6.387388	0.885311
H	0.552115	-0.521890	-2.468335	H	3.145579	-5.762715	-0.164568
H	1.074228	1.039471	-0.886722	C	0.357927	-1.784514	1.167884
C	-0.917039	1.700381	-1.436076	H	-0.907222	-0.897675	-1.813954
N	2.980499	-1.474822	0.250447	C	0.756487	-0.210443	3.007822
N	2.460525	-2.271895	-2.286174	H	1.426208	0.489909	3.512323
H	-0.193255	0.440252	0.183269	C	-1.356168	-1.343692	2.871315
C	-0.506586	1.996013	-2.900579	H	-2.352139	-1.540249	3.267497
N	1.726702	-4.313343	0.530693	C	-1.055406	-3.459584	-1.700201
C	0.926144	2.401849	-3.033780	C	-0.519972	-0.433552	3.513180
H	-0.682279	1.108813	-3.525014	H	-0.853223	0.087316	4.408844
N	1.257124	-5.005910	-2.152667	C	-0.910222	-2.008812	1.729546
C	1.829497	1.739636	-3.754922	H	-1.584049	-2.728456	1.258187
H	-1.155238	2.788357	-3.302436	C	-2.361233	-5.084956	-3.009417
C	-2.333940	1.127556	-1.332463	H	-2.376565	-5.963732	-3.656826
C	3.918857	-2.480338	0.798707	C	-3.554244	-4.470926	-2.648132
H	1.231064	3.292775	-2.478933	H	-4.504121	-4.865756	-3.003889
				C	-3.515534	-3.347877	-1.829749
				H	-4.436108	-2.841968	-1.540427

C	-2.290432	-2.866977	-1.372268	H	0.273097	-4.143815	-4.184114
H	-2.323933	-1.986750	-0.720689	C	2.708935	-3.539864	-4.093271
TS_{BC}				H	2.249694	-3.770690	-5.065023
Zr	0.951513	-2.674965	-0.856006	H	3.788632	-3.455294	-4.282862
N	-0.176485	-0.697141	-0.939849	C	2.019707	-5.534353	-0.219483
C	-0.005804	0.713902	-0.654415	H	1.858956	-6.381433	0.472493
H	-1.130545	-0.868708	-1.250855	H	3.104267	-5.572010	-0.466451
H	1.051285	0.993968	-0.785355	C	0.112490	-1.765463	1.504422
C	-0.856924	1.627129	-1.565936	H	-0.141011	-1.227482	0.296140
N	2.833244	-1.479036	0.480830	C	1.062751	-1.165754	3.666117
N	2.427858	-1.983196	-2.167728	H	1.877807	-0.730064	4.246427
H	-0.265193	0.947756	0.399374	C	-1.065074	-2.291218	3.574863
C	-0.294036	1.530690	-3.009755	H	-1.923430	-2.729058	4.080933
N	1.610748	-4.287780	0.388423	C	-1.142134	-3.385687	-1.632329
C	1.034807	2.197398	-3.178152	C	-0.036945	-1.717314	4.317253
H	-0.199679	0.466422	-3.270742	H	-0.088216	-1.702568	5.404026
N	1.219407	-4.659157	-2.384858	C	-0.987861	-2.301233	2.184147
C	2.190002	1.537558	-3.221738	H	-1.801259	-2.751883	1.613277
H	-1.016795	1.984784	-3.703719	C	-2.403286	-4.911291	-3.095873
C	-2.300901	1.132696	-1.479270	H	-2.395601	-5.673137	-3.877273
C	3.761036	-2.524323	0.980170	C	-3.609972	-4.487987	-2.550882
H	1.030889	3.287297	-3.245913	H	-4.548636	-4.917477	-2.895612
H	3.144835	2.046188	-3.337891	C	-3.599902	-3.510882	-1.561784
C	-2.931666	0.433391	-2.509203	H	-4.535955	-3.159027	-1.129652
H	4.683269	-2.020723	1.329218	C	-2.388275	-2.979343	-1.123490
H	2.204704	0.450406	-3.130452	H	-2.439986	-2.200816	-0.355243
C	-4.219275	-0.076209	-2.347765	C			
H	4.042179	-3.135330	0.112768	Zr	0.694922	-2.630707	-1.386036
C	-4.898436	0.103945	-1.150795	N	-0.423203	-1.016107	-0.691352
C	3.720412	-1.460047	-1.822356	C	-0.185866	0.405426	-0.582195
H	-2.414664	0.260861	-3.450406	H	-1.404521	-1.216915	-0.488664
C	-4.279766	0.795976	-0.111202	H	0.854271	0.604444	-0.880914
H	-4.682998	-0.627539	-3.162867	C	-1.102777	1.306134	-1.454658
H	4.091564	-0.761738	-2.596589	N	2.617065	-1.429115	0.601070
C	-2.998807	1.303319	-0.275855	N	2.437785	-1.950986	-2.296131
H	4.508906	-2.236077	-1.730962	H	-0.275650	0.754028	0.464364
H	-5.902097	-0.296026	-1.023087	C	-0.665939	1.152932	-2.936484
C	2.162430	-2.213397	-3.565685	N	0.979828	-4.110334	0.053185
C	-0.787355	3.087797	-1.126413	C	0.613856	1.862854	-3.257986
H	-4.799546	0.942606	0.833235	H	-0.580964	0.077553	-3.161655
C	-1.674981	4.007815	-1.696597	N	1.377800	-4.755471	-2.661838
H	2.549403	-1.386424	-4.188293	C	1.804605	1.279399	-3.379396
H	-2.526416	1.851821	0.538418	H	-1.454173	1.562664	-3.584258
H	-2.437165	3.648975	-2.388145	C	-2.550001	0.874060	-1.219256
H	1.066794	-2.187084	-3.720786	C	3.266497	-2.608319	1.198134
C	-1.611872	5.359268	-1.385703	H	0.537240	2.945623	-3.381629
C	-0.655631	5.826271	-0.487368	H	2.696832	1.856495	-3.614437
H	-2.316568	6.051240	-1.842065	C	-3.384494	0.369566	-2.216782
C	0.230935	4.925988	0.088615	H	4.148111	-2.288437	1.792937
C	1.983716	-4.225985	1.790362	H	1.925552	0.205027	-3.230388
H	-0.605785	6.883666	-0.237835	C	-4.691505	-0.024732	-1.929810
C	0.167340	3.571101	-0.230105	H	3.663923	-3.199848	0.363561
H	2.093421	-5.246394	2.193682	C	-5.186533	0.065273	-0.636494
H	0.982589	5.275822	0.793261	C	3.698727	-1.631549	-1.678272
H	1.172117	-3.775682	2.367734	H	-3.018318	0.250392	-3.233792
H	0.882236	2.891737	0.229428	C	-4.364486	0.563108	0.372475
C	3.567607	-0.684517	-0.526518	H	-5.321147	-0.408142	-2.730564
H	4.543836	-0.356817	-0.123068	H	4.306040	-0.999435	-2.357190
H	2.975617	0.212894	-0.747911	C	-3.069116	0.966275	0.080194
C	2.340421	-0.614019	1.570857	H	4.325463	-2.526479	-1.483492
H	2.057337	0.345420	1.112419	H	-6.204282	-0.246180	-0.413212
H	3.153980	-0.391562	2.286427	C	2.545755	-2.320647	-3.691210
C	2.512821	-4.675972	-3.100188	C	-0.962854	2.782242	-1.076628
H	2.632596	-5.649993	-3.608833	H	-4.738122	0.645451	1.390946
H	3.295020	-4.617136	-2.333661	C	-1.916760	3.695558	-1.540253
C	1.139542	-1.190942	2.274880	H	3.066512	-1.529957	-4.264066
C	1.182389	-5.800260	-1.445448	H	-2.443988	1.374980	0.874380
H	1.499542	-6.719382	-1.970893	H	-2.777237	3.326131	-2.097843
H	0.139829	-5.927589	-1.130994	H	1.529220	-2.352405	-4.124349
C	-1.200707	-4.363329	-2.648502	C	-1.791435	5.056764	-1.296027
C	3.285260	-3.451925	2.083060	C	-0.705117	5.540251	-0.571649
H	3.181229	-2.904605	3.029879	H	-2.547740	5.743662	-1.670193
H	4.120878	-4.151165	2.235695	C	0.250581	4.647312	-0.104486
C	0.080197	-4.785141	-3.313572	C	1.003657	-3.813872	1.468186
H	0.025669	-5.820245	-3.700485	H	-0.605721	6.605274	-0.374481

C	0.126019	3.283723	-0.359471	H	2.640105	-3.014331	0.471790
H	0.551743	-4.644985	2.041977	C	-4.179725	-0.438535	-3.609400
H	1.106997	5.010059	0.460168	C	2.337748	-1.365493	-1.584961
H	0.361598	-2.945545	1.651536	H	-0.930524	0.209274	-2.886733
H	0.904224	2.612263	-0.003279	C	-4.776653	0.269294	-2.568902
C	3.505526	-0.828450	-0.409254	H	-2.312866	-0.994070	-4.521665
H	4.496786	-0.606478	0.038344	H	2.792516	-0.800539	-2.422084
H	3.060014	0.134018	-0.699923	C	-3.995157	0.945686	-1.643232
C	2.398666	-0.352817	1.594898	H	2.918704	-2.310853	-1.532510
H	1.908683	0.468564	1.055729	H	-4.790210	-0.982055	-4.326593
H	3.390044	0.026894	1.917557	C	0.670992	-2.043794	-3.183238
C	2.814124	-4.762434	-2.980559	C	-2.379568	3.067570	-0.462029
H	3.102086	-5.749573	-3.389965	H	-5.860594	0.288705	-2.475192
H	3.352678	-4.650465	-2.030308	C	-2.490381	3.904629	-1.579864
C	1.603508	-0.657216	2.834031	H	1.080556	-1.331595	-3.925904
C	1.062941	-5.804868	-1.672394	H	-4.477328	1.505898	-0.842247
H	1.516136	-6.763953	-1.985591	H	-2.187518	3.527593	-2.556469
H	-0.027038	-5.928648	-1.676259	H	-0.419435	-2.033472	-3.353059
C	-0.837999	-4.417536	-3.659401	C	-2.995680	5.191318	-1.471907
C	2.390324	-3.529756	2.046465	C	-3.409693	5.679397	-0.234418
H	2.262560	-3.136178	3.062307	H	-3.071766	5.816494	-2.359090
H	2.950891	-4.470542	2.158281	C	-3.306491	4.864326	0.883616
C	0.547608	-4.968515	-3.858541	C	0.394281	-3.188399	2.324499
H	0.528505	-6.043054	-4.122923	H	-3.811122	6.686434	-0.146516
H	1.025251	-4.461194	-4.707467	C	-2.792877	3.572936	0.771005
C	3.248947	-3.658525	-3.940713	H	0.033441	-3.931569	3.060567
H	3.090434	-3.957438	-4.986314	H	-3.627251	5.229396	1.857118
H	4.335895	-3.538110	-3.832578	H	-0.092621	-2.240494	2.596686
C	1.493569	-5.419088	-0.273323	H	-2.723878	2.963472	1.668589
H	1.096295	-6.181033	0.424587	C	2.560151	-0.555058	-0.324387
H	2.597943	-5.487282	-0.175464	H	3.645654	-0.432278	-0.148240
C	0.216645	-0.830632	2.797858	H	2.148520	0.450959	-0.484296
H	-0.303687	-0.793715	1.839679	C	1.725589	-0.100750	1.903698
C	2.251653	-0.711710	4.069729	H	1.188701	-0.562847	2.741181
H	3.331096	-0.562746	4.108264	H	1.050928	0.661059	1.494527
C	0.169943	-1.168960	5.188166	C	0.974833	-4.456537	-2.376890
H	-0.387459	-1.374452	6.099280	H	1.089606	-5.483055	-2.774787
C	-1.021668	-3.352339	-2.752956	H	1.747446	-4.334714	-1.605667
C	1.545570	-0.970783	5.239602	C	2.998346	0.543991	2.402685
H	2.070103	-1.017595	6.191389	C	-0.444632	-5.318154	-0.611605
C	-0.491759	-1.092751	3.965537	H	-0.123152	-6.312809	-0.972079
H	-1.569202	-1.235932	3.919673	H	-1.508192	-5.378266	-0.352814
C	-1.889587	-4.949090	-4.406546	C	-2.715222	-3.940678	-2.061142
H	-1.705149	-5.780335	-5.089261	C	1.910114	-3.038676	2.484005
C	-3.171146	-4.424132	-4.283020	H	2.115135	-2.535828	3.440328
H	-3.991071	-4.840295	-4.865303	H	2.382463	-4.027631	2.572007
C	-3.393447	-3.372938	-3.399957	C	-1.451493	-4.521785	-2.634561
H	-4.392506	-2.953660	-3.282529	H	-1.564967	-5.596541	-2.875353
C	-2.334544	-2.860348	-2.654258	H	-1.206666	-4.024272	-3.582484
H	-2.553930	-2.036758	-1.974161	C	1.210455	-3.444690	-3.495740
C'				H	0.771836	-3.795512	-4.440543
Zr	-0.535813	-2.118352	-0.432578	H	2.293688	-3.401810	-3.674824
N	-1.411886	-0.528656	0.570240	C	0.326415	-4.903741	0.623916
C	-1.851578	0.850957	0.659674	H	0.073682	-5.611981	1.436304
H	-1.987083	-1.056020	1.236001	H	1.417072	-5.033414	0.455746
H	-1.272023	1.399675	1.427561	C	3.737999	-0.024342	3.443557
C	-1.785801	1.667226	-0.656753	H	3.374299	-0.931704	3.925532
N	1.889298	-1.122353	0.850144	C	3.470937	1.726653	1.826047
N	0.932342	-1.587798	-1.835816	H	2.899556	2.195556	1.024561
H	-2.899866	0.886848	1.001787	C	5.382309	1.730969	3.296519
C	-0.312792	1.845674	-1.092541	H	6.304607	2.191393	3.643585
N	-0.027770	-3.552928	0.991607	C	-2.608757	-2.873893	-1.144271
C	0.476825	2.767934	-0.221011	C	4.651521	2.314882	2.266686
H	0.165479	0.853640	-1.124664	H	4.999275	3.237531	1.806764
N	-0.326817	-4.328730	-1.703026	C	4.920147	0.559124	3.886574
C	1.253060	3.749292	-0.675864	H	5.477570	0.100357	4.700373
H	-0.277661	2.229475	-2.122045	C	-3.944620	-4.458486	-2.467912
C	-2.598239	0.936295	-1.726122	H	-3.978013	-5.287719	-3.177029
C	2.588034	-2.322358	1.322960	C	-5.126568	-3.930431	-1.960249
H	0.402114	2.621461	0.860525	H	-6.086717	-4.337181	-2.272391
H	1.816232	4.393805	-0.004766	C	-5.064726	-2.891291	-1.038599
C	-2.013391	0.234962	-2.781624	H	-5.982349	-2.471432	-0.627608
H	3.635589	-2.085541	1.593303	C	-3.827712	-2.381454	-0.649510
H	1.342786	3.951649	-1.742986	H	-3.819396	-1.547523	0.054446
C	-2.796717	-0.448967	-3.711619				

TS^{cD}

Zr	-0.218663	-2.046648	-0.348716
N	-1.142423	-0.480317	0.250109
C	-1.808611	0.769567	0.407812
H	-2.047007	-1.407975	-0.418423
H	-1.369451	1.308904	1.266741
C	-1.736889	1.699464	-0.841964
N	1.996544	-1.289968	0.825952
N	1.261871	-1.698518	-1.825062
H	-2.878992	0.647484	0.663217
C	-0.253535	2.022757	-1.136339
N	0.012195	-3.580666	1.080672
C	0.398556	2.883820	-0.104704
H	0.281835	1.061682	-1.209721
N	-0.497384	-4.144181	-1.669649
C	1.010865	4.038024	-0.359385
H	-0.167718	2.520849	-2.112852
C	-2.387958	0.950950	-2.003306
C	2.682570	-2.498292	1.328415
H	0.362612	2.532065	0.930600
H	1.478269	4.625571	0.427654
C	-1.669801	0.422925	-3.077426
H	3.727936	-2.254276	1.592848
H	1.054922	4.443760	-1.370011
C	-2.310994	-0.293817	-4.088987
H	2.736317	-3.194283	0.480695
C	-3.682807	-0.503924	-4.043475
C	2.655001	-1.476219	-1.568881
H	-0.592902	0.564076	-3.139676
C	-4.412882	0.019125	-2.978765
H	-1.724563	-0.683328	-4.920811
H	3.129104	-0.877935	-2.372179
C	-3.772574	0.742884	-1.982458
H	3.257889	-2.410238	-1.512092
H	-4.181901	-1.068415	-4.827860
C	0.895790	-2.043386	-3.172333
C	-2.473871	3.020270	-0.623356
H	-5.488408	-0.135582	-2.925054
C	-2.623884	3.890257	-1.710469
H	1.424984	-1.405903	-3.907481
H	-4.357434	1.162763	-1.164243
H	-2.264426	3.576671	-2.690660
H	-0.171784	-1.794951	-3.313642
C	-3.231873	5.128943	-1.567570
C	-3.715103	5.530524	-0.324334
H	-3.333225	5.783554	-2.430756
C	-3.581455	4.677300	0.762247
C	0.493908	-3.344180	2.414069
H	-4.194385	6.499960	-0.207144
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H	0.170957	-4.145153	3.106376
H	-3.957133	4.975324	1.739080
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C	2.777546	-0.689423	-0.279620
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C	1.765372	-0.269627	1.882851
H	1.232635	-0.756269	2.707111
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C	0.708990	-4.489538	-2.447899
H	0.582612	-5.501674	-2.876618
H	1.533019	-4.557348	-1.726379
C	2.994241	0.437047	2.401651
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H	-0.538299	-6.172624	-1.037845
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C	2.021543	-3.209496	2.506978
H	2.279241	-2.722486	3.459085
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C	-1.700218	-4.045206	-2.517254
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H	-1.470092	-3.379913	-3.360097
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H	1.262971	-5.168869	0.340671
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H	3.238918	-2.479348	-1.535621
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C	0.620157	-4.405377	-2.202127
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C	3.207902	0.488034	2.307877
C	-0.881576	-5.003242	-0.414223
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H	1.098874	-5.167504	0.477455
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H	3.711015	-1.032541	3.751531
C	3.599776	1.717788	1.770370
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C	4.773266	2.337356	2.185128
H	5.058006	3.295615	1.756302
C	5.190609	0.521784	3.705419
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H	-0.753236	-1.803015	-3.385320
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C	-2.057155	0.401250	-4.003223
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C	-1.149507	1.776205	4.350783
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C	3.601407	0.895889	-3.408236
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C	2.455599	0.078011	-1.447508
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C	-2.297277	4.243133	1.571190
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C	-2.872987	4.168495	-0.776612
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H	-3.248966	5.215990	-0.751962
H	2.432629	-0.060858	-0.368352
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C	0.379497	-4.682485	-0.058971
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C	0.371293	3.367572	-3.615960	C	2.523858	5.360694	-6.045927
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H	-0.550716	-1.404408	-2.987081	H	1.872550	6.457917	-7.780885
H	-0.488730	2.758852	-3.921832	C	0.230617	5.508338	-6.760805
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H	2.839726	2.173258	2.737705	N	-2.097296	3.738975	-0.191856
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C	1.682437	0.005334	-2.865469	C	0.631795	-1.516064	-1.015321
H	-2.379395	3.256721	-3.180956	N	1.547347	3.167128	-0.520400
H	-3.242688	4.771061	-3.140896	C	-1.099361	1.675371	2.526016
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C	-0.151218	4.710548	-5.687964	H	0.904836	-0.650354	1.004556
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H	-1.199286	4.436684	-5.560627	C	-0.555939	-1.240475	-1.966131
C	4.043859	0.501112	-2.747071	C	0.169040	3.502973	-3.796160
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H	-1.052984	5.567280	-3.408106	H	0.929713	2.736168	-3.592849
H	-1.225486	5.591964	-1.650367	H	-0.247714	-1.084470	-3.006736
H	0.734721	0.141454	-3.383721	H	-0.739841	2.961139	-4.073436
C	2.663391	2.571574	0.630623	C	-2.328464	2.397247	4.620956
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H	3.394283	3.384672	0.819029	H	-3.111249	2.818870	3.990201
H	2.730111	1.244046	-4.281267	H	-1.216658	-2.116474	-1.969302
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H	4.927478	0.994792	-3.145058	H	-2.269304	-0.376605	-0.973205
C	-2.488784	3.906338	1.119768	H	2.797223	1.851823	2.359285
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H	5.091101	-0.430983	-1.110242	C	2.021354	0.113253	-2.453385
H	-3.004661	4.887874	1.094316	H	-2.545006	3.393947	-3.064260
C	-3.090549	3.875800	-1.194669	H	-3.383659	4.937630	-3.110907
C	1.251221	-3.677064	-2.178357	H	-1.066583	1.050332	-3.259564
H	-3.570731	4.821127	-0.866151	C	-0.340582	4.878564	-5.845027
H	3.091526	-1.569394	-0.229374	C	3.235674	0.716126	-2.780230
H	1.367343	-3.115078	-3.105140	H	-1.395322	4.645511	-5.692928
H	-3.937427	3.164120	-1.318711	C	4.394064	0.387800	-2.087356
C	1.104862	4.857059	-1.811665	C	-1.293872	5.097403	-2.633634
C	1.498400	-5.042934	-2.167160	H	-1.201751	5.686918	-3.559125
C	1.379294	-5.765240	-0.982330	H	-1.242450	5.809054	-1.800154
H	0.689916	5.432422	-0.972926	H	1.132696	0.389171	-3.017735
H	1.791284	-5.546106	-3.086362	C	2.550183	2.653893	0.391684
H	1.472349	5.579441	-2.561582	C	4.325172	-0.549689	-1.059573
C	1.011867	-5.104191	0.182309	H	3.219293	3.486609	0.696679
C	0.979724	3.207461	2.417891	H	3.272438	1.443176	-3.591687
H	1.576302	-6.834782	-0.968906	H	3.201519	1.903330	-0.095586
H	0.938492	3.302411	3.514096	C	3.113398	-1.149653	-0.741466
C	0.757638	-3.734167	0.166017	C	-0.266991	1.190665	4.853326
H	1.244948	4.196879	2.021851	H	0.576926	0.668649	4.399499
C	-1.238273	4.097391	1.954304	H	5.342279	0.853690	-2.345924
H	0.920609	-5.654475	1.116563	C	-2.436591	4.066703	1.169742
H	-0.658439	4.914027	1.502043	H	-3.206516	3.391816	1.604468

C	0.875038	-3.005983	-0.854010	H	-0.544653	1.749419	-4.150389
H	5.222078	-0.821312	-0.506611	C	1.914332	-0.435296	-0.545178
H	-2.880273	5.079901	1.236915	H	-3.419905	3.661084	-3.059000
C	-3.110999	4.192746	-1.122142	H	-4.619522	4.919668	-2.818844
C	1.188920	-3.761207	-1.990384	H	0.752889	1.598327	-2.957030
H	-3.478276	5.186488	-0.789410	C	-2.316411	3.576046	-5.353508
H	3.077675	-1.895177	0.052863	C	2.993103	-0.168775	0.299203
H	1.257717	-3.258437	-2.955238	H	-2.123814	2.709815	-4.724615
H	-4.004717	3.535925	-1.127229	C	3.001463	-0.646560	1.603487
C	1.049797	4.965577	-2.034091	C	-2.592923	5.584266	-2.523154
C	1.424310	-5.125703	-1.906065	H	-2.753489	6.234458	-3.394324
C	1.357512	-5.770846	-0.672753	H	-2.665759	6.227801	-1.636806
H	0.700301	5.581848	-1.195154	H	1.924563	-0.026096	-1.552868
H	1.664763	-5.689953	-2.804762	C	2.017565	3.305939	-0.494770
H	1.422990	5.645443	-2.817964	C	1.923200	-1.407304	2.052537
C	1.057684	-5.034176	0.465369	H	2.980983	3.566255	-0.970356
C	0.970773	2.994802	2.337760	H	3.826576	0.426940	-0.071312
H	1.542240	-6.840348	-0.601587	H	1.913949	2.216358	-0.630299
H	0.988248	2.890260	3.432886	C	0.858379	-1.676453	1.204158
C	0.819689	-3.663420	0.375696	C	1.125804	1.858362	4.156281
H	1.263496	4.028884	2.115984	H	2.025993	2.134922	3.608225
C	-1.179998	4.074578	2.010061	H	3.838854	-0.433438	2.264643
H	1.008125	-5.524779	1.435442	C	-2.842641	3.222634	1.014711
H	-0.538503	4.881850	1.631629	H	-3.062567	2.140104	1.120255
H	0.590409	-3.106176	1.282152	C	-0.803314	-2.901181	-0.872810
H	-1.385990	4.280603	3.073817	H	1.910464	-1.788248	3.071609
C	2.126668	4.053155	-1.498359	H	-3.711361	3.743989	1.456802
H	2.650978	3.506374	-2.312804	C	-3.892763	4.065807	-0.987981
H	2.904444	4.694570	-1.040032	C	0.029596	-3.840923	-1.492198
C	1.956000	4.632810	-5.190730	H	-4.333511	4.913838	-0.419722
H	2.708203	4.215611	-4.519970	H	0.025033	-2.277974	1.567107
C	-2.441083	2.473131	6.005206	H	0.925510	-3.492826	-2.006928
H	-3.301819	2.966108	6.451671	H	-4.662733	3.268810	-0.973480
C	-1.461431	1.910108	6.817162	C	-0.322306	5.900721	-1.766887
H	-1.550504	1.966685	7.899543	C	-0.261994	-5.197056	-1.453432
C	-0.374994	1.262324	6.237719	C	-1.395826	-5.649449	-0.781802
H	0.386814	0.805559	6.865441	H	-0.799033	6.015694	-0.783802
C	2.349316	5.411410	-6.273560	H	0.399607	-5.906653	-1.946026
H	3.405611	5.607063	-6.444104	H	-0.266052	6.900701	-2.236005
C	1.394669	5.930852	-7.142477	C	-2.224602	-4.731267	-0.150651
H	1.701333	6.536801	-7.991918	C	0.747835	3.946917	1.629756
C	0.047046	5.659629	-6.928186	H	-1.627460	-6.711703	-0.749328
H	-0.703644	6.048564	-7.612398	H	0.852962	4.095648	2.718886

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Zr	-0.885259	2.869592	-1.198368
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C	-1.525226	-0.456639	-0.414048
N	-2.664526	3.633063	-0.371331
H	-2.510957	-0.815119	-0.779280
C	-1.658317	4.779865	-5.083598
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C	-0.132594	1.670060	1.952718
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H	-0.956494	1.038011	1.613208
C	-0.331711	-0.938228	-2.413663
C	-0.663129	4.936333	-3.961621
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H	0.698263	-0.895431	-2.786374
H	0.058822	4.108515	-3.969126
C	-1.180825	1.201752	4.188560
C	-0.344530	1.652858	-3.080244
H	-2.101589	0.965128	3.653162
H	-0.868333	-1.634991	-3.069514
C	-0.055094	1.591125	3.456933
C	2.093985	3.585660	1.021034
C	0.824955	-1.189629	-0.110215
H	2.555127	2.719848	1.520878
H	-2.016617	0.321132	-2.897157
H	2.756313	4.438334	1.229400
C	-3.677204	4.519709	-2.421127

H	-0.544653	1.749419	-4.150389
C	1.914332	-0.435296	-0.545178
H	-3.419905	3.661084	-3.059000
H	-4.619522	4.919668	-2.818844
H	0.752889	1.598327	-2.957030
C	-2.316411	3.576046	-5.353508
C	2.993103	-0.168775	0.299203
H	-2.123814	2.709815	-4.724615
C	3.001463	-0.646560	1.603487
C	-2.592923	5.584266	-2.523154
H	-2.753489	6.234458	-3.394324
H	-2.665759	6.227801	-1.636806
H	1.924563	-0.026096	-1.552868
C	2.017565	3.305939	-0.494770
C	1.923200	-1.407304	2.052537
H	2.980983	3.566255	-0.970356
H	3.826576	0.426940	-0.071312
H	1.913949	2.216358	-0.630299
C	0.858379	-1.676453	1.204158
C	1.125804	1.858362	4.156281
H	2.025993	2.134922	3.608225
H	3.838854	-0.433438	2.264643
C	-2.842641	3.222634	1.014711
H	-3.062567	2.140104	1.120255
C	-0.803314	-2.901181	-0.872810
H	1.910464	-1.788248	3.071609
H	-3.711361	3.743989	1.456802
C	-3.892763	4.065807	-0.987981
C	0.029596	-3.840923	-1.492198
H	-4.333511	4.913838	-0.419722
H	0.025033	-2.277974	1.567107
H	0.925510	-3.492826	-2.006928
H	-4.662733	3.268810	-0.973480
C	-0.322306	5.900721	-1.766887
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C	-1.395826	-5.649449	-0.781802
H	-0.799033	6.015694	-0.783802
H	0.399607	-5.906653	-1.946026
H	-0.266052	6.900701	-2.236005
C	-2.224602	-4.731267	-0.150651
C	0.747835	3.946917	1.629756
H	-1.627460	-6.711703	-0.749328
H	0.852962	4.095648	2.718886
C	-1.929252	-3.369694	-0.195079
H	0.441435	4.912479	1.209171
C	-1.634546	3.614648	1.844947
H	-3.109731	-5.071421	0.383235
H	-1.531100	4.703679	1.758146
H	-2.590578	-2.668085	0.309418
H	-1.783932	3.387880	2.912771
C	1.059520	5.311452	-1.549123
H	1.684800	5.405575	-2.461151
H	1.560765	5.940022	-0.784142
C	-1.920590	5.873858	-5.913279
H	-1.409621	6.817963	-5.721933
C	-1.139863	1.099857	5.574929
H	-2.028116	0.793469	6.122936
C	0.038929	1.383231	6.256473
H	0.077494	1.302726	7.340354
C	1.172756	1.759249	5.542562
H	2.102062	1.969436	6.067667
C	-2.817030	5.779840	-6.972533
H	-3.003232	6.646405	-7.602932
C	-3.470901	4.578661	-7.221834
H	-4.173234	4.497887	-8.048277
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TSF'G

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C	-1.454028	-0.273168	-1.029697
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H	-2.306404	-0.655413	-1.629093

H	-3.828398	5.301503	0.076939	C	-1.096943	4.897523	-5.195582
H	-0.775010	-1.905092	1.232109	C	2.563024	-1.161401	-3.903416
H	0.751707	-3.580228	-1.795343	H	-2.169066	4.782213	-5.030402
H	-4.826407	4.060415	-0.684820	C	3.274720	-0.017636	-3.549773
C	-0.155639	6.287326	-1.689022	C	-1.918850	5.431144	-1.978957
C	-0.873834	-4.949555	-1.479708	H	-1.885369	5.831507	-3.001449
C	-2.216143	-5.093755	-1.135649	H	-1.684741	6.267024	-1.309080
H	-0.510781	6.418131	-0.656772	H	0.797728	-2.336454	-3.583401
H	-0.269048	-5.827072	-1.698432	C	1.894966	2.582553	1.047588
H	-0.016192	7.294092	-2.126253	C	2.739965	0.846750	-2.603704
C	-2.971430	-3.963588	-0.852415	H	2.700953	3.317307	-1.260910
C	0.633199	4.079906	1.449140	H	2.968673	-1.851956	-4.639862
H	-2.666641	-6.082359	-1.084103	H	2.397091	1.740789	0.523702
H	0.769209	4.219713	2.538037	C	1.502538	0.579390	-2.016403
C	-2.395093	-2.696216	-0.919514	C	-3.930400	1.417393	3.616373
H	0.279855	5.043124	1.058680	H	-3.905871	1.499945	4.704311
C	-1.731201	3.602095	1.688059	H	4.239448	0.192535	-4.006353
H	-4.019057	-4.062474	-0.575754	C	-2.610574	4.908025	2.070181
H	-1.749865	4.695881	1.571994	H	-3.441507	4.325736	2.520828
H	-3.006416	-1.826005	-0.687802	C	-0.343945	-2.204944	-0.864464
H	-1.851007	3.385649	2.763533	H	3.290769	1.739244	-2.306409
C	1.139967	5.498789	-1.649117	H	-2.866357	5.976001	2.217116
H	1.725303	5.642007	-2.579689	C	-3.562031	5.058965	-0.122426
H	1.764018	5.941845	-0.850334	C	-1.340642	-3.173854	-0.724236
C	-2.370660	4.574694	-5.714506	H	-3.753295	6.135804	0.070827
H	-2.259372	5.514037	-6.258545	H	1.095874	1.277603	-1.286677
C	-1.073161	0.928783	5.294912	H	-2.277246	-3.078012	-1.269137
H	-1.934640	0.533769	5.828892	H	-4.497735	4.530698	0.156352
C	0.093443	1.241758	5.984915	C	0.403020	5.007748	-1.354570
H	0.148576	1.096398	7.061323	C	-1.165014	-4.271698	0.113643
C	1.194264	1.731790	5.288219	C	0.010010	-4.419320	0.840099
H	2.114531	1.966002	5.819153	H	0.142389	5.676908	-0.523482
C	-3.164852	3.555006	-6.236579	H	-1.956225	-5.013703	0.198692
H	-3.668458	3.691428	-7.191739	H	0.848744	5.624116	-2.153434
C	-3.324271	2.372295	-5.522207	C	1.005317	-3.453557	0.725593
H	-3.958564	1.580608	-5.918437	C	0.608150	3.200389	3.107014
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N	-2.442231	4.610918	0.666637
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C	-0.203642	4.343462	-4.273763
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N	0.865754	3.197935	0.247502
C	-1.593104	2.328921	3.530749
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H	-0.310341	0.237743	0.087912
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C	-1.617367	-1.171901	-2.806578
C	-0.708412	3.604345	-3.062289
C	-1.562506	-0.226897	-3.968155
H	-0.068779	2.745876	-2.834153
H	-1.547179	-2.197065	-3.197231
H	-1.699077	3.186560	-3.285718
C	-2.817963	1.754165	1.455016
C	-1.685705	-0.605627	-5.236913
H	-2.256823	1.345909	-1.823387
H	-2.609415	-1.103515	-2.326818
C	-2.836043	1.832302	2.856114
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C	0.782574	-0.565479	-2.359140
H	0.698372	1.219375	2.247915
H	-1.402818	0.827152	-3.736146
H	2.198038	1.738170	2.999550
C	-3.296572	4.892967	-1.614677
H	-1.655397	0.108819	-6.055504
C	1.336898	-1.429148	-3.311209
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H	-4.078688	5.414122	-2.181318
H	-1.815353	-1.654535	-5.504814

C	-1.096943	4.897523	-5.195582
C	2.563024	-1.161401	-3.903416
H	-2.169066	4.782213	-5.030402
C	3.274720	-0.017636	-3.549773
C	-1.918850	5.431144	-1.978957
H	-1.885369	5.831507	-3.001449
H	-1.684741	6.267024	-1.309080
H	0.797728	-2.336454	-3.583401
C	1.894966	2.582553	1.047588
C	2.739965	0.846750	-2.603704
H	2.700953	3.317307	-1.260910
H	2.968673	-1.851956	-4.639862
H	2.397091	1.740789	0.523702
C	1.502538	0.579390	-2.016403
C	-3.930400	1.417393	3.616373
H	-3.905871	1.499945	4.704311
H	4.239448	0.192535	-4.006353
C	-2.610574	4.908025	2.070181
H	-3.441507	4.325736	2.520828
C	-0.343945	-2.204944	-0.864464
H	3.290769	1.739244	-2.306409
H	-2.866357	5.976001	2.217116
C	-3.562031	5.058965	-0.122426
C	-1.340642	-3.173854	-0.724236
H	-3.753295	6.135804	0.070827
H	1.095874	1.277603	-1.286677
H	-2.277246	-3.078012	-1.269137
H	-4.497735	4.530698	0.156352
C	0.403020	5.007748	-1.354570
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C	1.005317	-3.453557	0.725593
C	0.608150	3.200389	3.107014
H	0.149133	-5.277971	1.493010
H	0.653253	3.086269	4.203052
C	0.827884	-2.361262	-0.114494
H	1.084818	4.158754	2.866897
C	-1.317882	4.656855	2.821755
H	1.930230	-3.552298	1.290242
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H	1.618400	-1.616256	-0.204161
H	-1.422699	4.913275	3.891061
C	1.407390	3.994371	-0.833139
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H	2.280622	4.579842	-0.482161
C	1.166030	4.448826	-4.534346
H	1.875560	3.978616	-3.852837
C	-3.971344	1.224141	0.854988
H	-4.013686	1.129455	-0.235170
C	-5.076548	0.806670	1.594120
H	-5.954441	0.404323	1.090373
C	-5.056251	0.903365	2.982981
H	-5.915316	0.583524	3.569519
C	1.628346	5.118551	-5.661758
H	2.697605	5.187440	-5.848752
C	0.726108	5.686018	-6.556718
H	1.087505	6.206365	-7.440714
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C	0.399690	4.012146	-4.416841
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C	-2.073859	2.448846	3.232622
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H	0.303393	2.446316	-2.957353
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H	-1.236135	2.857907	-3.710252
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H	-3.365375	0.084893	-0.389768
H	1.806972	1.862880	3.227843
C	-3.118270	4.734691	-2.214838
H	-3.364980	1.837422	-1.967920
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C	0.781495	-0.137779	-4.556704
H	-1.380446	4.241603	-5.600421
C	1.928297	0.617416	-4.331191
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H	-1.459332	6.038907	-1.903138
H	-0.802231	-1.282352	-3.698224
C	1.621601	2.373272	1.159092
C	2.331882	0.849212	-3.022067
H	2.394220	3.147979	1.346758
H	0.449918	-0.338141	-5.573160
H	2.200570	1.490443	0.810084
C	1.594087	0.346877	-1.952000
C	-4.552538	2.133320	3.364402
H	-4.478106	2.246652	4.447589
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H	1.930681	0.568796	-0.943108
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C	0.454810	4.706095	-1.444963
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H	0.043004	5.348239	-0.656362
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H	1.983580	-6.082524	-0.792534
H	0.084666	3.227123	4.104592
C	1.661768	-2.706570	-0.584569
H	0.710638	4.157546	2.741309
C	-1.632050	4.722135	2.440114
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C	1.379509	3.710641	-0.787723
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C	1.780613	4.234723	-4.386272
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C	1.699875	5.315055	-6.541043
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H	-0.244290	5.406826	-7.462657

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C	-2.180023	2.513269	3.257703
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H	-3.136118	1.444660	-2.055076
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C	1.951673	0.602815	-4.349295
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H	2.344883	3.178446	1.446871
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C	1.645886	0.279432	-1.973692
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H	0.127706	5.470401	-0.686084	H	0.202212	0.596851	-2.859639
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C	2.238323	-4.128608	-0.360714	H	2.550908	3.170580	0.538725
C	0.120306	3.179094	3.088591	H	2.269975	1.630651	-3.681327
H	2.049918	-6.199235	-0.929828	H	2.058189	1.591488	-0.088682
H	0.012983	3.079108	4.182656	C	2.423497	-1.034383	-0.897291
C	1.654821	-2.868209	-0.390487	C	-4.147826	2.242327	3.490514
H	0.688798	4.101127	2.914294	H	-3.974508	2.532182	4.527737
C	-1.593621	4.778247	2.521353	H	4.470707	0.981949	-2.714632
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H	-0.706099	5.332155	2.187680	H	-3.630844	4.431521	1.972752
H	2.178511	-2.026581	0.061846	C	0.180916	-2.865831	-0.784317
H	-1.811190	5.081796	3.561889	H	4.549725	-0.738355	-0.916221
C	1.381991	3.757030	-0.772039	H	-2.948618	5.999632	1.534699
H	1.899625	3.117780	-1.520713	C	-3.703708	4.890076	-0.687358
H	2.192997	4.339905	-0.289794	C	0.337905	-3.614633	-1.956428
C	1.661254	4.197394	-4.450970	H	-3.909508	5.966831	-0.508957
H	2.274895	3.872317	-3.611035	H	2.475618	-1.800141	-0.123821
C	-4.686867	2.048926	0.506094	H	0.270062	-3.107505	-2.919044
H	-4.736034	1.987355	-0.585230	H	-4.633162	4.355123	-0.397310
C	-5.884835	1.965373	1.214980	C	0.199759	5.041969	-1.823426
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C	-5.877254	2.040539	2.604782	C	0.694857	-5.629957	-0.684531
H	-6.806723	1.979557	3.167523	H	-0.148197	5.645933	-0.975388
C	2.261712	4.791965	-5.554909	H	0.700201	-5.538111	-2.838236
H	3.338385	4.946915	-5.566922	H	0.596794	5.727880	-2.589607
C	1.489531	5.179032	-6.646460	C	0.556874	-4.898440	0.487487
H	1.959121	5.641813	-7.511507	C	0.486387	3.265702	2.506132
C	0.116584	4.959062	-6.629931	H	0.890590	-6.699104	-0.645075
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N	0.664458	3.179245	-0.358101
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C	-3.248955	1.724367	1.276993
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H	-1.992254	-1.983323	-1.721764
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C	1.223517	2.123996	1.831978
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C	2.324091	0.884362	-2.888370
H	-2.124014	4.378123	-5.688524
C	3.553674	0.523353	-2.351677
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C	1.679225	2.495537	0.423865
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H	2.550908	3.170580	0.538725
H	2.269975	1.630651	-3.681327
H	2.058189	1.591488	-0.088682
C	2.423497	-1.034383	-0.897291
C	-4.147826	2.242327	3.490514
H	-3.974508	2.532182	4.527737
H	4.470707	0.981949	-2.714632
C	-2.755597	4.908378	1.491138
H	-3.630844	4.431521	1.972752
C	0.180916	-2.865831	-0.784317
H	4.549725	-0.738355	-0.916221
H	-2.948618	5.999632	1.534699
C	-3.703708	4.890076	-0.687358
C	0.337905	-3.614633	-1.956428
H	-3.909508	5.966831	-0.508957
H	2.475618	-1.800141	-0.123821
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H	-0.148197	5.645933	-0.975388
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C	0.556874	-4.898440	0.487487
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H	0.890590	-6.699104	-0.645075
H	0.586037	3.227714	3.604972
C	0.303664	-3.528535	0.437507
H	0.925721	4.215031	2.174755
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C	1.251151	4.088805	-1.309559
H	1.763710	3.550564	-2.137907
H	2.044113	4.702163	-0.836398
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C	-4.566024	1.544781	0.833167
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H	-6.668508	1.576255	1.316579
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C	0.687477	5.718149	-7.039151
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C	-0.075839	4.475258	-4.907689
C	-0.100788	-1.317865	-0.927572
N	0.896421	3.351963	-0.480275
C	-1.660805	2.013234	2.841583
H	-1.379062	2.247407	3.884130
H	0.232102	-0.464755	1.089735
H	-1.170248	2.070278	2.573022
C	-1.286352	-0.995726	-1.867713
C	-0.512510	3.655504	-3.720471
C	-2.003331	0.226495	-1.237908

H	0.239159	2.883483	-3.504732	C	0.710541	5.960589	-7.154489
H	-0.975700	-0.813371	-2.903178	H	1.015940	6.535545	-8.025655
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C	-3.784061	1.184361	1.742160	H	-1.390805	6.087342	-7.608578
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H	-3.165471	0.755046	0.957941	E'			
H	-1.965540	-1.856713	-1.897393	Zr	0.068411	2.320286	1.587667
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C	1.304104	2.235198	1.694602	N	0.320675	-0.137057	2.029248
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H	0.784914	1.292920	1.482049	C	0.044097	-1.682694	0.183977
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H	-2.079654	4.756375	-5.637145	C	1.272607	2.988551	-1.742546
C	3.706274	0.462517	-2.051567	C	-0.588502	-0.442377	0.839430
C	-1.929234	5.313077	-2.594399	H	0.418003	2.372595	-2.052541
H	-1.838797	5.856513	-3.547487	H	2.018610	-1.133392	2.820330
H	-1.844535	6.060824	-1.796066	H	1.398315	3.769318	-2.512559
H	0.425368	0.610588	-2.896909	C	-1.874414	1.667811	2.757199
C	1.897467	2.816553	0.418377	C	-0.712125	0.810724	-0.007136
C	3.624820	-0.486034	-1.034904	H	-0.173997	-0.426443	2.872708
H	2.587465	3.633405	0.720582	H	2.196859	-0.494202	1.172514
H	2.591485	1.583780	-3.512890	C	-1.875275	1.759692	4.162507
H	2.528543	2.053588	-0.073716	C	2.458254	1.457402	4.041971
C	2.398762	-1.046150	-0.698770	C	0.291817	-3.139151	2.293187
C	-3.940363	2.365015	3.829186	H	1.758364	0.615398	3.966904
H	-3.457498	2.863945	4.669886	H	-1.566315	-0.687202	1.272116
H	4.665489	0.895475	-2.326221	H	3.249674	1.135498	4.732520
C	-2.989393	4.507023	1.259629	C	-1.590845	4.275932	-0.485171
H	-3.857628	3.966210	1.677045	H	-1.760901	1.006867	-0.267865
C	0.092817	-2.815881	-0.775265	C	1.064157	-3.696127	3.320549
H	4.522898	-0.798653	-0.506070	H	-1.721513	3.198305	-0.669955
H	-3.275043	5.579126	1.282268	H	-2.301033	4.786381	-1.148575
C	-3.714861	4.510556	-1.002871	H	-0.169982	0.715733	-0.956784
C	0.364787	-3.576625	-1.918780	C	3.679133	2.724987	-2.359870
H	-4.067455	5.519595	-0.707334	C	0.485445	-4.459566	4.324314
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H							

C	2.694628	-4.961598	-0.886754	H	6.293388	-1.568356	-2.748741
C	1.733246	2.660652	4.616671	C	0.017397	6.724062	-2.743510
H	4.804574	-5.322832	-1.149139	C	5.187511	2.159514	1.104305
H	1.670825	2.611086	5.717980	H	3.447072	10.249807	-2.809270
C	1.729999	-4.179124	-0.267402	C	9.467224	2.580215	0.491764
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C	-0.001445	4.261291	4.115704	C	8.963047	0.265865	-3.996838
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H	0.877600	4.820345	3.766681	H	8.931105	1.624094	0.440113
H	0.673530	-4.389733	-0.432366	H	-0.358063	7.778690	-0.905518
H	-0.197785	4.560332	5.161637	H	5.147569	0.261949	-1.942805
C	2.924219	3.421165	0.975454	C	-1.956476	8.075544	-2.305588
H	3.661412	2.922680	0.320652	H	10.384864	2.375303	1.059595
H	3.524393	4.091780	1.628182	C	-2.444737	7.807161	-3.582309
C	2.641995	0.908385	-1.188909	C	6.348973	7.039114	-2.608695
H	1.766922	0.462940	-0.727993	H	-2.523272	8.708755	-1.626112
C	-3.137939	1.480821	2.172888	H	4.788197	2.009799	-3.466129
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H	-5.268403	1.232835	2.411767	H	-3.394788	8.224952	-3.907646
C	-4.266100	1.450355	4.304665	H	5.390085	7.580419	-2.615198
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C	3.842339	0.207951	-1.209200	H	7.123309	7.802863	-2.777248
H	3.888868	-0.790374	-0.774050	H	-2.066447	6.787254	-5.437633
C	4.970297	0.770884	-1.800389	H	6.425200	1.875245	-4.113465
H	5.909459	0.222519	-1.818227	H	0.069192	5.839688	-4.713448
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H	3.146757	3.927945	-2.364856	H	7.428356	0.426828	-5.506977
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H	1.508264	4.683576	-3.823417	C	11.098281	1.246716	-4.636036
C	8.253915	-0.076134	-1.560700	H	10.632828	3.856725	-0.746150
C	1.327057	6.137266	-2.212868	H	8.823501	1.629995	-7.118529
N	5.820105	5.217891	-0.971546	H	10.434644	2.236952	-1.399642
H	2.395223	6.172863	-4.097536	C	10.301702	0.570811	-3.721022
H	8.172594	-0.931837	-0.873828	C	4.179252	1.800564	1.998886
C	0.979343	5.106081	-1.109032	H	4.405673	1.696123	3.061600
C	7.363646	4.816520	-6.259087	H	11.193949	2.158758	-6.590571
C	0.167755	3.947421	-1.596746	C	5.375478	5.197861	0.415511
C	8.180649	-0.606909	-3.006742	H	4.523603	4.521544	0.545514
H	1.914126	4.719712	-0.672294	C	8.777013	-2.007275	-3.141632
N	8.809862	3.559102	-1.729578	H	12.134503	1.466386	-4.387729
C	-1.120247	3.761845	-1.321587	H	5.025212	6.197944	0.729704
C	6.577039	2.412175	1.614339	C	6.566334	6.447020	-1.222619
H	0.434733	5.612129	-0.299948	C	8.439041	-2.787098	-4.252473
H	6.583682	2.600558	2.704979	H	7.653405	6.325477	-1.040222
C	2.187070	7.284843	-1.677823	H	10.743987	0.247136	-2.779438
H	9.201034	0.431329	-1.343846	H	7.747888	-2.389549	-4.994464
H	0.684264	3.213747	-2.222706	H	6.251819	7.226442	-0.504647
H	7.216078	1.528920	1.459742	C	8.592049	5.265105	-3.491110
H	-1.673122	2.904814	-1.697770	C	8.974731	-4.055628	-4.429659
C	6.651779	-0.633233	-3.202967	C	9.874894	-4.572011	-3.501975
C	2.737302	7.316055	-0.396931	H	8.625221	6.070839	-2.752516
C	7.030445	4.111806	-4.966384	H	8.689608	-4.643938	-5.299211
H	-1.673297	4.475807	-0.711349	H	9.034175	5.665486	-4.418413
C	3.527027	8.388503	0.020461	C	10.233105	-3.803054	-2.402063
C	6.073521	0.565143	-2.443855	C	8.638307	3.605956	1.244784
H	7.663101	3.222539	-4.882290	H	10.296462	-5.565066	-3.638995
C	3.796220	9.444113	-0.839013	H	8.758853	3.492539	2.338017
H	6.323153	-0.649491	-4.246882	C	9.690292	-2.532620	-2.225876
H	2.556260	6.503015	0.302024	H	9.006106	4.606621	0.981953
H	5.988336	3.771899	-4.994523	C	6.527808	4.812434	1.334752
C	3.255804	9.426738	-2.124031	H	10.940140	-4.190514	-1.671539
C	4.958619	2.341265	-0.274579	H	7.276769	5.613020	1.277881
H	3.932926	8.390576	1.030893	H	9.992102	-1.949970	-1.356873
C	5.841246	1.864978	-3.188750	H	6.217941	4.736157	2.392583
C	2.461094	8.364498	-2.529901	C	9.394922	4.102902	-2.952535
H	6.673792	0.613125	-0.463454	H	9.541975	3.323789	-3.725289
H	4.413120	10.278121	-0.512265	H	10.410345	4.489542	-2.744883
				C	8.660316	4.782168	-6.782028
				H	9.437554	4.243232	-6.239104

C	3.645056	2.077737	-0.693658
H	3.403326	2.123432	-1.759969
C	2.614137	1.737231	0.184386
H	1.602469	1.584292	-0.192018
C	2.879787	1.603314	1.542953
H	2.084732	1.346673	2.239962
C	8.959657	5.394985	-7.994844
H	9.974393	5.355815	-8.385393
C	7.961383	6.047036	-8.711286
H	8.192491	6.523663	-9.661316
C	6.662441	6.074452	-8.212983
H	5.873018	6.570012	-8.773756

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N	7.294050	3.439433	1.087462
C	2.565942	5.023716	-3.028989
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N	7.025461	5.067585	-3.444385
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C	1.598014	6.022767	-2.343011
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H	2.936198	5.480481	-3.961035
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C	0.998652	5.352848	-1.075816
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C	2.408653	7.272809	-1.998714
H	9.150463	0.455859	-1.429052
H	0.872187	3.166250	-1.392518
H	7.351850	1.388782	1.499157
H	-1.534450	3.036425	-1.753110
C	6.512681	-0.582144	-3.162603
C	2.786743	7.618250	-0.700267
C	6.557679	4.442263	-4.715275
H	-1.682166	4.872210	-1.528034
C	3.547354	8.760716	-0.450384
C	5.985195	0.603212	-2.350509
H	7.080670	3.487252	-4.824455
C	3.948627	9.579737	-1.496882
H	6.132927	-0.576892	-4.188969
H	2.478627	7.003108	0.141761
H	5.493041	4.216266	-4.564713
C	3.595666	9.239247	-2.801898
C	4.968314	2.289072	-0.012014
H	3.821368	9.006331	0.573836
C	5.760784	1.933256	-3.036157
C	2.838107	8.101992	-3.044802
H	6.649917	0.519552	-0.394861
H	4.537097	10.473452	-1.301952
H	6.172749	-1.524076	-2.707614
C	0.434963	6.412420	-3.252590
C	5.306248	2.010229	1.327889
H	3.906182	9.867942	-3.633834
C	9.536979	2.497360	0.459020
C	-0.396477	7.471546	-2.867283
C	8.781706	0.333405	-4.051061
H	2.546221	7.859445	-4.066854
H	9.014683	1.533099	0.403296
H	-0.153011	8.034733	-1.966169
H	5.065558	0.305227	-1.834497
C	-1.514065	7.821818	-3.611783
H	10.495809	2.289667	0.953298
C	-1.825311	7.121499	-4.774776
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C	8.205737	0.785320	-5.239806
H	-2.699898	7.392269	-5.362045
H	5.892293	7.903256	-1.932509
C	0.113990	5.726434	-4.424286
H	7.611705	7.790148	-2.257702
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H	6.357042	1.988312	-3.952411
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C	5.766261	6.090444	-6.472241
H	4.211358	5.359245	-1.784213
C	8.947034	1.508078	-6.173770
H	4.839917	6.208385	-5.909180
C	10.289308	1.786141	-5.945087
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H	5.271960	6.152887	-3.293960
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C	9.842401	3.020581	-0.934147
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H	10.574674	3.850061	-0.820784
H	8.464006	1.852418	-7.086818
H	10.396122	2.231810	-1.486786
C	10.139366	0.610256	-3.846639
C	4.392948	1.496334	2.249313
H	4.702448	1.321219	3.281369
H	10.868073	2.346881	-6.676031
C	5.541370	5.200652	0.767846
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C	8.631541	-1.962674	-3.247941
H	11.936871	1.525857	-4.579043
H	5.244238	6.192348	1.164120
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H	7.974244	6.106361	-0.673477
H	10.634361	0.238903	-2.949763
H	7.508343	-2.281709	-5.057526
H	6.762470	7.140230	0.060237
C	8.492098	5.219735	-3.427004
C	8.751572	-3.970385	-4.608556
C	9.694716	-4.519711	-3.744350
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H	8.419659	-4.529477	-5.480754
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H	8.954735	3.310347	2.389065
C	9.587279	-2.520714	-2.396872
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H	6.324254	4.472727	2.688877
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C	3.652811	1.943472	-0.369968
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C	2.722885	1.427499	0.534200
H	1.711952	1.189721	0.203130
C	3.088811	1.212481	1.858222
H	2.370667	0.821835	2.576221
C	8.103301	5.766217	-7.935408
H	9.016705	5.626299	-8.509574
C	7.116133	6.631884	-8.394463
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N	6.712050	0.951113	-1.346257	C	9.701266	3.041806	-1.023875
H	3.776417	4.252054	-0.910174	C	10.547267	1.259662	-5.058067
N	7.016797	5.419948	-3.257581	H	10.376496	3.921326	-0.918134
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C	7.905897	0.178947	-1.751701	H	10.294237	2.305346	-1.607725
C	1.913348	5.634513	-2.422462	C	9.799761	0.593903	-4.095538
N	6.215020	5.508650	-0.336207	C	4.466426	1.439758	2.421144
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C	1.207242	5.193088	-1.111570	C	5.756736	5.363422	1.023970
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C	6.765889	2.188709	1.798316	H	8.298218	5.990668	-0.473278
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H	8.788902	0.823907	-1.735504	C	8.483068	5.321298	-3.323223
H	0.998445	3.010308	-1.437020	C	8.098990	-3.945301	-4.547739
H	7.328021	1.325444	1.409713	C	9.067240	-4.491122	-3.709748
H	-1.415139	2.885778	-1.155992	H	8.912001	5.935629	-2.524925
C	6.132289	-0.346144	-3.258844	H	7.683095	-4.537370	-5.360136
C	2.958495	7.535979	-1.044633	H	8.870993	5.716449	-4.277743
C	6.401043	4.999473	-4.543955	C	9.593117	-3.714848	-2.685408
H	-1.492166	4.715462	-0.864887	C	8.787497	3.407635	1.316035
C	3.649953	8.742904	-0.962951	H	9.412421	-5.511481	-3.859217
C	5.706174	0.893285	-2.471735	H	9.054609	3.182696	2.366436
H	6.723357	3.974505	-4.745876	C	9.148853	-2.408855	-2.492442
C	3.963335	9.452910	-2.115180	H	9.139316	4.427602	1.109198
H	5.731366	-0.351504	-4.277319	C	6.759839	4.602602	1.888465
H	2.734538	7.002385	-0.123558	H	10.356484	-4.123573	-2.026695
H	5.318792	4.957045	-4.375647	H	7.595918	5.275481	2.120663
C	3.578526	8.944661	-3.353579	H	9.588982	-1.822545	-1.687756
C	4.862501	2.430809	0.200210	H	6.321923	4.300794	2.853795
H	3.951110	9.120907	0.011969	C	8.908562	3.891438	-3.083156
C	5.708265	2.250513	-3.137861	H	8.509937	3.229892	-3.873007
C	2.890785	7.739861	-3.430683	H	10.003707	3.840405	-3.198617
H	6.294570	0.517490	-0.527384	C	7.764022	5.536390	-6.599888
H	4.504397	10.394279	-2.051055	H	8.384397	4.667667	-6.371216
H	5.742599	-1.246644	-2.760518	C	3.514244	2.132523	-0.065730
C	0.852212	5.670681	-3.520373	H	3.095445	2.358976	-1.052261
C	5.308635	2.025316	1.475516	C	2.654623	1.537803	0.859538
H	3.816879	9.488384	-4.266032	H	1.613850	1.350129	0.595377
C	9.498225	2.465572	0.365184	C	3.129402	1.199068	2.120539
C	-0.160425	6.634677	-3.443473	H	2.469397	0.751991	2.860998
C	8.423934	0.383677	-4.249492	C	8.033704	6.307718	-7.725940
H	2.587462	7.354409	-4.404376	H	8.874196	6.053242	-8.368099
H	8.980959	1.498405	0.312636	C	7.224162	7.395994	-8.035312
H	-0.132815	7.368105	-2.637691	H	7.432611	7.998666	-8.916454
H	4.724349	0.719533	-2.012912	C	6.137813	7.700625	-7.220438
C	-1.184378	6.681772	-4.377982	H	5.490449	8.539805	-7.466441
H	10.493908	2.249638	0.776861				
C	-1.218516	5.762508	-5.424235				
C	7.150929	7.393238	-1.651600	TS _{HI}			
H	-1.958107	7.441784	-4.292355	Zr	6.148540	3.518870	-1.065659
H	4.743086	2.477982	-3.609733	N	4.344730	4.427455	-2.141744
C	-0.218637	4.805060	-5.518514	N	6.869518	3.318626	1.379000
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H	-2.018184	5.797591	-6.160460	N	6.449158	0.972685	-1.566265
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C	0.805697	4.758249	-4.573831	N	7.129063	5.734077	-3.115934
H	8.124260	7.858160	-1.870547	H	2.530324	3.410468	-2.315985
H	-0.229089	4.082528	-6.331693	C	7.701837	0.302332	-1.973108
H	6.478515	2.285152	-3.917396	C	2.092016	5.518381	-2.394287
C	1.568309	3.990567	-4.677710	N	6.183497	5.444569	-0.196456
C	5.873548	6.927712	-6.095318	H	3.041766	4.192915	-3.808585
H	4.509456	5.539117	-1.556306	H	7.902206	-0.512498	-1.267373
C	8.575995	1.510320	-6.398904	C	1.896771	5.660088	-0.861701
H	5.014598	7.159501	-5.463456	C	7.198124	6.230490	-5.606391
C	9.935912	1.730213	-6.217000	C	1.305797	4.457817	-0.193373
C	6.560132	6.777053	-2.911893	C	7.538102	-0.242410	-3.426602

H	2.876739	5.866953	-0.410906	H	5.245285	6.331735	1.491947
N	8.257847	3.480130	-1.533128	C	7.287657	6.377003	-0.181641
C	0.004860	4.253977	-0.000874	C	7.557572	-2.445489	-4.661762
C	6.391017	2.057700	1.970137	H	8.247905	5.843642	-0.297622
H	1.258136	6.535826	-0.679699	H	10.159736	0.427264	-3.277315
H	6.455291	2.106093	3.073381	H	6.811324	-2.022782	-5.332854
C	2.716450	6.786719	-2.985610	H	7.353021	6.887173	0.797997
H	8.526184	1.019323	-1.913596	C	8.559698	5.449654	-3.035222
H	2.012347	3.702285	0.152087	C	8.014513	-3.738028	-4.883712
H	7.075769	1.252443	1.666391	C	8.981051	-4.291961	-4.049562
H	-0.358862	3.353818	0.490468	H	8.987781	5.996134	-2.188008
C	6.006832	-0.166855	-3.597527	H	7.614113	-4.315194	-5.714341
C	3.201533	7.845029	-2.213742	H	9.102076	5.795853	-3.933266
C	6.580197	5.465047	-4.460695	C	9.487541	-3.534268	-3.001530
H	-0.746333	4.970873	-0.334557	C	8.331790	3.421344	1.558481
C	3.726924	8.990701	-2.812451	H	9.340022	-5.304213	-4.219813
C	5.551270	1.024813	-2.756984	H	8.569967	3.214570	2.618529
H	6.696058	4.393761	-4.664804	C	9.025386	-2.239105	-2.782171
C	3.784947	9.097296	-4.195080	H	8.624320	4.461439	1.362567
H	5.662631	-0.108397	-4.635291	C	6.195055	4.68521	2.061359
H	3.178307	7.789770	-1.127772	H	10.249460	-3.949409	-2.345272
H	5.498323	5.661531	-4.411766	H	6.962111	5.053132	2.589229
C	3.317934	8.043254	-4.980073	H	9.451005	-1.665689	-1.960599
C	4.626357	2.197903	0.218209	H	5.501620	4.089023	2.833817
H	4.093958	9.800985	-2.185382	C	8.769432	3.964477	-2.818303
C	5.660027	2.400244	-3.390801	H	8.322822	3.412638	-3.662744
C	2.793200	6.907576	-4.380283	H	9.848646	3.754488	-2.905297
H	5.987795	0.420537	-0.848154	C	8.223239	5.649038	-6.358629
H	4.190080	9.992786	-4.662048	H	8.549828	4.637092	-6.112137
H	5.581449	-1.088840	-3.174363	C	3.375821	1.728698	-0.217803
C	0.709078	5.331730	-3.024989	H	3.006004	2.011300	-1.204614
C	5.007204	1.737220	1.494428	C	2.546658	0.911101	0.551150
H	3.360855	8.109881	-6.065434	H	1.580745	0.594749	0.158453
C	9.120473	2.511397	0.635405	C	2.947206	0.519844	1.823503
C	-0.177432	6.416316	-3.039328	H	2.303674	-0.101593	2.442838
C	8.344589	0.599630	-4.429844	C	8.819430	6.335658	-7.410763
H	2.404167	6.102502	-5.003014	H	9.615980	5.863151	-7.982647
H	8.617292	1.540969	0.521001	C	8.394109	7.620954	-7.732296
H	0.158134	7.382082	-2.661558	H	8.856573	8.160315	-8.556063
H	4.523439	0.866298	-2.404610	C	7.368182	8.208550	-6.998646
C	-1.468901	6.288572	-3.530403	H	7.023517	9.209389	-7.251075
H	10.088207	2.291154	1.106200				
C	-1.908419	5.066053	-4.032078	I			
C	7.206021	7.468607	-1.251025	Zr	6.404400	4.615087	-0.373419
H	-2.134504	7.149207	-3.525885	N	4.587381	5.187537	-1.240283
H	4.958069	2.465943	-4.239800	N	6.992433	4.193683	2.013831
C	-1.038780	3.984111	-4.036741	C	3.594635	4.525852	-2.041409
C	7.815862	1.092084	-5.624478	N	5.812471	2.076067	-3.641597
H	-2.919318	4.961648	-4.419630	H	4.536530	6.199244	-1.372042
H	6.499844	8.246030	-0.919522	N	7.411217	5.752071	-2.417997
C	0.255016	4.116184	-3.537085	H	3.397684	3.543835	-1.592173
H	8.188201	7.963085	-1.307241	C	6.522276	0.924313	-3.119620
H	-1.365832	3.022861	-4.427707	C	2.255961	5.292551	-2.144971
H	6.655394	2.532511	-3.825831	N	6.817454	6.499641	0.492671
H	0.904600	3.244972	-3.545824	H	3.933971	4.329603	-3.083685
C	6.774552	7.517788	-5.946614	H	5.895591	0.281395	-2.468810
H	5.021170	3.563870	-2.852609	C	1.674413	5.471464	-0.718090
C	8.602964	1.814372	-6.518614	C	7.115814	5.776375	-4.961573
H	5.958560	7.973375	-5.386409	C	1.528566	4.180841	0.026951
C	9.944605	2.051299	-6.244330	C	6.862285	0.147234	-4.400943
C	6.736500	7.061216	-2.647884	H	2.349242	6.118020	-0.142479
H	5.638030	7.081767	-2.670571	N	8.150337	3.529774	-0.915540
H	7.061672	7.852494	-3.351339	C	0.384408	3.520207	0.181568
H	6.768015	0.936832	-5.868361	C	5.829325	3.559387	2.677936
C	9.405336	3.113431	-0.725143	H	0.702750	5.981564	-0.791614
C	10.494393	1.546285	-5.069487	H	5.144883	4.371208	2.966716
H	10.055331	4.002607	-0.561341	C	2.574752	6.625233	-2.825417
H	8.157431	2.197661	-7.434730	H	7.391699	1.245721	-2.531072
H	10.055960	2.394538	-1.267115	H	2.446947	3.766077	0.451940
C	9.703473	0.827504	-4.182723	H	6.158132	3.088112	3.623565
C	4.188249	0.935031	2.290934	H	0.341252	2.579011	0.724996
H	4.529496	0.628470	3.281469	C	5.492765	0.253690	-5.116225
H	10.556597	2.620596	-6.941030	C	2.650982	7.842821	-2.145739
C	5.453315	5.342095	1.044043	C	6.613952	5.328697	-3.613080
H	4.468544	4.884749	0.853922	H	-0.550194	3.892136	-0.240444
C	8.042593	-1.675921	-3.598952	C	3.063638	9.007199	-2.794533
H	11.545102	1.711780	-4.840952				

C	4.855851	1.577758	-4.639207	H	8.335093	3.037362	3.153431
H	6.557917	4.232449	-3.613821	C	7.646228	-1.757763	-2.890977
C	3.402556	8.979129	-4.140509	H	9.065002	3.984890	1.844627
H	5.550334	0.184543	-6.207719	C	7.234904	5.509688	2.655784
H	2.386341	7.898837	-1.092809	H	8.312918	-3.424338	-1.708983
H	5.598769	5.710421	-3.450760	H	8.299775	5.756648	2.562116
C	3.317307	7.775084	-4.838135	H	7.664536	-1.074886	-2.042585
C	5.199290	2.737427	0.399455	H	7.003485	5.467160	3.733641
H	3.112925	9.940557	-2.237608	C	8.838990	3.778786	-2.171001
C	4.616163	2.621137	-5.713508	H	8.421712	3.181592	-3.005904
C	2.912676	6.618200	-4.187041	H	9.901737	3.478673	-2.101670
H	5.336086	2.600348	-2.913104	C	7.929979	4.936196	-5.727418
H	3.721228	9.887306	-4.647559	H	8.202194	3.950779	-5.344584
H	4.880594	-0.594859	-4.787899	C	4.488630	1.776054	-0.341753
C	1.236530	4.520603	-2.979869	H	4.529144	1.781855	-1.432808
C	5.094955	2.590567	1.796600	C	3.704320	0.779403	0.237895
H	3.574008	7.735464	-5.895265	H	3.174381	0.067532	-0.393539
C	8.246979	2.120292	1.190467	C	3.607508	0.695537	1.622428
C	0.071810	5.173386	-3.399466	H	3.001581	-0.077206	-2.090991
C	8.016482	0.827842	-5.144418	C	8.379986	5.332532	-6.982654
H	2.846085	5.684844	-4.746046	H	9.014401	4.660274	-7.557535
H	7.275952	1.617159	1.175054	C	8.014755	6.572112	-7.498210
H	-0.056274	6.229424	-3.160655	H	8.364885	6.881499	-8.480625
H	3.884237	1.338032	-4.161326	C	7.187623	7.409207	-6.755330
C	-0.910466	4.509794	-4.122327	H	6.882742	8.373211	-7.157674
H	8.952230	1.405163	1.636344	TSeJ			
C	-0.747038	3.166954	-4.453345	Zr	0.436054	2.436759	1.408678
C	8.123004	7.854703	-1.139287	N	0.773382	2.723637	3.902069
H	-1.805017	5.045112	-4.433904	N	0.498055	-0.129191	1.933072
H	3.901898	2.265888	-6.466468	N	0.646902	4.041855	-0.561004
C	0.401940	2.503552	-4.043950	C	0.451820	-1.689401	0.145455
C	7.937798	1.263696	-6.466844	N	-0.746199	4.165988	1.858282
H	-1.511459	2.644285	-5.023867	H	1.271551	-1.288365	-0.467540
H	7.702923	8.863928	-1.030777	C	2.114977	2.368274	-1.629122
C	1.379208	3.171776	-3.309922	C	1.063429	-2.427237	1.348441
H	9.173266	8.000254	-1.430102	N	2.402466	3.264214	1.714046
H	0.545253	1.452892	-4.289806	C	-0.083508	1.776260	4.647537
H	5.559646	2.889833	-6.207115	H	-0.174930	2.111390	5.698457
H	2.254261	2.611982	-2.986360	H	-0.157192	-2.319433	-0.512127
C	6.739973	7.011023	-5.500222	H	0.471590	0.822799	4.683852
H	4.204558	3.538701	-5.268517	C	1.463207	-1.212997	2.217193
C	9.034814	1.841615	-7.104325	C	1.026473	3.369130	-1.823304
H	6.071464	7.657502	-4.931186	C	-0.349518	-0.543927	0.742614
C	10.236251	2.006554	-6.427698	H	0.113755	2.882463	-2.205015
C	7.340703	7.222311	-2.285543	H	1.468621	-1.442165	3.290426
H	6.273375	7.469377	-2.186968	H	1.319480	4.130182	-2.570242
H	7.686062	7.692056	-3.221215	C	-1.515456	1.654278	2.612350
H	7.010208	1.163564	-7.025168	C	-0.597062	0.629633	-0.190553
C	8.747649	2.402443	-0.224576	H	-0.146387	-0.051856	2.715423
C	10.334082	1.571177	-5.108352	H	2.474685	-0.883324	1.960725
H	9.842317	2.578868	-0.155191	C	-1.429465	1.587527	4.016699
H	8.939693	2.166815	-8.138897	C	3.087890	1.825813	3.575560
H	8.647478	1.460239	-0.806315	C	0.064414	-3.313057	2.104216
C	9.242697	0.981669	-4.484529	H	2.589500	0.903615	3.240953
C	4.319479	1.599929	2.401320	H	-1.299869	-0.926918	1.141991
H	4.276558	1.532451	3.489936	H	3.970268	1.515488	4.150765
H	11.090029	2.464342	-6.922609	C	-1.822572	4.338610	-0.351853
C	6.429812	6.545379	1.885191	H	-1.599823	1.050122	-0.089023
H	5.351902	6.318995	1.974965	C	0.468195	-3.893233	3.312930
C	7.254593	-1.298881	-4.149303	H	-1.877946	3.265749	-0.599886
H	11.269489	1.681928	-4.563553	H	-2.672257	4.815289	-0.857955
H	6.566864	7.549456	2.325271	H	-0.487960	0.333185	-1.244062
C	8.086175	7.150753	0.220144	C	3.193308	2.314631	-2.510304
C	7.258140	-2.203746	-5.215517	C	-0.375558	-4.726630	4.033236
H	8.944051	6.449580	0.284028	H	3.232915	2.999513	-3.358445
H	9.350254	0.625235	-3.459785	C	-1.653103	-5.007872	3.555978
H	6.974890	-1.854459	-6.208460	C	-0.523685	4.913953	-0.871551
H	8.290455	7.913516	0.993565	H	-0.563266	5.082694	-1.957536
C	8.797267	5.256625	-2.496644	H	-0.367915	5.897867	-0.412123
C	7.622065	-3.530368	-5.027647	H	1.474468	-3.703334	3.686898
C	8.001231	-3.978510	-3.764884	C	3.521200	2.669841	2.391897
H	9.386247	5.787810	-1.740663	C	-2.065303	-4.451137	2.353335
H	7.612772	-4.217736	-5.870809	H	4.204283	3.461105	2.774029
H	9.243813	5.474006	-3.481054	H	-0.032532	-5.163055	4.968787
C	8.015002	-3.086968	-2.699404	H	4.140791	2.056451	1.699352
C	8.209402	3.343124	2.099014				
H	8.286586	-5.017190	-3.614689				

C	-1.213712	-3.614687	1.634109	C	2.691970	1.171171	3.025729
C	-2.535403	1.370705	4.842308	C	0.306975	-4.370587	2.678821
H	-2.405789	1.342256	5.925760	H	1.840351	0.676269	2.525591
H	-2.318671	-5.658722	4.117978	H	-2.187118	-2.539140	1.315845
C	-0.913110	4.497230	3.254809	H	3.296874	0.358459	3.448100
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C	2.240541	-3.298267	0.929545	H	-2.661039	-0.675802	-0.297741
H	-3.058995	-4.663099	1.964869	C	1.075175	-4.476903	3.846973
H	-1.050085	5.591659	3.373696	H	-0.976350	5.414194	-0.351404
C	-1.930350	4.573200	1.142376	H	-1.165170	7.149958	-0.149026
C	3.506288	-3.209269	1.511096	H	-2.481362	-2.228834	-1.142363
H	-2.107820	5.659498	1.298471	C	2.071532	2.613709	-2.828955
H	-1.569341	-3.196948	0.695397	C	0.849398	-5.485401	4.772682
H	3.696659	-2.492311	2.307980	H	2.547078	3.220050	-3.601858
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C	1.755105	4.886191	-0.025411	C	0.879232	6.459785	-0.001118
C	4.546354	-4.036965	1.092760	H	1.086888	7.065696	-0.898254
C	4.337815	-4.971791	0.087656	H	1.307747	6.996498	0.853944
H	1.284580	5.540290	0.717128	H	1.873060	-3.754391	4.017753
H	5.524495	-3.946048	1.560349	C	3.520191	1.943001	2.004715
H	2.157621	5.513383	-0.841642	C	-0.940017	-6.320680	3.411679
C	3.075695	-5.081654	-0.490627	H	4.503664	2.186435	2.460349
C	2.152128	2.618559	4.462408	H	1.465564	-5.543739	5.667500
H	5.150310	-5.615884	-0.240307	H	3.740382	1.283104	1.138249
H	2.089165	2.189053	5.473627	C	-0.709574	-5.304423	2.485449
C	2.041532	-4.257883	-0.068875	C	-2.594375	1.203664	3.517127
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C	0.312942	4.131427	4.059584	H	-0.341075	-7.212400	5.278431
H	2.895891	-5.816347	-1.272426	C	-0.386803	4.879524	3.711791
H	1.139417	4.754105	3.698023	H	-1.388720	4.423970	3.863817
H	1.052363	-4.366380	-0.512820	C	2.026410	-3.072160	1.350738
H	0.156692	4.345869	5.132232	H	-1.738390	-7.067562	3.231486
C	2.882685	4.149383	0.677709	H	-0.404069	5.843512	4.257566
H	3.541254	3.635392	-0.049000	C	-0.938591	6.090840	1.709708
C	3.515291	4.943859	1.127226	C	2.532653	-1.843993	0.906505
C	2.018813	1.529787	-0.510593	H	-0.805395	7.067159	2.223807
H	0.664564	1.214311	-0.268114	H	-1.350385	-5.247036	1.608953
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C	4.161199	0.562708	-1.191845	C	4.174457	-4.075834	0.833963
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C	4.221210	1.402907	-2.298370	H	5.692683	-2.761826	0.052514
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Zr	0.767989	3.406012	1.391886	H	2.890747	2.902483	4.280573
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C	1.521098	3.219257	-1.698374	H	3.788037	3.359847	-0.303721
C	0.557842	-3.184085	1.756982	H	4.637509	4.129514	1.046527
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C	-0.225307	1.757744	4.097794	H	-1.154394	-1.038110	-1.158066
H	-0.557089	1.962814	5.131900	C	-2.209017	2.083866	0.914556
H	-0.707791	-4.122985	0.168953	H	-2.076365	2.402099	-0.122500
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C	-1.370443	-2.088907	0.707999	H	-4.586801	0.672113	2.896885
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C	-1.369659	1.752390	3.124734	Zr	-0.057607	2.089031	-1.763952

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N	1.606404	3.294139	-1.552954	C	0.778178	-1.054198	2.820045
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H	0.872366	3.431873	3.600401	C	-0.075169	-1.259478	3.909872
H	0.127066	-0.946032	0.365433	H	-0.362316	-2.272176	4.185524
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C	1.240036	-1.933438	-2.281775	H	-1.211358	-0.322049	5.480612
C	-1.371270	4.269995	-3.948791	C	-0.155004	2.180729	-6.860290
C	1.758938	-0.550471	-1.855157	H	-0.076730	2.262095	-7.942684
H	-2.448516	4.063982	-3.864932	C	0.230460	1.011531	-6.213550
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H	-1.289818	5.235972	-4.480288	C	0.141330	0.928325	-4.824650
C	1.138439	0.238165	2.462482	H	0.455659	0.001372	-4.340100
C	2.838088	-0.641604	-0.780819				
H	1.788939	0.404433	1.602328				
H	0.919340	-1.894061	-3.329118				
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C	2.358779	4.424603	0.570117				
C	0.169260	-3.262180	-0.296772				
H	3.101736	4.290575	1.370603				
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H	2.578807	5.411982	0.134322				
C	-3.092575	4.110943	-1.423166				
H	3.716264	-1.189044	-1.148224				
C	1.389191	-3.841622	0.052180				
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H	2.469111	-1.167906	0.110244				
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C	0.378433	-4.992861	1.921151				
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H	-2.172312	5.970907	-2.049401				
H	-1.361443	5.150652	-0.714854				
H	2.285837	-3.625497	-0.523770				
C	2.568526	3.326317	-0.474102				
C	-0.848552	-4.423300	1.585295				
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H	2.522504	2.353855	0.039134				
C	-0.946697	-3.571885	0.494352				
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H	-0.543462	1.976782	4.835399				
H	0.460250	-5.662462	2.774263				
C	-1.821720	2.191811	0.956289				
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C	-1.160386	-2.587700	-2.324823				
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H	-2.601122	-5.299896	-3.801362				
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C	-2.876414	-1.923147	-3.909193				
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H	-3.907615	-3.514202	-4.935803				
H	0.911809	5.231426	1.959317				
C	-1.897469	-1.595293	-2.978214				
H	0.294475	4.881145	0.341983				
C	-1.077655	3.280257	1.722755				
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N	0.429295	-0.007285	-1.112336
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C	-0.672390	-0.884754	-1.531419
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H	-1.105868	-0.520253	-2.471875
C	-1.061702	3.016863	-4.116214
C	-0.077999	-2.298539	-1.748752
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C	1.524093	2.588050	2.225661
H	1.811155	3.169082	3.125808
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H	2.457438	2.323912	1.709182
C	1.353004	-1.934420	-2.205601
C	-1.687586	4.149123	-3.366921
C	1.718738	-0.577158	-1.576257
H	-2.725863	3.891897	-3.120922
H	2.095331	-2.708394	-1.979570
H	-1.737962	5.071869	-3.973125
C	0.302554	0.498293	1.590240
C	2.735462	-0.663649	-0.445248
H	0.454668	0.149760	0.036442
H	1.337746	-1.844786	-3.299092
C	0.781172	1.343522	2.608695
C	2.843836	4.472827	0.347771
C	-0.157504	-3.122142	-0.460336
H	3.633300	4.225301	1.071629
H	2.149516	0.069919	-2.358120
H	3.131655	5.441935	-0.086548
C	-3.133598	4.436220	-0.783011
H	3.661357	-1.124793	-0.810956
C	0.949767	-3.554356	0.266123
H	-3.939211	4.589620	-1.514741
H	-3.488651	4.904628	0.146146
H	2.354487	-1.246272	0.401077
C	-0.501844	1.959292	-3.368990
C	0.797442	-4.277559	1.448504
H	2.990999	0.330732	-0.058454
C	-0.467897	-4.595455	1.919761
C	-1.860317	5.174244	-1.191946
H	-2.118103	6.145646	-1.653087
H	-1.270571	5.398246	-0.296765
H	1.955907	-3.321750	-0.072683
C	2.818145	3.392600	-0.738840
C	-1.585668	-4.194202	1.190369
H	3.705575	3.510634	-1.384454
H	1.680570	-4.587641	2.002664
H	2.953257	2.409936	-0.260795
C	-1.427564	-3.474013	0.016013
C	0.553301	1.099271	3.964885
H	0.938523	1.797199	4.711929
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C	-1.715702	2.931689	1.579936

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H	-2.585227	-4.446856	1.537602	C	0.998987	-3.706365	-0.186619
H	-2.641519	3.462899	1.862723	H	-3.865738	5.163183	-1.285803
C	-2.922982	2.932135	-0.558913	H	-3.295534	5.479685	0.337294
C	-0.178923	-4.277020	-3.293938	H	2.245935	-1.397627	0.360941
H	-3.813357	2.509700	-0.062151	C	-0.646644	1.987657	-3.148813
H	-2.308939	-3.177424	-0.552740	C	0.856129	-4.358585	1.410228
H	0.766500	-4.590391	-2.851599	H	2.723301	0.259771	-0.025229
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C	0.260762	5.213582	-2.365733	C	-1.718350	5.471601	-1.089169
C	-0.766185	-5.054616	-4.281650	H	-1.883084	6.431210	-1.617715
C	-1.988030	-4.676298	-4.833533	H	-1.070746	5.700800	-0.235982
H	0.435634	5.841258	-1.483070	H	2.002141	-3.558541	-0.206140
H	-0.271505	-5.962721	-4.619600	C	2.743524	3.284202	-0.663580
H	0.086701	5.896245	-3.215164	C	-1.526679	-4.152771	1.236602
C	-2.610713	-3.521868	-4.379429	H	3.633648	3.275068	-1.318430
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H	-2.452550	-5.282848	-5.607519	H	2.823847	2.353604	-0.079045
H	1.672742	5.242944	1.991535	C	-1.377607	-3.500054	0.021588
C	-2.015075	-2.740360	-3.390582	C	0.654370	0.859424	3.697810
H	0.874514	5.321006	0.421819	H	1.206235	1.289181	4.535639
C	-0.545099	3.835608	1.956075	H	-0.517750	-5.087361	2.899414
H	-3.569932	-3.219280	-4.794071	C	-1.753872	3.287938	1.748506
H	-0.782537	4.856305	1.625112	H	-1.748366	2.395506	2.392902
H	-2.531508	-1.846013	-3.048146	C	-0.637294	-3.467494	-2.927824
H	-0.433047	3.883795	3.053925	H	-2.523971	-4.331051	1.633337
C	1.496825	4.349922	-2.586318	H	-2.628012	3.885363	2.064202
H	1.455882	3.881749	-3.582942	C	-3.051398	3.419148	-0.301779
H	2.373050	5.020617	-2.589763	C	0.051644	-4.629914	-3.290359
C	-1.076030	3.043544	-5.510647	H	-3.952547	3.174732	0.289745
H	-1.516200	3.895971	-6.030313	H	-2.267718	-3.193196	-0.527449
C	-0.423742	-0.613898	2.048523	H	1.006177	-4.853142	-2.813859
H	-0.823475	-1.334789	1.332322	H	-3.188076	2.871436	-1.246962
C	-0.662884	-0.879904	3.398421	C	0.317888	5.172967	-2.347204
H	-1.232402	-1.765066	3.683874	C	-0.467501	-5.505347	-4.234116
C	-0.170714	-0.017892	4.369742	C	-1.698504	-5.241656	-4.829761
H	-0.348554	-0.206489	5.427014	H	0.604167	5.859590	-1.539953
C	-0.525813	1.994177	-6.235068	H	0.089161	-6.400273	-4.503888
H	-0.532684	2.011538	-7.322843	H	0.174958	5.790385	-3.252968
C	0.045830	0.932230	-5.544935	C	-2.400198	-4.099162	-4.467954
H	0.494356	0.102752	-6.089303	C	1.576102	4.819266	1.044656
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H	0.528014	0.081714	-3.669133	H	1.820608	5.404474	1.953230
K				C	-1.873757	-3.219718	-3.524512
Zr	-0.185232	2.248799	-0.753011	H	0.963585	5.476342	0.416492
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N	-1.861143	2.924772	0.348039	H	-0.366229	4.254338	3.124493
H	-0.965895	-0.803318	-2.803126	C	1.454336	4.172765	-2.546006
C	-1.206441	3.063631	-3.881233	H	1.322146	3.645832	-3.503517
C	-0.028999	-2.543849	-1.882465	H	2.390096	4.752427	-2.634985
N	1.531986	3.229339	-1.444869	C	-1.203532	3.136420	-5.276078
C	1.461040	2.763972	2.298541	H	-1.651208	4.002718	-5.766159
H	1.621535	3.253628	3.279963	C	-0.792848	-0.128158	1.581651
H	-1.629081	-1.153996	-1.206022	H	-1.445579	-0.523081	0.796133
H	2.461470	2.588496	1.880434	C	-0.873402	-0.758661	2.822823
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C	-1.774970	4.230851	-3.139492	C	-0.125063	-0.275411	3.889273
C	1.638313	-0.727314	-1.622145	H	-0.173534	-0.753833	4.865326
H	-2.798691	4.011984	-2.816295	C	-0.613048	2.140067	-6.039828
H	2.177151	-2.823151	-2.059085	H	-0.608668	2.199354	-7.126199
H	-1.847598	5.123765	-3.790952	C	0.005351	1.091415	-5.374322
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H	1.394388	-1.982397	-3.383922	TS_{KJ'}			
C	0.712491	1.475366	2.447154	Zr	-0.261320	2.458292	-0.768138
C	2.862766	4.473031	0.298191	N	0.805656	3.641985	1.416144
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H	2.028016	-0.015641	-2.361424	C	-0.565745	-1.392755	-1.999209
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C	0.077806	-2.791997	-1.897122
N	1.452030	3.424778	-1.469133
C	1.483868	2.601124	2.204463
H	1.710028	2.976578	3.222244
H	-1.540849	-1.308035	-1.503550
H	2.454072	2.391117	1.732854
C	1.533560	-2.417240	-2.257759
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C	1.731411	-0.942766	-1.823115
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H	2.281228	-3.092120	-1.824741
H	-1.911575	5.422433	-3.692097
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C	0.639090	1.361266	2.252613
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H	-3.884851	5.450095	-1.080281
H	-3.257971	5.731376	0.529518
H	2.461156	-1.234599	0.201629
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H	2.864508	0.340103	-0.497574
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C	-1.725234	5.718900	-0.941294
H	-1.878360	6.705090	-1.422118
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H	1.949677	-3.348267	0.146555
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H	3.555376	3.341893	-1.483816
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C	-1.418065	-3.650992	-0.070235
C	0.527958	0.650278	3.448522
H	1.105117	0.964297	4.319909
H	-0.827872	-4.753684	3.088577
C	-1.676838	3.412439	1.844715
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H	-2.500995	4.035523	2.235133
C	-3.056922	3.679336	-0.152639
C	0.150958	-5.058897	-2.981120
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H	-2.241666	-3.512910	-0.770851
H	1.002027	-5.278825	-2.336303
H	-3.244104	3.152603	-1.101661
C	0.264776	5.421148	-2.260170
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C	-1.403817	-5.757087	-4.684568
H	0.589342	6.055204	-1.423611
H	0.204443	-6.980840	-3.936234
H	0.117855	6.088944	-3.129138
C	-2.045312	-4.529833	-4.585328
C	1.714042	4.758239	1.114240
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C	-1.585578	-3.564994	-3.690505
H	1.123645	5.488197	0.546651
C	-0.380172	4.165789	2.133906
H	-2.912074	-4.314038	-5.206283
H	-0.516691	5.204084	1.802654
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H	-0.175842	4.202497	3.220140
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C	-0.971485	-0.063971	1.250519
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H	-1.817594	-1.603160	2.499790
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H	-0.902313	2.408302	-7.037083
C	-0.253789	1.304383	-5.296149
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H	0.313144	0.455121	-3.441159

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C	1.402567	2.121501	1.810684
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H	2.264368	1.674672	1.293032
C	2.062962	-2.977497	-1.606226
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C	2.180490	-1.463998	-1.275416
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H	-2.484742	5.849595	-3.594012
C	-0.632925	1.603466	0.441360
C	2.806246	-1.132872	0.063411
H	0.389899	-0.867456	-0.459389
H	2.548393	-3.189834	-2.567013
C	0.191302	1.273886	1.532968
C	3.160475	3.467064	-0.351517
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H	3.569825	2.456682	-0.205477
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H	4.005045	4.102666	-0.650490
C	-3.142658	5.920205	0.016759
H	3.833012	-1.509862	0.130590
C	0.499734	-3.883664	0.742745
H	-4.087468	5.738727	-0.514719
H	-3.365046	6.663688	0.794306
H	2.223719	-1.560453	0.890782
C	-1.228753	2.863229	-2.538797
C	-0.204958	-4.251595	1.888483
H	2.831960	-0.043867	0.205809
C	-1.585925	-4.386685	1.850790
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H	-2.526220	7.360404	-1.491441
H	-1.312088	6.976150	-0.251631
H	1.581073	-3.790978	0.806965
C	2.109903	3.438647	-1.465348
C	-2.258109	-4.154138	0.652219
H	2.572691	3.271026	-2.450216
H	0.336725	-4.434257	2.814418
H	1.516543	2.480908	-1.316412
C	-1.550429	-3.789222	-0.484168
C	-0.025468	0.134505	2.312398
H	0.635598	-0.087004	3.152863
H	-2.136518	-4.676911	2.742819
C	-0.844835	4.345865	2.373936
H	-1.206528	3.348593	2.692942
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H	-1.200690	5.067309	3.133118
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H	-2.086828	-3.632744	-1.419892
H	1.522117	-5.770524	-1.727961
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C	0.678274	-6.644127	-3.500436
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H	0.157176	6.969481	-1.681173
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H	-0.511469	6.774280	-3.314349
C	-0.756320	-5.217492	-4.794469
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C	-0.538826	-4.179172	-3.890819
H	2.474335	5.126217	0.787963
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H	1.093006	4.141199	3.361346
C	0.947709	5.281239	-2.684441
H	0.695271	4.586653	-3.506447
H	1.793046	5.898385	-3.042167
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C	-1.080482	-0.721463	2.015336
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C	-1.784730	2.239803	-5.256380
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H	-0.794992	0.370690	-4.859679
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N	3.450331	4.865362	-2.858442
H	-2.628324	1.280127	-3.700216
C	2.561488	-0.487356	-1.448560
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H	1.886156	-0.655251	-2.313686
C	-1.495710	-0.954284	-2.528802
C	3.208544	3.496744	-4.857522
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C	3.346235	-1.801708	-1.176879
H	-0.438422	-0.654367	-2.475116
N	5.150750	3.421685	-1.349119
C	-0.941155	-1.274286	-4.937301
C	3.493892	1.496476	1.776406
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H	1.931918	-0.187065	-0.594262
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H	2.709215	0.833004	1.388374
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C	4.424809	-1.694663	-2.280402
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C	-0.569352	-0.077566	1.549357
C	4.430928	-0.216337	-2.735863
H	4.056071	5.503677	-4.798841

C	-1.226203	0.916535	2.262809
H	5.408728	-2.037433	-1.936068
H	-0.358053	-1.117884	-0.303452
H	5.050534	4.236870	-4.060021
C	-2.211683	1.669324	1.627271
C	2.165493	1.267324	3.901559
H	0.207124	-0.674989	2.029158
C	5.822377	0.362425	-2.899450
C	-2.535059	1.417226	0.301557
H	1.299718	1.056465	3.273672
H	-0.982365	1.101455	3.308025
H	4.150664	-2.346218	-3.118430
C	-3.807098	-0.297281	-1.823586
C	3.389830	1.528498	3.282333
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C	3.894497	-1.732360	0.245256
H	-3.334693	1.989283	-0.167790
H	6.211831	2.461832	1.735651
H	-3.375544	-1.871843	-0.418324
H	3.942787	-0.180776	-3.730025
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H	0.085886	5.607248	-3.132810
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C	5.635125	-1.304116	1.884984
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C	4.756746	-1.576034	2.925522
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H	2.221873	6.189448	-3.956773
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C	5.968961	2.711704	-0.387505
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H	7.034622	2.705626	-0.688750
H	6.665594	-1.024466	2.099014
H	5.659998	1.655448	-0.383506
C	3.018744	-1.993324	1.308760
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H	5.476020	1.930180	3.636143
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C	1.073263	2.819208	0.278557
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H	0.680327	5.206034	-0.762519
H	1.987717	-2.273744	1.083769
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C	4.413722	5.609606	-2.027375
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H	3.879886	5.875685	-1.102908
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H	4.716523	6.550837	-2.523884
C	0.647876	-4.386036	-2.109172
C	4.457553	3.719979	1.418206
H	0.782397	-6.527422	-1.915275
H	4.423090	3.979303	2.492874
C	1.288053	-3.163536	-1.910111

H	4.250840	4.647888	0.868561	C	-4.555243	-0.717167	-1.868516
C	2.051411	3.398944	1.282155	C	4.455832	-1.663373	0.097541
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H	2.137672	4.478877	1.093964	H	6.289186	1.987726	1.342699
H	0.773076	-2.255871	-2.210008	H	-4.256437	-1.211739	-0.944162
H	1.709856	3.279196	2.324601	H	2.965754	-0.473251	-3.801802
C	5.608605	4.752082	-1.659291	C	-5.873932	-0.798152	-2.292172
H	6.366335	4.750929	-2.468720	H	6.617041	3.635504	0.863343
H	6.107900	5.239797	-0.801428	C	-6.274685	-0.148464	-3.457148
C	2.832341	3.585117	-6.194728	C	0.439104	4.756935	-2.446317
H	3.128489	4.449198	-6.791783	H	-6.594224	-1.366623	-1.707838
C	2.044328	1.255221	5.286612	H	5.316860	-0.353776	-4.459455
H	1.079813	1.044942	5.745269	C	-5.342026	0.578428	-4.184273
C	3.157818	1.505381	6.082298	C	5.717525	-1.114830	-0.144822
H	3.070104	1.494647	7.166264	H	-7.307960	-0.206824	-3.791171
C	4.387830	1.757884	5.482122	H	0.384600	3.918337	-3.156573
H	5.266086	1.942215	6.097101	C	-4.017059	0.654335	-3.757178
C	2.060399	2.575066	-6.764488	H	-0.440122	5.386675	-2.644211
H	1.751485	2.643975	-7.805561	H	-5.640688	1.095131	-5.093861
C	1.678393	1.485785	-5.988588	H	5.766837	0.373494	-2.899778
H	1.065318	0.695810	-6.422430	H	-3.311503	1.230335	-4.350493
C	2.074673	1.414156	-4.652365	C	2.452421	2.646600	-4.255214
H	1.750284	0.545717	-4.067990	H	0.112800	1.252321	-1.412688

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Zr	2.783033	2.507859	-1.949541	C	6.327438	-1.316524	2.183644
N	0.090264	1.132722	-2.424714	C	1.665561	5.608225	-2.738806
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H	0.572219	0.263030	-2.637402	C	5.608074	2.414910	-0.650059
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H	-1.265929	0.780559	-3.942181	H	6.590922	2.358461	-1.163356
C	2.497142	-0.539980	-1.057822	H	7.615117	-0.507910	0.656846
C	-2.153422	0.020646	-2.096885	H	5.212371	1.393314	-0.644355
N	1.311006	3.243248	-0.658676	C	4.157243	-2.034939	1.415550
H	-1.750116	2.038799	-2.809888	C	4.775150	1.455720	4.264858
H	1.535370	-0.880953	-1.500457	H	5.708594	1.521755	3.704692
C	-1.553242	-1.393326	-2.295489	H	7.048340	-1.182279	2.987281
C	2.845782	3.836888	-4.897659	C	1.104262	2.761066	0.701601
C	-1.388586	-1.788366	-3.726729	H	1.056224	1.653821	0.740408
C	3.395390	-1.808674	-0.995594	C	2.575466	-3.066729	-0.747325
H	-0.569256	-1.459162	-1.810562	H	4.806614	-2.156851	3.458022
N	4.674646	3.241140	-1.393763	H	0.115631	3.087508	1.067346
C	-0.237841	-2.218621	-4.240240	C	0.328635	4.243032	-1.018861
C	3.544113	1.239568	2.061587	C	3.084227	-4.317382	-1.109653
H	-2.197191	-2.121823	-1.777641	H	0.384287	5.116894	-0.330258
H	4.438937	0.727814	1.686943	H	3.185078	-2.469919	1.641360
C	-2.130514	0.434844	-0.621544	H	4.073550	-4.376023	-1.562812
H	2.254554	-0.131425	-0.063429	H	-0.695167	3.835007	-0.885601
H	-2.272836	-1.709964	-4.364200	C	3.897101	5.503546	-1.742541
H	2.687815	0.621017	1.753441	C	2.351935	-5.480054	-0.902367
H	-0.142285	-2.510069	-5.282977	C	1.089420	-5.419235	-0.318557
C	3.977914	-1.787340	-2.429380	H	3.349894	5.600675	-0.793862
C	-1.508051	-0.310081	0.383183	H	2.768309	-6.439561	-1.201438
C	3.567587	4.844942	-4.055339	H	4.190600	6.518101	-2.072338
H	0.654063	-2.318491	-3.617572	C	0.579206	-4.187001	0.071898
C	-1.448657	0.153469	1.697707	C	4.615002	3.375932	1.509431
C	3.726909	-0.368014	-2.999863	H	0.511835	-6.327481	-0.163649
H	3.569033	5.854227	-4.507661	H	4.851409	3.594230	2.570202
C	-2.018988	1.373102	2.037644	C	1.320476	-3.026511	-0.133593
H	5.040219	-2.059185	-2.450893	H	4.352572	4.338925	1.052793
H	-1.066731	-1.277588	0.155921	C	2.186267	3.227405	1.655849
H	4.617339	4.542839	-3.947595	H	-0.401354	-4.121998	0.541305
C	-2.659100	2.121303	1.051588	H	2.338026	4.303113	1.489670
C	2.394804	1.152814	4.306485	H	0.913739	-2.072790	0.202437
H	-0.952762	-0.451539	2.455151	H	1.873657	3.113671	2.709841
C	4.954124	0.265177	-3.629797	C	5.104196	4.613630	-1.522842
C	-2.713006	1.655933	-0.255698	H	5.849699	4.743941	-2.334232
H	1.455650	0.988673	3.773547	H	5.616010	4.982391	-0.615415
H	-1.971455	1.737968	3.061300	C	2.603664	4.083118	-6.247394
H	3.460289	-2.530692	-3.046534	H	2.912852	5.030109	-6.693013
C	-3.599733	0.005901	-2.593578	C	2.405293	1.217488	5.695979
C	3.575120	1.282184	3.569521	H	1.475743	1.113682	6.251810
H	-3.120510	3.074189	1.302264	C	3.605857	1.406093	6.373211
C	5.854348	2.844811	0.804931	H	3.618963	1.454440	7.459693
				C	4.792188	1.520005	5.653956

H	5.736375	1.652472	6.178174
C	1.966110	3.119987	-7.022913
H	1.770301	3.305629	-8.077321
C	1.571217	1.924962	-6.431236
H	1.064993	1.164539	-7.024703
C	1.808587	1.705753	-5.074708
H	1.458707	0.763381	-4.649645

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Zr	2.530040	2.241354	-2.061966
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N	2.910532	2.620934	1.238464
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N	3.276160	0.233192	-1.860498
H	0.632294	0.103598	-2.892906
N	2.801400	4.467009	-3.214572
H	-1.047345	1.570515	-3.364111
C	2.650214	-0.870932	-1.177874
C	-2.045069	0.298472	-1.889866
N	1.062431	3.348890	-1.001804
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H	1.882491	-1.369389	-1.819168
C	-2.002836	-0.935085	-2.827443
C	2.858349	3.047646	-5.185509
C	-2.265873	-0.606950	-4.261655
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H	-1.022362	-1.428477	-2.758851
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C	-1.413181	-0.860383	-5.251098
C	3.062995	1.379521	2.001878
H	-2.741748	-1.668206	-2.468395
H	3.999368	0.900277	1.689673
C	-1.772040	-0.086458	-0.431671
H	2.150004	-0.569402	-0.241143
H	-3.220204	-0.124677	-4.484281
H	2.254197	0.696110	1.693724
H	-1.635835	-0.606254	-6.284234
C	4.537490	-1.793482	-2.248673
C	-1.147277	-1.281037	-0.059045
C	3.531689	4.177411	-4.465620
H	-0.453196	-1.345016	-5.064783
C	-0.779617	-1.523548	1.264738
C	4.131383	-0.426485	-2.859008
H	3.606893	5.091164	-5.084243
C	-1.038398	-0.576200	2.247688
H	5.621646	-1.878984	-2.105204
H	-0.938587	-2.048497	-0.802862
H	4.557067	3.887860	-4.202360
C	-1.681557	0.609237	1.897575
C	1.839842	1.277261	4.206213
H	-0.287882	-2.461181	1.521112
C	5.320202	0.389528	-3.330302
C	-2.043733	0.845303	0.577801
H	0.955297	0.966105	3.646719
H	-0.755066	-0.766197	3.280817
H	4.254107	-2.605535	-2.928817
C	-3.427559	0.939070	-1.999631
C	3.025446	1.513849	3.505537
H	-1.892281	1.360796	2.656535
C	5.346649	3.060575	0.842547
C	-4.536903	0.220700	-1.537042
C	4.540390	-1.583297	0.328153
H	-2.538559	1.780357	0.315435
H	5.788443	2.314430	1.521471
H	-4.381919	-0.751788	-1.069926
H	3.518439	-0.647821	-3.759341
C	-5.822546	0.731396	-1.641851
H	6.039884	3.914522	0.866309
C	-6.030925	1.984468	-2.213089
C	0.304163	4.832660	-2.814078
H	-6.665727	0.151140	-1.273701
H	5.885780	-0.181142	-4.077439
C	-4.941109	2.713242	-2.669392
C	5.783353	-0.950685	0.302911
H	-7.036560	2.389646	-2.297402
H	-0.101538	3.912018	-3.261475

C	-3.650601	2.196054	-2.564592
H	-0.434420	5.625306	-3.002481
H	-5.088276	3.695416	-3.113343
H	5.994717	0.634935	-2.500525
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C	2.339167	2.007450	-4.386468
H	0.453353	0.209350	-1.287924
C	6.456728	-0.633026	1.482417
H	5.004274	1.329762	-3.796899
C	5.897775	-0.939585	2.716403
C	1.571288	5.233695	-3.549395
H	1.386487	5.120487	-4.624800
H	1.783889	6.302641	-3.378205
H	6.245002	-0.685382	-0.645063
C	5.273748	2.433969	-0.557882
C	4.651058	-1.560376	2.760951
H	6.307972	2.388651	-0.962522
H	7.425835	-0.140054	1.425891
H	4.942183	1.394896	-0.454818
C	3.987316	-1.875064	1.583462
C	4.160717	1.883384	4.233521
H	5.104300	2.039700	3.710409
H	6.422724	-0.695222	3.637400
C	0.680406	2.819004	0.285662
H	0.686824	1.709659	0.275207
C	3.191991	-3.345417	-0.767130
H	4.191539	-1.793399	3.719458
H	-0.365608	3.092933	0.530809
C	0.423859	4.602058	-1.314013
C	4.060558	-4.439445	-0.837725
H	0.909953	5.487822	-0.843560
H	3.013294	-2.362983	1.634614
H	5.121497	-4.261973	-1.014529
H	-0.607314	4.596313	-0.903829
C	3.644862	5.252475	-2.295081
C	3.595230	-5.738145	-0.677332
C	2.245053	-5.974530	-0.429059
H	3.013872	5.536276	-1.442439
H	4.291067	-6.571954	-0.742248
H	3.979705	6.183752	-2.790144
C	1.372090	-4.897642	-0.339841
C	4.012262	3.565460	1.367095
H	1.879543	-6.990985	-0.302548
H	4.133300	3.921691	2.410280
C	1.844343	-3.598035	-0.507767
H	3.723550	4.444927	0.775340
C	1.600463	3.244860	1.417179
H	0.314178	-5.062433	-0.138754
H	1.711693	4.337911	1.393108
H	1.147366	-2.766728	-0.425721
H	1.156351	3.001695	2.398615
C	4.815894	4.434270	-1.797304
H	5.647222	4.434760	-2.534871
H	5.227898	4.962130	-0.917329
C	2.802997	3.034017	-6.577590
H	3.207972	3.872651	-7.146331
C	1.779894	1.420495	5.588902
H	0.846799	1.229331	6.115217
C	2.914687	1.801150	6.297206
H	2.873161	1.911919	7.378460
C	4.106734	2.029476	5.615204
H	5.001303	2.315328	6.164691
C	2.234451	1.950879	-7.240226
H	2.183430	1.936184	-8.327002
C	1.731658	0.890680	-6.495360
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H	1.394842	0.056989	-4.575177

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Zr	2.480995	2.574663	-1.716172
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C	-0.613898	0.912685	-2.090230
N	3.594927	0.786483	-1.440951
H	1.212817	-0.063862	-2.135741

N	2.539745	4.757142	-2.972061	H	6.221584	3.363118	-0.553168
H	-0.566047	0.990599	-3.185104	H	7.445990	-4.673136	-1.646654
C	3.540042	-0.311534	-0.502448	H	5.069292	2.096787	-0.151142
C	-1.656662	-0.153666	-1.680167	C	5.438641	-2.321495	0.656140
N	0.762806	3.466651	-0.833761	C	3.745245	2.348364	4.488224
H	-0.921608	1.892671	-1.704131	H	4.713331	2.581952	4.044492
H	2.551574	-0.380398	-0.016184	H	8.071996	-4.472030	0.754460
C	-1.272966	-1.512479	-2.322313	C	0.376185	3.044411	0.495661
C	2.788206	3.247362	-4.851378	H	0.390103	1.940229	0.596790
C	-1.369835	-1.519522	-3.815070	C	2.736946	-2.645861	-1.242240
C	3.885705	-1.637109	-1.280637	H	6.745682	-2.970688	2.230075
H	-0.255096	-1.800068	-2.036565	H	-0.670246	3.328014	0.713236
N	4.221014	3.687890	-1.161027	C	-0.072293	4.529314	-1.340825
C	-0.362327	-1.816461	-4.633299	C	2.292099	-3.315112	-2.385442
C	2.856730	1.835499	2.168382	H	0.133736	5.518411	-0.868519
H	-1.931658	-2.292559	-1.908213	H	4.876522	-1.681379	1.333018
H	3.861720	1.466679	1.921706	H	2.742351	-3.093873	-3.351743
C	-1.651335	-0.217798	-0.151246	H	-1.131365	4.310924	-1.088100
H	4.259791	-0.170370	0.323417	C	3.230850	5.694305	-2.068850
H	-2.343893	-1.267102	-4.240463	C	1.286035	-4.277872	-2.316705
H	2.148944	1.082530	1.785281	C	0.712934	-4.608138	-1.095472
H	-0.484345	-1.818708	-5.711375	H	2.527492	5.930367	-1.257505
C	4.164409	-1.073952	-2.693139	H	0.951107	-4.767603	-3.228994
C	-0.932380	-1.185473	0.554651	H	3.459647	6.637922	-2.599572
C	3.361153	4.452638	-4.162517	C	1.163201	-3.970124	0.058229
H	0.624935	-2.078987	-4.248347	C	3.647344	4.107153	1.636353
C	-0.846204	-1.146909	1.945587	H	-0.069553	-5.361003	-1.038541
C	4.571744	0.379217	-2.457993	H	3.639729	4.444510	2.692073
H	3.415426	5.334647	-4.827773	C	2.156000	-3.000863	-0.017490
C	-1.493832	-0.147250	2.660970	H	3.326500	4.967800	1.035406
H	4.901428	-1.646180	-3.267326	C	1.287119	3.614878	1.562937
H	-0.423454	-1.988357	0.027000	H	0.732988	-4.225447	1.025446
H	4.383521	4.238072	-3.824959	H	1.330329	4.703549	1.422809
C	-2.218913	0.822571	1.971425	H	2.495143	-2.515768	0.898278
C	1.475684	1.601480	4.261272	H	0.888821	3.444224	2.578191
H	-0.274301	-1.912985	2.467149	C	4.476969	5.068138	-1.487136
C	6.044173	0.530085	-2.077831	H	5.334584	5.172467	-2.186155
C	-2.291111	0.787441	0.584788	H	4.764314	5.675281	-0.606970
H	0.657824	1.254035	3.626952	C	2.786739	3.158337	-6.242145
H	-1.439680	-0.124516	3.747835	H	3.180114	3.981508	-6.841024
H	3.232811	-1.055867	-3.275696	C	1.299408	1.701103	5.636921
C	-3.053753	0.234154	-2.164516	H	0.341331	1.438226	6.081634
C	2.696280	1.930063	3.665769	C	2.349597	2.129414	6.443032
H	-2.728888	1.614163	2.516540	H	2.216950	2.206154	7.519820
C	5.064757	3.758766	1.221263	C	3.574225	2.450159	5.865231
C	-4.137947	-0.572535	-1.797500	H	4.403590	2.773465	6.490589
C	5.092386	-2.392252	-0.697196	C	2.281036	2.021733	-6.866019
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H	5.529019	3.048539	1.922457	C	1.777079	0.987760	-6.084776
H	-3.963947	-1.430016	-1.147395	H	1.371228	0.092364	-6.555092
H	4.404232	0.959285	-3.378472	C	1.784210	1.100089	-4.694671
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C	-0.004485	4.683260	-2.852881	Zr	2.366071	2.832280	-1.696450
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H	-0.125105	3.691842	-3.314990	N	2.971850	4.985168	-2.815127
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H	-4.774314	2.500812	-4.035961	C	-1.444586	-0.083572	-1.665325
H	6.279708	0.071496	-1.109016	N	0.817263	4.098271	-1.003710
H	-2.501285	2.001469	-3.284277	H	-1.159548	2.064371	-1.547970
C	2.280293	2.226822	-4.020610	H	2.247942	-0.549711	-0.102313
H	0.709835	0.342642	-0.648425	C	-0.810790	-1.289193	-2.404182
C	6.890286	-4.007761	-0.989292	C	2.917227	3.563451	-4.774950
H	6.323336	1.587758	-2.031032	C	-1.001739	-1.302370	-3.887461
C	7.239270	-3.899725	0.352477	C	3.675345	-1.821905	-1.169681
C	1.242554	5.344579	-3.406860	H	0.265656	-1.328453	-2.181666
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H	2.599910	-1.772484	-3.055489
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H	0.680666	0.866939	-0.460195
C	6.824370	-3.961426	-0.994862
H	5.375576	1.449465	-2.975015
C	7.662218	-3.250710	-0.139245
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H	1.870704	6.763030	-2.539559
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H	7.154430	-4.904444	-1.425466
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C	5.942694	-1.568940	0.095052
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C	0.247507	3.836857	0.308465
H	-0.248662	2.846884	0.374834
C	2.721784	-2.902751	-0.657547
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C	1.907374	-3.686446	-1.475482
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H	1.931911	-3.565371	-2.556831
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C	3.672385	3.582433	1.614900
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H	3.716999	4.565596	1.131882
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H	1.782662	-4.217936	2.349752
H	1.746791	4.964772	1.272679
H	3.302018	-2.533450	1.383218
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H	5.781959	4.667065	-1.968588
H	5.282284	5.136255	-0.352701
C	2.831308	3.600591	-6.164170
H	3.350551	4.381386	-6.722156
C	0.599291	2.032436	5.371850
H	-0.381838	2.186981	5.816133
C	1.718981	1.886685	6.184633
H	1.619083	1.931546	7.266693
C	2.965674	1.671282	5.606080
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C	1.423196	1.655840	-6.110281
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H	4.173557	5.023307	-4.692500
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H	6.465827	0.680783	-3.452564
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C	6.994429	-4.443632	-1.627761
H	5.686926	1.771851	-2.273813
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H	2.680172	-3.191167	-3.937380
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C	0.940998	4.580511	1.123443
H	1.082779	-4.645185	0.514139

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H	2.957371	-3.068331	0.350366
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C	-0.350432	3.152477	5.213702
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C	1.879295	2.436160	5.760619
H	2.645797	2.213071	6.499652
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C	0.423754	-1.572046	6.093287
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C	1.463606	-1.877913	5.210700
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C	4.134185	-1.053689	2.374966
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H	3.468543	-1.848573	2.011240

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H	-1.121598	0.444277	-0.733024
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H	0.300589	3.613571	-3.552480
C	4.952535	-1.966149	-2.362153
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C	4.938880	-2.969960	-1.395522
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H	3.735126	-0.665911	-3.572675
H	5.035779	-0.842920	0.436737
C	3.733390	-3.426349	-0.879644
C	2.569644	-2.574649	5.707925
H	3.369099	-2.862194	5.024027
H	5.894680	-1.606307	-2.769748
C	0.109465	1.318882	3.314180
H	-0.574963	0.460392	3.219452
C	1.165835	-4.937430	-0.898219
H	5.873759	-3.403759	-1.045951
H	-0.432682	2.087993	3.898045
C	1.034531	3.137751	2.053286
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H	2.126633	3.112080	2.250343
H	3.735308	-4.229302	-0.142041
H	0.951498	-4.701816	-3.025062
H	0.613660	3.684715	2.917704
C	3.229553	2.810921	-0.426346
C	0.959571	-6.778128	-2.469173
C	1.061056	-7.697493	-1.427242
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H	0.840050	-7.125496	-3.493356
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C	1.221285	-7.237394	-0.126913
C	3.457628	-0.253269	3.486084
H	1.019579	-8.765049	-1.631322
H	3.737368	-0.628057	4.484295
C	1.274025	-5.869671	0.134572
H	3.809758	0.785667	3.429027
C	1.366382	0.900663	4.065150
H	1.307920	-7.945164	0.695047
H	2.072395	1.740975	4.064462
H	1.401860	-5.533146	1.161593
H	1.176121	0.652089	5.121274
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H	4.430236	1.173075	-1.227024
H	5.106338	2.006450	0.167900
C	3.602746	2.879433	-3.688902
H	4.335809	2.203415	-3.247505
C	0.495945	-1.925081	7.436304
H	-0.326075	-1.681249	8.105625
C	1.613626	-2.598924	7.919576
H	1.670824	-2.879208	8.968868
C	2.649333	-2.927357	7.050944
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C	3.992885	3.769030	-4.684556
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H	1.945184	-3.228866	1.640629
H	-4.796635	-1.079153	1.303514
H	0.205388	-1.287480	3.526171
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C	0.208024	-3.169755	-1.218555
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C	1.397738	1.846830	-2.575214
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C	-0.114775	-1.815024	-0.532238
H	2.064925	0.990908	-2.735708
C	-2.511849	5.606285	0.440639
H	0.456588	-3.054269	-2.279823
H	-3.687142	3.121440	2.422306
H	0.373742	1.469211	-2.654013
C	-2.660321	4.986807	-0.799280
C	0.592438	-1.181708	6.166639
H	-2.746914	5.378297	2.567551
C	0.080749	-0.534946	-1.328506
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H	-2.109342	6.614654	0.507063
H	-0.668736	-3.829378	-1.177253
C	-5.236802	1.649911	-1.011704
C	1.522813	-1.570869	5.199049
H	-2.372035	5.509464	-1.709673
C	3.953212	-0.965913	2.140737
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C	2.750675	-3.471569	-0.856790
H	-3.326351	3.243508	-1.857191
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H	-6.266331	3.308980	-0.106009
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C	-7.270710	2.657506	-1.885720
H	4.863833	-1.446917	2.524573
C	-7.267550	1.770722	-2.959926
C	0.745038	4.056705	0.475983
H	-8.056849	3.404112	-1.794531
H	-0.854647	-0.121190	-1.720288
C	-6.249683	0.832973	-3.060667
C	3.034156	-2.604233	-1.912261
H	-8.051040	1.816266	-3.712849
H	-0.205546	4.587071	0.617850
C	-5.245598	0.771679	-2.095269
H	1.517638	4.836441	0.403207
H	-6.229867	0.136444	-3.896137
H	0.759772	-0.712430	-2.175496

H	-4.468296	0.020758	-2.208343	C	-3.860921	1.569545	-0.112240
C	0.590123	3.677408	-4.118999	N	0.409269	2.103048	1.804133
H	-1.576428	1.373318	1.054706	H	-2.085743	1.372033	-1.341673
C	4.348254	-2.328197	-2.288364	H	-0.141036	-3.508289	1.465475
H	-0.407095	3.548895	-3.694562	C	-4.520591	0.843031	1.087833
C	5.412092	-2.913238	-1.613805	C	1.155592	3.186661	-3.558349
C	0.593172	3.346550	-0.857719	C	-4.901248	-0.575452	0.800763
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H	0.614043	4.122191	-1.640882	H	-3.829696	0.858264	1.943176
H	2.225021	-2.130699	-2.462165	N	3.029639	0.557349	0.150958
C	4.339720	-0.198831	0.885343	C	-6.153481	-1.004960	0.678140
C	5.147930	-3.776015	-0.552503	C	1.241658	-1.234215	3.781349
H	5.166076	0.486968	1.167991	H	-5.408856	1.407421	1.401961
H	4.534383	-1.652594	-3.121650	H	1.527828	-2.082343	3.160996
H	4.775574	-0.905934	0.154828	C	-3.457757	3.006179	0.231234
C	3.836651	-4.049776	-0.185978	H	1.574950	-3.787938	1.783475
C	2.672560	-2.246216	5.620135	H	-4.083259	-1.292634	0.683727
H	3.387003	-2.595717	4.873687	H	0.149536	-1.150289	3.692038
H	6.437096	-2.702296	-1.910633	H	-6.387093	-2.045333	0.467987
C	0.029592	1.515196	3.052361	C	0.120680	-3.209282	-1.218847
H	-0.661695	0.654796	3.040095	C	-3.243487	3.453466	1.536597
C	1.196824	-5.326257	-0.338076	C	0.909888	2.143074	-2.496789
H	5.967605	-4.249641	-0.015806	H	-6.996104	-0.320895	0.777480
H	-0.502133	2.326368	3.587804	C	-2.788090	4.746918	1.789145
C	1.024458	3.205187	1.711178	C	-0.168296	-1.794399	-0.655889
C	1.187493	-6.042595	-1.540548	H	1.414727	1.214889	-2.780281
H	2.121691	3.122258	1.860755	C	-2.535786	5.620756	0.740209
H	3.645687	-4.748031	0.629119	H	0.446949	-3.682931	-2.264249
H	1.281663	-5.496782	-2.479456	H	-3.429767	2.797193	2.384019
H	0.674426	3.790354	2.583171	H	-0.161482	1.913523	-2.455189
C	2.972992	2.686907	-0.917300	C	-2.735430	5.188041	-0.569198
C	1.072717	-7.425526	-1.553459	C	0.802663	-1.146478	6.275868
C	0.973545	-8.130399	-0.355742	H	-2.628670	5.065514	2.817197
H	3.009639	3.255321	0.015951	C	0.228328	-0.577457	-1.467760
H	1.064720	-7.958321	-2.502199	C	-3.189342	3.899489	-0.815593
H	3.352596	3.347576	-1.714353	H	-2.183181	6.630544	0.938048
C	0.992813	-7.434949	0.846072	H	-0.795194	-3.814967	-1.197048
C	3.341242	-0.073319	3.219205	C	-4.871428	1.584411	-1.259908
H	0.885526	-9.214442	-0.362335	C	1.618615	-1.534717	5.210106
H	3.697473	-0.352382	4.225015	H	-2.538697	5.859378	-1.402976
C	1.104424	-6.045659	0.853941	C	3.796087	-0.987052	1.987051
H	3.672020	0.959815	3.046278	C	-6.059245	2.308003	-1.094779
C	1.278926	1.119243	3.823553	C	2.601738	-3.613054	-0.622674
H	0.921804	-7.972937	1.789337	H	-3.350892	3.573517	-1.843248
H	2.001499	1.942348	3.768694	H	3.075873	-1.793038	1.799185
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H	1.086903	0.949274	4.894899	H	-1.258475	-1.753636	-0.444212
C	3.836634	1.458837	-0.734990	C	-7.036195	2.328206	-2.079061
H	3.998088	0.928238	-1.696969	H	4.720787	-1.489176	2.305422
H	4.841103	1.806619	-0.430452	C	-6.844323	1.627992	-3.268013
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H	3.714442	2.384064	-3.906223	H	-7.949727	2.897351	-1.920772
C	0.816277	-1.429604	7.516782	H	-0.571147	-0.213565	-2.122615
H	0.079164	-1.119768	8.254251	C	-5.666762	0.917773	-3.453468
C	1.976911	-2.081614	7.921198	C	3.022102	-2.961126	-1.782384
H	2.153411	-2.278794	8.976141	H	-7.606427	1.642481	-4.043604
C	2.902991	-2.495475	6.968681	H	0.100756	4.907322	0.953410
H	3.802769	-3.023853	7.275999	C	-4.690399	0.894234	-2.458462
C	3.114728	3.964849	-5.238166	H	1.806899	4.929347	0.547261
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C	2.067274	4.766275	-5.680572	H	1.114469	-0.808419	-2.081414
H	2.233717	5.498438	-6.467382	H	-3.783334	0.323517	-2.641789
C	0.801533	4.616821	-5.121803	C	0.183874	4.141287	-3.873972
H	-0.026397	5.227731	-5.474721	H	-1.425548	1.600032	1.049658
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N				H	-0.762263	4.132425	-3.330725
Zr	0.968591	0.363913	0.490133	C	5.344714	-3.319874	-1.221196
N	-1.585506	0.706383	0.567218	C	0.544727	3.640945	-0.646572
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N	0.579924	-1.701988	0.631999	H	2.291416	-2.550952	-2.474402
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N	1.325642	2.473978	-1.104816	C	4.943713	-3.967903	-0.055135
H	-2.784229	-0.175052	-0.882064	H	4.976855	0.405938	0.893381
C	0.783264	-3.066670	1.034209	H	4.670275	-2.305009	-2.994750
				H	4.461938	-0.992368	-0.054593
				C	3.593112	-4.114515	0.231291

C	2.785125	-2.250883	5.497024	H	-3.575275	0.948923	-3.258851
H	3.411835	-2.597237	4.674165	H	0.556650	-0.328538	2.990682
H	6.401255	-3.210467	-1.455424	H	-5.648907	2.034426	-3.921265
C	0.097323	1.700148	3.158195	C	1.261427	-3.183653	-0.872875
H	-0.678078	0.907962	3.158636	C	-3.403239	-1.002588	1.236271
C	0.925095	-5.353090	-0.148169	C	0.975249	1.813489	-3.522235
H	5.686692	-4.374850	0.628075	H	-6.430819	1.565632	-2.305650
H	-0.339633	2.537405	3.740890	C	-3.046407	-1.650935	2.419037
C	1.234708	3.294126	1.828034	C	0.533951	-1.847990	-1.043732
C	0.926705	-6.118262	-1.319634	H	1.603340	0.925950	-3.627508
H	2.322168	3.065891	1.843621	C	-2.605376	-0.923133	3.515698
H	3.295792	-4.657941	1.128598	H	2.329153	-2.975006	-1.007040
H	1.074180	-5.615730	-2.275536	H	-3.732737	-1.608155	0.394670
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C	0.755529	-7.494989	-1.281858	C	1.158389	0.181620	5.498706
C	0.585750	-8.144295	-0.061047	H	-3.112570	-2.736419	2.470887
H	3.001365	3.227686	-0.105159	C	1.077785	-0.846394	-2.035509
H	0.757505	-8.065929	-2.208113	C	-2.905760	1.109189	2.250824
H	3.143240	3.308227	-1.862168	H	-2.313316	-1.428803	4.433765
C	0.592901	-7.400419	1.111494	H	0.964032	-3.915771	-1.632642
C	3.295289	-0.063888	3.094385	C	-4.583740	2.297699	0.119744
H	0.452533	-9.223205	-0.026277	C	2.006139	-0.399361	4.550994
H	3.725366	-0.335657	4.073255	H	-2.210014	1.056856	4.278923
C	0.762110	-6.017478	1.068312	C	4.097838	-0.498411	1.191736
H	3.633883	0.958331	2.877096	C	-5.786387	2.001740	0.771755
C	1.330692	1.180596	3.878735	C	2.196707	-3.884367	1.436041
H	0.466025	-7.895038	2.072512	H	-2.854015	2.194671	2.194953
H	2.106486	1.954802	3.842310	H	3.365469	-1.316969	1.216777
H	0.766343	-5.457010	2.001367	H	-5.966204	0.983878	1.118293
H	1.153062	0.980231	4.946961	H	-0.538581	-2.072031	-1.270215
C	3.520686	1.364060	-0.952139	C	-6.746578	2.979151	0.991840
H	3.473249	0.817148	-1.918012	H	5.049995	-0.946713	1.507128
H	4.590916	1.601865	-0.809576	C	-6.519901	4.287355	0.570976
C	2.343480	3.185017	-4.295021	C	0.750129	4.508069	-0.817584
H	3.094194	2.421555	-4.089622	H	-7.673459	2.720712	1.499379
C	1.153212	-1.437134	7.590305	H	0.459959	-0.795932	-2.939191
H	0.502865	-1.128075	8.405633	C	-5.325193	4.599965	-0.063061
C	2.328418	-2.130898	7.860061	C	3.464114	-4.121341	0.896964
H	2.603203	-2.361741	8.886743	H	-7.269420	5.056722	0.741375
C	3.142163	-2.542327	6.808931	H	-0.186529	5.053616	-0.629851
H	4.053373	-3.100980	7.011181	C	-4.366058	3.613977	-0.287132
C	2.569994	4.126469	-5.293279	H	1.497545	5.275169	-1.068524
H	3.500813	4.106767	-5.855767	H	-5.131837	5.618820	-0.391607
C	1.601821	5.083430	-5.579707	H	2.106870	-1.100645	-2.337265
H	1.774321	5.819113	-6.361965	H	-3.443005	3.889290	-0.792978
C	0.404177	5.085113	-4.871078	C	-0.025265	3.365402	-5.252517
H	-0.364861	5.819216	-5.101328	H	-1.409723	-0.137050	-0.267405
H	-0.130568	-0.622172	6.066133	C	4.566534	-4.363596	1.713578
N'				H	-0.968655	3.310838	-4.707348
Zr	1.153428	0.664437	-0.246313	C	4.427505	-4.388780	3.095436
N	-1.260052	0.642460	-0.914204	C	0.470910	3.633040	-2.030659
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C	-2.250628	1.693682	-0.668512	H	0.499894	4.283044	-2.921165
N	0.593118	-1.278577	0.330519	H	3.609264	-4.116460	-0.180794
H	-1.348257	0.246792	-1.846851	C	4.259083	0.022695	-0.233069
N	1.337960	2.456787	-2.229596	C	3.165883	-4.191977	3.650184
H	-2.392851	2.247909	-1.605805	H	5.233314	0.550982	-0.287307
C	0.136168	-2.406859	1.094295	H	5.540515	-4.533479	1.258909
C	-3.608295	1.158880	-0.166848	H	4.352822	-0.842306	-0.926917
N	0.528121	2.545763	0.704699	C	2.071362	-3.949842	2.830034
H	-1.808894	2.393838	0.056566	C	3.160587	-1.046435	5.002501
H	-0.932367	-2.595691	0.860302	H	3.801960	-1.554416	4.281062
C	-4.239214	0.253574	-1.260291	H	5.288126	-4.576052	3.733661
C	1.078620	2.656736	-4.769433	C	0.411089	2.319371	2.132710
C	-4.432327	0.940133	-2.578574	H	-0.267552	1.469876	2.326228
C	0.946574	-3.641690	0.578151	C	0.147978	-4.941515	0.631214
H	-3.599911	-0.628207	-1.411636	H	3.030566	-4.222729	4.729805
N	3.215959	0.934201	-0.661085	H	-0.060819	3.184387	2.642872
C	-5.557132	1.540681	-2.957296	C	1.186366	3.809664	0.464498
C	1.650137	-0.380580	3.086572	C	0.583512	-6.052407	-0.099621
H	-5.204465	-0.120553	-0.892741	H	2.294540	3.719627	0.462673
H	1.966647	-1.323586	2.633765	H	1.093156	-3.812848	3.290534
C	-3.331436	0.387857	1.127481	H	1.476276	-5.963816	-0.718070
H	0.192798	-2.268558	2.177706	H	0.972286	4.511956	1.293518
				C	2.773929	2.793825	-2.198527
				C	-0.088997	-7.265694	-0.041124

C	-1.216015	-7.403341	0.764719
H	2.934582	3.523069	-1.400221
H	0.270367	-8.110147	-0.625586
H	3.091142	3.276098	-3.138168
C	-1.649191	-6.317697	1.515037
C	3.685101	0.605185	2.157988
H	-1.746241	-8.351819	0.811801
H	4.126067	0.464153	3.158019
C	-0.972038	-5.102269	1.450881
H	4.053200	1.567320	1.779011
C	1.763982	2.020781	2.762371
H	-2.521822	-6.412618	2.158342
H	2.484072	2.782184	2.438947
H	-1.326333	-4.269479	2.056966
C	1.750669	2.049179	3.863813
C	3.621498	1.577978	-1.890879
H	3.615989	0.866701	-2.747311
H	4.670412	1.925981	-1.817599
C	2.267027	2.705052	-5.503726
H	3.124306	2.121751	-5.167681
C	1.464762	0.144564	6.854768
H	0.791299	0.601674	7.576524
C	2.627262	-0.486430	7.286603
H	2.868777	-0.520176	8.346608
C	3.471776	-1.087048	6.357708
H	4.372762	-1.598396	6.690384
C	2.360515	3.464584	-6.665404
H	3.294156	3.487951	-7.223002
C	1.258293	4.180939	-7.120340
H	1.327854	4.772042	-8.030610
C	0.060548	4.124111	-6.414191
H	-0.810949	4.667627	-6.772486
H	0.237497	0.659997	5.159640

TS_{N'O}

Zr	1.040984	0.694929	0.001874
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H	-0.353804	0.128515	-1.627161
N	1.246134	2.495758	-2.001217
H	-2.184373	2.169268	-1.800985
C	0.174798	-2.471038	1.219348
C	-3.514932	1.236837	-0.382527
N	0.651000	2.554721	0.964799
H	-1.828435	2.571413	-0.112302
H	-0.915628	-2.638522	1.097035
C	-3.988717	0.179303	-1.417201
C	0.733206	2.784326	-4.499665
C	-4.004417	0.679381	-2.828267
C	0.911264	-3.698654	0.589948
H	-3.318952	-0.690416	-1.375355
N	3.066927	0.806108	-0.631675
C	-5.090154	1.103635	-3.468695
C	1.673170	-0.486846	3.254001
H	-4.991567	-0.168881	-1.131968
H	1.948611	-1.406600	2.734430
C	-3.376353	0.648174	1.025335
H	0.352311	-2.365388	2.291139
H	-3.040766	0.688221	-3.346125
H	0.575096	-0.431928	3.253886
H	-5.050782	1.460084	-4.495005
C	1.009875	-3.236114	-0.892476
C	-3.388785	-0.721893	1.295230
C	0.706656	1.915661	-3.267206
H	-6.065699	1.113815	-2.981996
C	-3.126812	-1.207511	2.576787
C	0.298016	-1.882908	-0.918943
H	1.259836	0.993045	-3.463322
C	-2.857733	-0.330950	3.619090
H	2.044836	-3.064585	-1.209640
H	-3.594425	-1.439097	0.503548
H	-0.330491	1.622023	-3.063573
C	-2.866354	1.040998	3.370902
C	1.375548	-0.079426	5.727819

H	-3.138116	-2.281853	2.752042
C	0.634012	-0.873971	-1.988087
C	-3.121071	1.519673	2.092905
H	-2.656704	-0.709610	4.619007
H	0.562412	-3.952790	-1.591252
C	-4.540235	2.368356	-0.367066
C	2.160607	-0.564555	4.677855
H	-2.665693	1.744792	4.177232
C	4.013083	-0.556784	1.264049
C	-5.792860	2.135777	0.212800
C	2.269735	-3.916127	1.271212
H	-3.113360	2.593914	1.909122
H	3.319187	-1.399965	1.367214
H	-5.984138	1.174677	0.690451
H	-0.798769	-2.084825	-0.987938
C	-6.786475	3.104762	0.200178
H	4.995028	-0.957433	1.551045
C	-6.547387	4.342082	-0.392338
C	0.983049	4.551541	-0.497207
H	-7.750629	2.895715	0.658931
H	0.134842	-1.106854	-2.937881
C	-5.307847	4.591411	-0.966454
C	3.473493	-4.066813	0.578122
H	-7.322007	5.105455	-0.403166
H	0.127843	5.191186	-0.237310
C	-4.315383	3.613931	-0.955097
H	1.796424	5.239923	-0.769803
H	-5.106002	5.554123	-1.431574
H	1.716788	-0.841203	-2.190647
H	-3.358589	3.837607	-1.422586
C	-0.381854	3.549362	-4.854184
H	-1.469341	-0.099375	-0.216470
C	4.676613	-4.275316	1.249744
H	-1.269241	3.518419	-4.219577
C	4.706867	-4.350568	2.636074
C	0.532286	3.756839	-1.716023
H	-0.522274	3.489903	-1.598439
H	0.594070	4.425393	-2.590672
H	3.491155	-4.023517	-0.507748
C	4.095440	-0.124003	-0.200009
C	3.512429	-4.239778	3.343480
H	5.081581	0.360773	-0.346050
H	5.596052	-4.378951	0.677008
H	4.119445	-1.038513	-0.833310
C	2.316888	-4.032582	2.667464
C	3.380243	-1.175243	4.987319
H	3.975800	-1.613966	4.185962
H	5.646613	-4.510784	3.159837
C	0.427993	2.322087	2.374392
H	-0.309208	1.508292	2.509743
C	0.140750	-5.006447	0.747159
H	3.507960	-4.313969	4.429483
H	-0.019801	3.202800	2.874260
C	1.412432	3.766223	0.739128
C	0.501072	-6.116675	-0.024361
H	2.504256	3.574269	0.680211
H	1.394781	-3.967354	3.244743
H	1.311616	-6.019417	-0.746574
H	1.298102	4.447619	1.602265
C	2.701159	2.708661	-2.104538
C	-0.143775	-7.337514	0.120617
C	-1.166037	-7.482235	1.055117
H	2.999674	3.403669	-1.314336
H	0.155032	-8.182415	-0.496368
H	2.966817	3.182789	-3.063777
C	-1.525293	-6.395147	1.841029
C	3.624344	0.573602	2.209325
H	-1.673344	-8.437241	1.171560
H	4.136399	0.483620	3.180828
C	-0.876387	-5.171904	1.690048
H	3.928198	1.533576	1.772021
C	1.736549	1.923232	3.035706
H	-2.316859	-6.495104	2.581045
H	2.497077	2.685118	2.825688
H	-1.172727	-4.338039	2.324404
H	1.672906	1.841583	4.130092
C	3.454771	1.418028	-1.883115

H	3.321433	0.727140	-2.745883
H	4.533747	1.662387	-1.880269
C	1.843998	2.799757	-5.347962
H	2.703418	2.171469	-5.113044
C	1.806842	-0.169701	7.046717
H	1.181024	0.213070	7.849822
C	3.034173	-0.757715	7.337120
H	3.374098	-0.831360	8.367612
C	3.816866	-1.266005	6.304683
H	4.768095	-1.745273	6.526686
C	1.854527	3.583211	-6.497382
H	2.728180	3.581526	-7.145370
C	0.744842	4.355392	-6.824371
H	0.749898	4.964842	-7.725181
C	-0.378475	4.331691	-6.003063
H	-1.256910	4.918359	-6.262475
H	0.404869	0.365107	5.499453

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Zr	1.325487	1.088134	-0.186655
N	-0.761070	0.804230	-0.496896
N	2.459464	0.927696	2.107672
C	-1.926664	1.641914	-0.402920
N	1.305742	-1.078295	-0.288237
H	2.863536	-0.624189	-2.625207
N	1.196482	2.686422	-2.072762
H	-2.193532	2.116037	-1.371548
C	0.275182	-1.885645	0.337814
C	-3.217784	0.928928	0.070982
N	0.749085	2.804804	0.949691
H	-1.685529	2.471245	0.280183
H	-0.615617	-1.925991	-0.325580
C	-3.624671	-0.123915	-0.998414
C	0.399527	2.510644	-4.497374
C	-3.711601	0.422438	-2.389554
C	0.821260	-3.349543	0.458556
H	-2.893549	-0.947505	-0.984459
N	3.309868	1.376761	-0.992328
C	-4.843195	0.771761	-2.995234
C	1.994416	-0.338511	2.746906
H	-4.593236	-0.562971	-0.722518
H	2.216267	-1.150313	2.046325
C	-2.965554	0.279137	1.431451
H	-0.082128	-1.463810	1.285103
H	-2.765035	0.540221	-2.925088
H	0.897729	-0.273619	2.810204
H	-4.854333	1.169113	-4.007298
C	1.938336	-3.313483	-0.610850
C	-3.128798	-1.083798	1.682292
C	0.637272	1.838340	-3.172026
H	-5.806726	0.674324	-2.494941
C	-2.830289	-1.634586	2.928574
C	1.734523	-1.988652	-1.349141
H	1.326168	0.991448	-3.308051
C	-2.366100	-0.827135	3.959550
H	2.931137	-3.264464	-0.142848
H	-3.496996	-1.743547	0.899369
H	-0.301302	1.426132	-2.782746
C	-2.247144	0.544179	3.740405
C	1.804304	-0.379071	5.261275
H	-2.958692	-2.705579	3.083368
C	2.953032	-1.612467	-2.159953
C	-2.552699	1.085503	2.498316
H	-2.118393	-1.256333	4.928649
H	1.930935	-4.177097	-1.286684
C	-4.374735	1.922329	0.219763
C	2.540403	-0.668449	4.109252
H	-1.915735	1.201499	4.543292
C	4.441211	0.053741	0.815508
C	-5.575167	1.477452	0.787598
C	1.313147	-3.672485	1.875106
H	-2.458781	2.160912	2.347056
H	3.807857	-0.839992	0.722492
H	-5.643913	0.449945	1.145081
H	0.883809	-2.125587	-2.061400
C	-6.669522	2.319756	0.924197

H	5.446770	-0.302092	1.079288
C	-6.589058	3.643393	0.499095
C	0.701836	4.729562	-0.612098
H	-7.587665	1.943259	1.370490
H	3.106949	-2.354969	-2.952685
C	-5.403668	4.104436	-0.057236
C	2.517482	-4.332043	2.131372
H	-7.442596	4.308973	0.606053
H	-0.228412	5.221387	-0.293010
C	-4.309229	3.253159	-0.196680
H	1.360066	5.534488	-0.971061
H	-5.322812	5.137378	-0.389745
H	3.852299	-1.604813	-1.532846
H	-3.396912	3.647290	-0.638471
C	-0.839745	3.093180	-4.778551
H	-0.992003	-0.068922	-0.971481
C	2.894854	-4.671135	3.430095
H	-1.632146	3.044546	-4.030161
C	2.073373	-4.361342	4.505930
C	0.292429	3.821013	-1.774503
H	-0.689390	3.387046	-1.570730
H	0.187132	4.444799	-2.677810
H	3.173840	-4.608066	1.308730
C	4.542123	0.779570	-0.518567
C	0.861395	-3.719978	4.266624
H	5.310356	1.574631	-0.401550
H	3.842555	-5.180596	3.595316
H	4.968111	0.083932	-1.270140
C	0.486645	-3.391243	2.970901
C	3.757101	-1.341531	4.248569
H	4.308190	-1.637981	3.355443
H	2.377040	-4.605033	5.521789
C	0.654012	2.541130	2.362153
H	-0.079388	1.735578	2.531494
C	-0.238933	-4.411568	0.155316
H	0.203151	-3.466722	5.096392
H	0.288766	3.415094	2.935611
C	1.352280	4.074941	0.611051
C	0.143567	-5.702529	-0.222389
H	2.449314	4.004423	0.441555
H	-0.472421	-2.899311	2.810994
H	1.201139	-5.936720	-0.337423
H	1.246134	4.785149	1.452442
C	2.547995	3.179155	-2.400710
C	-0.797592	-6.701684	-0.438559
C	-2.153179	-6.438565	-0.266426
H	2.783759	3.975223	-1.687690
H	-0.468443	-7.694513	-0.738495
H	2.565859	3.624986	-3.408523
C	-2.549510	-5.167969	0.132579
C	3.930113	0.958272	1.929678
H	-2.891725	-7.219010	-0.434870
H	4.414894	0.728550	2.891705
C	-1.601829	-4.170341	0.342111
H	4.194474	1.994979	1.679548
C	2.008065	2.102248	2.895539
H	-3.604603	-4.945038	0.284110
H	2.726589	2.916619	2.737721
H	-1.931862	-3.186278	0.665678
H	2.010716	1.877890	3.973212
C	3.568180	2.079532	-2.225923
H	3.582458	1.397388	-3.106261
H	4.569558	2.550463	-2.221336
C	1.390325	2.540984	-5.481612
H	2.348497	2.057042	-5.289479
C	2.277163	-0.733100	6.520195
H	1.687330	-0.505426	7.405426
C	3.500923	-1.383857	6.644453
H	3.873353	-1.663235	7.627556
C	4.238517	-1.690625	5.505184
H	5.184740	-2.220242	5.594327
C	1.160895	3.161719	-6.705127
H	1.942503	3.174133	-7.461250
C	-0.069827	3.756843	-6.963209
H	-0.251766	4.240412	-7.920228
C	-1.072662	3.716650	-5.999125
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H	0.832042	0.105848	5.157980	C	3.656706	-4.682703	2.509336
TS_{Op}				H	-1.455153	3.716302	-3.806670
				C	3.133126	-4.650740	3.795184
Zr	1.260641	1.342563	-0.031274	C	0.725257	4.180605	-1.607605
N	-0.660080	1.101020	-0.403277	H	-0.284471	3.904952	-1.278241
N	2.352789	0.871083	2.183482	H	0.617956	4.788464	-2.520248
C	-1.918433	1.758726	-0.478981	H	3.316947	-4.321956	0.426434
N	0.496178	-1.125985	-0.355506	C	4.161911	0.094113	-0.590879
H	0.784534	-0.623408	-3.172670	C	1.836708	-4.178247	3.986773
N	1.401015	2.905389	-1.939779	H	5.170264	0.558664	-0.548455
H	-2.164947	2.051223	-1.521207	H	4.666370	-5.051418	2.338783
C	-0.082056	-2.077341	0.582560	H	4.248706	-0.718310	-1.344564
C	-3.110877	0.906747	0.023990	C	1.078321	-3.755062	2.903972
N	1.156143	3.156741	1.035760	C	3.115100	-1.325669	4.606616
H	-1.902089	2.710918	0.089092	H	3.606984	-1.844402	3.782348
H	-1.138905	-2.256172	0.314107	H	3.728065	-4.982399	4.643744
C	-3.259615	-0.327482	-0.909035	C	1.055178	2.911755	2.459866
C	0.504881	3.009675	-4.337235	H	0.152538	2.313162	2.676932
C	-3.273127	0.008147	-2.367163	C	-0.289262	-4.641086	0.325181
C	0.671908	-3.446090	0.418506	H	1.417707	-4.126092	4.989881
H	-2.421849	-1.011695	-0.715416	H	0.942262	3.850956	3.030370
N	3.187538	1.091808	-0.973565	C	1.946656	4.316374	0.687434
C	-4.374141	0.128044	-3.104293	C	0.157357	-5.850504	-0.218897
C	1.611167	-0.197445	2.922300	H	3.015240	4.068010	0.515156
H	-4.183709	-0.864348	-0.652965	H	0.061361	-3.400959	3.076372
H	1.710151	-1.116723	2.336733	H	1.174628	-5.919919	-0.601694
C	-2.837056	0.482055	1.468793	H	1.956362	5.035487	1.526147
H	-0.097906	-1.706206	1.612973	C	2.829023	3.089011	-2.275021
H	-2.294170	0.162841	-2.831424	C	-0.658386	-6.973624	-0.263310
H	0.544302	0.074615	2.912611	C	-1.948935	-6.922700	0.254310
H	-4.335602	0.377167	-4.161957	H	3.260809	3.762402	-1.528515
C	1.418087	-3.199880	-0.914867	H	-0.280355	-7.896133	-0.699238
C	-2.930440	-0.837549	1.914675	H	2.940798	3.574481	-3.258077
C	0.677069	2.227039	-3.061648	C	-2.400900	-5.739763	0.824620
H	-5.363357	-0.015679	-2.668480	C	3.756755	0.473579	1.897282
C	-2.634401	-1.184126	3.233081	H	-2.591510	-7.799503	0.220760
C	0.701042	-1.996006	-1.512285	H	4.227863	0.115664	2.825141
H	1.226020	1.303492	-3.274574	C	-1.579559	-4.616247	0.863397
C	-2.244767	-0.211106	4.144002	H	4.289684	1.388022	1.604720
H	2.461235	-2.901112	-0.735596	C	2.292479	2.160968	2.922218
H	-3.230052	-1.625779	1.226881	H	-3.402610	-5.684351	1.246052
H	-0.300181	1.930483	-2.664293	H	3.174492	2.751081	2.642870
C	-2.185443	1.118177	3.725946	H	-1.961347	-3.708823	1.328893
C	1.372985	0.118868	5.412876	H	2.343802	1.999267	4.008675
H	-2.714320	-2.224960	3.544057	C	3.567173	1.765641	-2.189161
C	1.419411	-1.371867	-2.684215	H	3.390573	1.145681	-3.096900
C	-2.485198	1.455930	2.412485	H	4.651957	1.986606	-2.206219
H	-2.004164	-0.478373	5.171109	C	1.480996	2.995505	-5.337211
H	1.429609	-4.069935	-1.582793	H	2.384951	2.403445	-5.193448
C	-4.422315	1.695396	-0.020110	C	1.768768	-0.127166	6.723144
C	2.048224	-0.464711	4.337090	H	1.231766	0.335224	7.548330
H	-1.907273	1.900977	4.431181	C	2.848041	-0.969144	6.975903
C	3.883073	-0.547320	0.766685	H	3.158529	-1.165390	7.999693
C	-5.559142	1.163220	0.601113	C	3.516450	-1.572410	5.915351
C	1.585762	-3.787558	1.597664	H	4.344348	-2.252428	6.105997
H	-2.436143	2.500497	2.105599	C	1.300053	3.703770	-6.520834
H	2.972483	-1.162284	0.699675	H	2.069158	3.678723	-7.289442
H	-5.475223	0.225780	1.150752	C	0.131006	4.429295	-6.726393
H	-0.291486	-2.354946	-1.877847	H	-0.014405	4.978598	-7.653700
C	-6.787177	1.807951	0.540850	C	-0.859201	4.434916	-5.748511
H	4.699031	-1.246921	0.993289	H	-1.783581	4.984581	-5.910680
C	-6.910905	3.015154	-0.141292	H	0.518100	0.766099	5.209571
C	1.396923	5.043378	-0.544454	P			
H	-7.651394	1.367321	1.033885				
H	1.664126	-2.132432	-3.435873	Zr	1.199021	1.962499	0.056181
C	-5.792568	3.561901	-0.756094	N	-0.538298	1.317402	-0.302107
C	2.889125	-4.259901	1.425032	N	1.966963	1.322894	2.248273
H	-7.870886	3.524399	-0.189590	C	-1.857105	1.870212	-0.370746
H	0.626501	5.758719	-0.226558	N	0.334457	-1.743938	-0.070117
C	-4.563560	2.908330	-0.696734	H	0.994288	-0.541469	-2.406094
H	2.198669	5.646856	-0.993743	N	1.550129	3.318777	-1.920060
H	-5.870894	4.506061	-1.291474	H	-2.119836	2.093870	-1.424852
H	2.347517	-0.884834	-2.357802	C	-0.298728	-2.740241	0.767400
H	-3.710042	3.360512	-1.195257	C	-2.987081	0.958590	0.173288
C	-0.672553	3.727390	-4.566671	N	1.123637	3.828778	1.055591
H	-0.383996	-0.117067	-0.532572	H	-1.937921	2.845593	0.157059

H	-1.386460	-2.828193	0.564139	C	0.942147	3.562814	2.473518
C	-3.001083	-0.353771	-0.650365	H	-0.058928	3.125860	2.639015
C	0.817954	3.309916	-4.363345	C	-0.458103	-5.289582	0.635864
C	-3.039366	-0.143012	-2.130745	H	3.019869	-5.275129	3.985613
C	0.374064	-4.056242	0.324038	H	0.965523	4.495614	3.066852
H	-2.092105	-0.916979	-0.406737	C	2.131632	4.812933	0.730981
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C	-4.129416	-0.275796	-2.881808	H	3.162353	4.392660	0.695598
C	0.997865	0.347913	2.849523	H	0.885018	-5.078198	2.783271
H	-3.862041	-0.965911	-0.345920	H	0.732703	-6.545257	-0.640894
H	0.804476	-0.427605	2.098205	H	2.179411	5.594689	1.512207
C	-2.729223	0.694881	1.657348	C	2.997361	3.230723	-2.221342
H	-0.170757	-2.528629	1.840697	C	-0.829960	-7.667719	0.317551
H	-2.089565	0.137958	-2.596218	C	-1.900860	-7.634377	1.207431
H	0.051279	0.884957	2.991927	H	3.517751	3.848845	-1.480740
H	-4.113091	-0.114465	-3.956919	H	-0.547053	-8.603029	-0.160796
C	0.475683	-3.812630	-1.209256	H	3.213505	3.653682	-3.216466
C	-2.595487	-0.582862	2.202575	C	-2.242629	-6.434329	1.817288
C	0.719665	2.687322	-2.994714	C	3.332267	0.748428	2.083750
H	-5.088705	-0.544139	-2.438145	H	-2.461111	-8.540454	1.426416
C	-2.355449	-0.772575	3.562983	H	3.679870	0.375902	3.059674
C	0.247796	-2.301159	-1.422508	C	-1.526174	-5.273411	1.533634
H	1.004552	1.629562	-3.043388	H	3.989729	1.581192	1.798734
C	-2.254023	0.317952	4.416408	C	2.004728	2.603115	3.012981
H	1.435491	-4.147871	-1.620904	H	-3.072437	-6.395210	2.519720
H	-2.680940	-1.460059	1.565611	H	2.993364	3.054243	2.855159
H	-0.318926	2.711992	-2.641218	H	-1.806770	-4.345221	2.030044
C	-2.400053	1.601870	3.893033	H	1.913471	2.412587	4.093665
C	1.137229	0.271473	5.374496	C	3.504921	1.803556	-2.074841
H	-2.248370	-1.783833	3.952943	H	3.222720	1.190216	-2.961819
C	1.201799	-1.619883	-2.379511	H	4.611680	1.849778	-2.106780
C	-2.638533	1.783139	2.536000	C	1.765770	2.866848	-5.289861
H	-2.062259	0.171001	5.477362	H	2.436924	2.052272	-5.016239
H	-0.301262	-4.388974	-1.723393	C	1.549954	-0.335083	6.556299
C	-4.365410	1.612357	0.030959	H	1.313159	0.124983	7.513246
C	1.429984	-0.303710	4.134378	C	2.253707	-1.535277	6.513670
H	-2.335236	2.469947	4.547547	H	2.574518	-2.012021	7.437261
C	3.418434	-0.341304	1.016903	C	2.530838	-2.129507	5.286325
C	-5.464008	1.018075	0.664409	H	3.065629	-3.076321	5.236947
C	1.734336	-4.180393	1.018892	C	1.849214	3.439497	-6.554516
H	-2.768497	2.792358	2.145584	H	2.591101	3.079160	-7.263601
H	2.458706	-0.871875	0.911625	C	0.977959	4.462554	-6.915012
H	-5.303877	0.140192	1.290440	H	1.040766	4.909311	-7.904587
H	-0.781540	-2.172567	-1.817612	C	0.017201	4.901699	-6.009480
C	-6.747279	1.528238	0.522779	H	-0.678149	5.689380	-6.290356
H	4.131302	-1.106098	1.351769	H	0.551128	1.190809	5.408676
C	-6.966831	2.661079	-0.256308				
C	1.841911	5.506570	-0.609962				
H	-7.579465	1.041247	1.027255				
H	1.096961	-2.020631	-3.394859				
C	-5.888107	3.269275	-0.883671				
C	2.926627	-3.733055	0.447539				
H	-7.969988	3.066300	-0.369225				
H	1.204876	6.382760	-0.427815				
C	-4.603002	2.749189	-0.743158				
H	2.781308	5.903499	-1.020142				
H	-6.041837	4.156635	-1.494520				
H	2.245029	-1.746516	-2.059270				
H	-3.782572	3.244309	-1.255569				
C	-0.062900	4.325076	-4.746884				
H	-0.114889	-0.820027	-0.033896				
C	4.138873	-3.842948	1.126069				
H	-0.829885	4.655971	-4.046562				
C	4.187024	-4.394184	2.400459				
C	1.095192	4.707678	-1.676079				
H	0.036762	4.628327	-1.391126				
H	1.139291	5.279704	-2.617622				
H	2.923418	-3.274639	-0.538540				
C	3.853135	0.161357	-0.356984				
C	3.004706	-4.833650	2.990466				
H	4.915325	0.486558	-0.294511				
H	5.050433	-3.488216	0.647401				
H	3.858572	-0.711780	-1.048454				
C	1.798812	-4.722322	2.309628				
C	2.120116	-1.519535	4.106421				
H	2.329896	-2.003130	3.149568				
H	5.134607	-4.486223	2.926617				

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