

Electronic Supplementary Information

Electronic Structures and Bonding of the Actinide Halides

An(TRENTIPS)X (An=Th-Pu, X=F-I): A Theoretical Perspective

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Table S1. Selected bond distances (Å) and angles (degrees) as well as the average relative error of the calculated values to the experimental ones in the four An(TREN^{TIPS})Cl complex using BP86, BLYP, B3LYP and M06L functionals with 6-31+G(d) basis set.

An(TREN ^{TIPS})Cl	Bond parameter	expt.	BP86	BLYP	B3LYP	M06L
Th(TREN ^{TIPS})Cl	Th-Cl	2.693(3)	2.704	2.722	2.712	2.736
	Th-N1	2.309(3)	2.327	2.354	2.335	2.314
	Th-N2	2.305(3)	2.325	2.351	2.333	2.327
	Th-N3	2.284(3)	2.318	2.343	2.333	2.303
	Th-N4	2.668(3)	2.721	2.730	2.716	2.767
	∠ClThN4	173.50	177.15	177.00	176.85	171.55
U(TREN ^{TIPS})Cl	U-Cl	2.6383(6)	2.637	2.663	2.651	2.671
	U-N1	2.249(2)	2.267	2.300	2.275	2.271
	U-N2	2.255(2)	2.278	2.310	2.284	2.265
	U-N3	2.231(2)	2.262	2.290	2.268	2.248
	U-N4	2.623(2)	2.660	2.669	2.660	2.710
	∠ClUN4	173.86	174.76	175.59	175.23	169.38
Np(TREN ^{TIPS})Cl	Np-Cl	2.6200(6)	2.632	2.660	2.641	2.661
	Np-N1	2.2322(19)	2.264	2.297	2.268	2.252
	Np-N2	2.2305(19)	2.276	2.307	2.264	2.272
	Np-N3	2.2056(19)	2.255	2.287	2.256	2.247
	Np-N4	2.605(2)	2.636	2.651	2.660	2.681
	∠ClNpN4	173.81	173.61	175.48	176.47	169.43
Pu(TREN ^{TIPS})Cl	Pu-Cl	2.6001(5)	2.631	2.653	2.633	2.658
	Pu-N1	2.2311(18)	2.270	2.307	2.267	2.262
	Pu-N2	2.2317(17)	2.286	2.327	2.266	2.297
	Pu-N3	2.2122(17)	2.283	2.316	2.259	2.273
	Pu-N4	2.577(2)	2.640	2.655	2.618	2.684
	∠ClPuN4	174.35	176.44	176.27	176.98	171.90
Average relative error			1.36%	2.33%	1.47%	1.84%

Table S2. The electronic energies (a.u.) of each state and the relative electronic energies (RE, kcal/mol) to each ground state for the An(TREN^{TIPS})Cl (An=U, Np, Pu) complexes.

Complexes	Spin state	E	RE
U(TREN ^{TIPS})Cl	1	-3327.707381	32.29
	3	-3327.758845	0.0
Np(TREN ^{TIPS})Cl	2	-3365.251962	16.04
	4	-3365.277523	0.0
Pu(TREN ^{TIPS})Cl	1	-3404.644651	66.61
	3	-3404.711357	24.75
	5	-3404.750794	0.0

Table S3. The calculated $\langle S^2 \rangle$ of the ground state for the An(TREN^{TIPS})X (An=Pa-U, X=F-I) complexes are obtained with the BP86/6-31+G(d)/RECP level of theory.

	-F $\langle S^2 \rangle$	-Cl $\langle S^2 \rangle$	-Br $\langle S^2 \rangle$	-I $\langle S^2 \rangle$	S(S+1)
Pa(TREN ^{TIPS})X	0.77	0.76	0.78	0.76	0.76
U(TREN ^{TIPS})X	2.02	2.02	2.02	2.02	2.00
Np(TREN ^{TIPS})X	3.80	3.81	3.81	3.82	3.75
Pu(TREN ^{TIPS})X	6.18	6.21	6.22	6.27	6.25

Table S4. Natural charge on the An (Q_{An}) and X (Q_X) atoms as well as population of valence electron of An and X atoms at the BP86/ECP-SEG/6-31+G(d) level of theory.

An(TREN ^{TIPS})X	Q_{An}	Q_X	An				X	
			7s	5f	6d	7p	ns	np
Th(TREN ^{TIPS})F	1.839	-0.623	0.11	0.16	1.05	0.24	1.90	5.72
Pa(TREN ^{TIPS})F	1.728	-0.568	0.31	1.52	1.08	0.24	1.89	5.67
U(TREN ^{TIPS})F	1.606	-0.548	0.12	2.85	1.10	0.25	1.89	5.65
Np(TREN ^{TIPS})F	1.589	-0.572	0.12	3.97	1.02	0.25	1.90	5.66
Pu(TREN ^{TIPS})F	1.580	-0.597	0.12	5.05	0.96	0.24	1.91	5.68
Th(TREN ^{TIPS})Cl	1.439	-0.329	0.13	0.17	1.25	0.29	1.80	5.52
Pa(TREN ^{TIPS})Cl	1.414	-0.317	0.17	1.63	1.29	0.29	1.81	5.50
U(TREN ^{TIPS})Cl	1.302	-0.338	0.13	2.90	1.27	0.30	1.83	5.50
Np(TREN ^{TIPS})Cl	1.270	-0.372	0.14	4.04	1.19	0.29	1.83	5.53
Pu(TREN ^{TIPS})Cl	1.324	-0.416	0.14	5.08	1.12	0.29	1.85	5.56
Th(TREN ^{TIPS})Br	1.331	-0.246	0.14	0.17	1.29	0.31	1.78	5.46
Pa(TREN ^{TIPS})Br	1.254	-0.246	0.38	1.49	1.32	0.31	1.80	5.44
U(TREN ^{TIPS})Br	1.246	-0.288	0.14	2.90	1.31	0.32	1.82	5.46
Np(TREN ^{TIPS})Br	1.201	-0.317	0.15	4.04	1.23	0.32	1.82	5.49
Pu(TREN ^{TIPS})Br	1.267	-0.363	0.15	5.07	1.15	0.31	1.83	5.52
Th(TREN ^{TIPS})I	1.250	-0.164	0.15	0.16	1.32	0.34	1.77	5.39
Pa(TREN ^{TIPS})I	1.265	-0.209	0.27	1.52	1.35	0.35	1.80	5.41
U(TREN ^{TIPS})I	1.205	-0.250	0.16	2.88	1.32	0.35	1.81	5.43
Np(TREN ^{TIPS})I	1.144	-0.265	0.17	4.04	1.24	0.35	1.81	5.45
Pu(TREN ^{TIPS})I	1.127	-0.280	0.18	5.14	1.16	0.35	1.82	5.46

Table S5. The composition and contribution of An and X atomic orbitals (AOs) to An-X bonds for the actinide halides An(TREN^{TIPS})X.

	An%	X%	Contribution of An AOs (%)	Contribution of X AOs(%)
Th-Cl	11.22	88.78	7s(5.97)7p(11.80)6d(42.02)5f(40.19)	3s(75.92)3p(24.05)
Pa-Cl	12.54	87.46	7s(6.96)7p(7.77)6d(48.68)5f(36.57)	3s(63.46)3p(36.50)
U-Cl	13.10	86.90	7s(5.56)7p(6.07)6d(52.69)5f(35.67)	3s(51.49)3p(48.47)
Np-Cl	12.97	87.03	7s(6.42)7p(5.69)6d(55.03)5f(32.84)	3s(47.65)3p(52.31)
Pu-Cl	12.61	87.39	7s(4.53)7p(2.83)6d(61.20)5f(31.44)	3s(39.05)3p(60.91)
Th-Br	12.88	87.12	7s(6.70)7p(13.88)6d(40.89)5f(38.51)	4s(69.43)4p(30.52)
Pa-Br	14.59	85.41	7s(24.86)7p(8.66)6d(48.21)5f(18.25)	4s(59.10)4p(40.83)
U-Br	14.28	85.72	7s(6.58)7p(8.80)6d(51.82)5f(32.80)	4s(48.60)4p(51.31)
Np-Br	14.27	85.73	7s(7.40)7p(8.79)6d(54.19)5f(29.62)	4s(45.99)4p(53.96)
Pu-Br	14.05	85.95	7s(5.19)7p(5.07)6d(61.26)5f(28.48)	4s(38.92)4p(61.00)
Th-I	15.47	84.53	7s(9.06)7p(13.71)6d(54.10)5f(23.12)	5s(48.81)5p(51.19)
Pa-I	16.45	83.55	7s(14.31)7p(12.63)6d(52.36)5f(20.69)	5s(49.71)5p(50.29)
U-I	16.49	83.51	7s(8.56)7p(13.86)6d(48.93)5f(28.65)	5s(40.61)5p(59.39)
Np-I	16.73	83.27	7s(9.42)7p(14.50)6d(50.38)5f(25.69)	5s(38.88)5p(61.12)
Pu-I	16.95	83.05	7s(9.86)7p(12.95)6d(51.20)5f(25.98)	5s(33.55)5p(66.45)

Table S6. Change of the Gibbs free energy (ΔG , kcal/mol) for the reactions $An^{IV}(TREN^{TIPS})X \rightarrow An^{III}(TREN^{TIPS}) + 0.5X_2$ (An=Th-Pu, X=F-I) at the BP86/ECP/6-31+G(d) level of theory.

Reaction	X=F	X=Cl	X=Br	X=I
$Th^{IV}(TREN^{TIPS})X \rightarrow Th^{III}(TREN^{TIPS}) + 0.5X_2$	139.99	92.85	88.25	74.72
$Pa^{IV}(TREN^{TIPS})X \rightarrow Pa^{III}(TREN^{TIPS}) + 0.5X_2$	125.32	85.47	72.46	67.13
$U^{IV}(TREN^{TIPS})X \rightarrow U^{III}(TREN^{TIPS}) + 0.5X_2$	118.46	71.15	66.49	53.41
$Np^{IV}(TREN^{TIPS})X \rightarrow Np^{III}(TREN^{TIPS}) + 0.5X_2$	97.29	53.19	49.20	36.44
$Pu^{IV}(TREN^{TIPS})X \rightarrow Pu^{III}(TREN^{TIPS}) + 0.5X_2$	85.15	39.05	33.07	22.47

The optimized Cartesian coordinates of the An(TREN^{TIPS})X (An=Th-Pu, X=F-Br) complexes at the BP86/ECP/6-31+G(d) level of theory as following:

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Th(TREN^{TIPS})F

Th	11.50345500	9.72229500	4.85304200
F	10.87930500	11.79023100	4.78044400
Si	15.10582500	10.73115300	4.69117300
Si	10.12759700	9.64601300	8.30195600
Si	9.48497800	8.91050200	1.84842700
N	13.80344700	9.54665700	4.45687100
N	11.14185500	8.93441400	7.02187600
N	10.33684400	8.38504700	3.31891500
C	16.36982800	10.22279600	6.08128300
H	16.97660800	11.14338700	6.22725000
C	15.68797200	9.90572000	7.42943000
H	14.99990600	10.70557300	7.75831000
H	16.43634400	9.76091300	8.23502200
H	15.09406300	8.97413400	7.36483900
C	17.36141900	9.09250000	5.71969100
H	16.84807100	8.11836400	5.60885000
H	18.11705100	8.96229400	6.52138500
H	17.91190600	9.28958700	4.78186500
C	16.15765300	10.89481700	3.07000500
H	16.68523800	9.91819700	2.99891300
C	17.25184500	11.98441900	3.15725100
H	16.81329300	12.99885200	3.20838200
H	17.90733800	11.96141600	2.26290800
H	17.90101000	11.85879000	4.04353600
C	15.33314900	11.04082800	1.77228500
H	14.55507700	10.26041300	1.69012700
H	15.98607000	10.95972000	0.87929200
H	14.82594700	12.02066700	1.71616700
C	14.27021800	12.38954500	5.23892700
H	13.40247500	12.09140200	5.87177500
C	15.16479200	13.29515400	6.12030200
H	15.48845600	12.80348000	7.05407700
H	14.61661600	14.21502200	6.40612800
H	16.07475400	13.61538600	5.57862000
C	13.70833600	13.22429800	4.06293900

H	14.52997100	13.64705900	3.45537600
H	13.10433500	14.07170800	4.44149000
H	13.05815600	12.64044500	3.39019000
C	14.24942600	8.21881600	3.96296200
H	15.35170800	8.13977300	3.86046700
H	13.85287700	8.01874200	2.94260200
C	13.78688100	7.10670100	4.91582100
H	14.13565500	6.10147100	4.58513300
H	14.21491500	7.30220600	5.91456500
C	9.02808500	8.25551600	9.09253600
H	9.76446400	7.55192100	9.53996600
C	8.12938600	8.74404400	10.25224300
H	8.69632300	9.29557200	11.02427400
H	7.63278700	7.88900600	10.75436800
H	7.32738000	9.41200400	9.88688100
C	8.19837200	7.44535800	8.07205400
H	7.36614100	8.04559700	7.66043500
H	7.74886100	6.54873100	8.54522100
H	8.81061300	7.10581900	7.21692000
C	9.13746300	11.09458800	7.49326000
H	9.91189600	11.71074600	6.98842400
C	8.43121100	12.02703300	8.50623000
H	7.63777300	11.50003600	9.06802600
H	7.94860500	12.87419600	7.97883200
H	9.13032500	12.45895100	9.24475800
C	8.13382000	10.65694800	6.40371100
H	8.55893900	9.93900200	5.67389400
H	7.77192200	11.52938000	5.82579700
H	7.24912700	10.16066400	6.84447200
C	11.17211500	10.42111000	9.73734500
H	10.42626400	10.89272500	10.41382900
C	11.96505100	9.39777100	10.58224700
H	11.31809400	8.60469400	11.00154600
H	12.46772900	9.89593600	11.43622600
H	12.75666800	8.90503900	9.98717700
C	12.10958200	11.53632500	9.22652300
H	12.85651000	11.12931600	8.51844100
H	12.66957500	12.00442100	10.06133200
H	11.56248500	12.34194500	8.70332100
C	11.91615200	7.73440000	7.42589200
H	11.55427100	7.28830200	8.37603600

H	12.98228900	7.99111900	7.61186400
C	11.83705300	6.62876100	6.36361100
H	12.42221200	5.73038100	6.66710900
H	10.78153900	6.32215200	6.25671000
C	7.57989200	8.55232100	1.89934700
H	7.18176300	9.06073100	0.99400400
C	6.89536000	9.19088900	3.12711600
H	7.24068100	8.71611500	4.06441900
H	5.79446600	9.06497300	3.08124900
H	7.09992200	10.27406400	3.21273300
C	7.17959600	7.06251700	1.78830000
H	7.61627700	6.56824900	0.90079400
H	6.07809700	6.95768900	1.71232100
H	7.49398600	6.48983400	2.68098700
C	10.17410800	7.95226100	0.30843400
H	9.89260400	6.89458000	0.50805100
C	11.71081300	7.98104100	0.15582600
H	12.07109700	8.97986600	-0.15076100
H	12.04630000	7.26271100	-0.61961400
H	12.22531500	7.72340200	1.09930700
C	9.49561500	8.34612700	-1.02497400
H	8.39271700	8.28996200	-0.97529900
H	9.82274400	7.67811700	-1.84759500
H	9.76309300	9.37724600	-1.32397700
C	9.70637800	10.82852600	1.75099000
H	9.48162100	11.19568000	2.77623800
C	11.14357900	11.28807400	1.41014100
H	11.93082200	10.77983100	2.00410000
H	11.26027000	12.37555100	1.58148600
H	11.38475700	11.09200300	0.34870300
C	8.70622700	11.54237100	0.80926500
H	8.85213100	11.24394100	-0.24558300
H	8.84631200	12.64073600	0.85920400
H	7.65394100	11.33421700	1.07195400
C	10.27448200	6.92834900	3.59168400
H	9.89259300	6.34072800	2.72980800
H	9.57139100	6.70713400	4.42563600
C	11.66442700	6.36738700	3.92103200
H	11.62113900	5.28116000	4.16555000
H	12.30409300	6.48369900	3.02925300
N	12.30034600	7.12260200	5.03689300

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Th(TREN^{TIPS})Cl

Th	11.49426400	9.77021500	4.88494600
Cl	10.57662800	12.31420900	4.90172700
Si	15.11335900	10.79034400	4.75051200
Si	10.01920200	9.41243100	8.27563200
Si	9.55216000	9.14778500	1.77504400
N	13.77661200	9.64135100	4.45016600
N	11.07120000	8.80799800	6.95846000
N	10.35731100	8.56721800	3.26182100
C	16.22262100	10.23950100	6.24741900
H	16.89236200	11.10868800	6.42845500
C	15.40159800	10.01582700	7.53452100
H	14.78090600	10.88972400	7.80378900
H	16.05937800	9.79803400	8.40039700
H	14.71608500	9.15489900	7.41884600
C	17.13342000	9.01815100	5.98573800
H	16.54470300	8.09761800	5.80823900
H	17.78116700	8.81629100	6.86317500
H	17.79885200	9.16191400	5.11521900
C	16.29970400	10.85156100	3.21794300
H	16.79046600	9.85375400	3.21596000
C	17.43305400	11.89366000	3.37899200
H	17.04222700	12.92812200	3.35860600
H	18.16518500	11.81011500	2.55021800
H	17.99318500	11.76867900	4.32425800
C	15.60755900	11.00388100	1.84542200
H	14.81424800	10.25018700	1.69376200
H	16.34154200	10.88738200	1.02208400
H	15.14192400	11.99861700	1.72829200
C	14.33229600	12.50507300	5.18189200
H	13.39520000	12.28512000	5.74284700
C	15.20404600	13.38592500	6.10949600
H	15.42622600	12.90144200	7.07606200
H	14.68530500	14.33980800	6.33026400
H	16.16982500	13.64334800	5.63553700
C	13.91783400	13.32550600	3.93731100
H	14.80710500	13.69364200	3.39149300
H	13.32171100	14.20897400	4.23654100

H	13.30249500	12.74603300	3.22856200
C	14.20788100	8.34771300	3.85235500
H	15.30728200	8.28068100	3.72062600
H	13.78560400	8.22159800	2.83069000
C	13.77444500	7.16661600	4.72953800
H	14.11181500	6.19198500	4.30956300
H	14.23471600	7.28193100	5.72662900
C	9.41490300	7.94713000	9.39921400
H	10.33935800	7.58812200	9.90170400
C	8.47071300	8.43303200	10.52565100
H	8.90000500	9.27046000	11.10496800
H	8.25563900	7.61252200	11.23987400
H	7.49859500	8.77149600	10.12152400
C	8.79650800	6.73013600	8.67439200
H	7.81034100	6.97072500	8.23941400
H	8.64359100	5.88946600	9.38153200
H	9.43236000	6.35869500	7.85100200
C	8.55846300	10.38155000	7.46564200
H	8.99739800	10.93023100	6.60327100
C	7.93256700	11.46302000	8.37960700
H	7.47276400	11.02276100	9.28447300
H	7.13228600	12.00678000	7.83912000
H	8.67031400	12.21460400	8.71040300
C	7.44740200	9.45992600	6.90965600
H	7.84339300	8.66670600	6.24881100
H	6.70926500	10.04402600	6.32587700
H	6.89187800	8.96400600	7.72747800
C	10.99796500	10.61535500	9.43347700
H	10.25012800	11.05701300	10.12758400
C	12.07286500	9.91212000	10.29362200
H	11.64650400	9.13728500	10.95672500
H	12.60041400	10.64258700	10.94027100
H	12.84223800	9.42820400	9.66215900
C	11.63241100	11.77463700	8.63483800
H	12.39207300	11.39461200	7.92234700
H	12.15214900	12.48768200	9.30668900
H	10.89511600	12.34764800	8.04483300
C	11.94143300	7.65791400	7.31442100
H	11.64179100	7.17193800	8.26444600
H	12.99538000	7.97706600	7.47048400
C	11.89228900	6.58881500	6.21749400

H	12.53151800	5.71118100	6.46451900
H	10.85185200	6.23201500	6.12408100
C	7.63658400	9.26413300	2.00816800
H	7.23265300	9.60612500	1.03054700
C	7.24363100	10.31595200	3.06752400
H	7.68737000	10.07672400	4.05210700
H	6.14358400	10.35011600	3.20479600
H	7.57465900	11.33479400	2.79803700
C	6.97510200	7.90444900	2.33183300
H	7.19650100	7.13005600	1.57324600
H	5.87213100	8.00429100	2.38675600
H	7.31213500	7.51850100	3.31247600
C	9.87225000	7.89955900	0.32010600
H	9.55701000	6.91459900	0.72823500
C	11.35462700	7.75987100	-0.09269500
H	11.70710400	8.65756000	-0.63326100
H	11.49890300	6.89613100	-0.77299600
H	12.02237400	7.61698900	0.77687500
C	8.99040100	8.14974300	-0.92619000
H	7.91358000	8.17732000	-0.68107700
H	9.13774300	7.34723500	-1.67725900
H	9.24310300	9.10518400	-1.42141900
C	10.19245100	10.93467200	1.44410900
H	9.91845700	11.49699200	2.36251700
C	11.72172900	11.06701400	1.27620200
H	12.30221300	10.57355100	2.08252100
H	12.02465800	12.13224600	1.26660700
H	12.06861500	10.61843200	0.32767500
C	9.47659000	11.63746000	0.26560200
H	9.74557400	11.17915600	-0.70449900
H	9.77194200	12.70420800	0.21358400
H	8.37576800	11.60566100	0.35560300
C	10.21752500	7.11702100	3.55732300
H	9.71654800	6.55431400	2.74381900
H	9.58678100	6.94972100	4.45821900
C	11.59832000	6.48609900	3.77675200
H	11.53300400	5.39134000	3.96946700
H	12.19860300	6.63365100	2.86251100
N	12.29389700	7.16921100	4.90492600

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Th(TREN^{TIPS})Br

Th	11.48527700	9.77611300	4.88622600
Br	10.49359300	12.47240700	4.87871400
Si	15.10505200	10.80664500	4.74639700
Si	10.01667700	9.41541500	8.28011600
Si	9.55627500	9.13027900	1.77369700
N	13.76433100	9.65856500	4.44728300
N	11.07535300	8.82057000	6.96219800
N	10.35480700	8.56444800	3.27188200
C	16.21030400	10.25664900	6.24638100
H	16.88139400	11.12536200	6.42449500
C	15.38793600	10.04018500	7.53377600
H	14.76399200	10.91396600	7.79586400
H	16.04499600	9.83056100	8.40220400
H	14.70565600	9.17614100	7.42338600
C	17.11954500	9.03291500	5.99068200
H	16.53001300	8.11264600	5.81444200
H	17.76470200	8.83273700	6.87039300
H	17.78742400	9.17295500	5.12144600
C	16.29468900	10.85552700	3.21567900
H	16.78162100	9.85592300	3.21849200
C	17.43235800	11.89310200	3.37625300
H	17.04658400	12.92929400	3.35169900
H	18.16603700	11.80332700	2.54952100
H	17.98962300	11.76846600	4.32324200
C	15.60677700	11.00597700	1.84084300
H	14.81106200	10.25476600	1.68948200
H	16.34252900	10.88402500	1.01989100
H	15.14507800	12.00195500	1.71948700
C	14.33545100	12.52807700	5.17008800
H	13.39128600	12.31882300	5.72356100
C	15.20828300	13.40200800	6.10330200
H	15.41459900	12.91875400	7.07398200
H	14.69796700	14.36244200	6.31494800
H	16.18185300	13.64678500	5.63865300
C	13.93861000	13.35042500	3.92111700
H	14.83501700	13.70617600	3.37890500
H	13.35199600	14.24194400	4.21528300
H	13.31813600	12.77723100	3.21176800
C	14.19797200	8.36551500	3.84857500

H	15.29676700	8.30357600	3.71087300
H	13.77035700	8.23618700	2.82964700
C	13.77551100	7.18380700	4.72978400
H	14.11518500	6.21030600	4.30934700
H	14.24082000	7.30287100	5.72401800
C	9.43244100	7.94690600	9.41036800
H	10.36050700	7.60071100	9.91531800
C	8.48198100	8.42910100	10.53314800
H	8.89962500	9.27718000	11.10533700
H	8.27793700	7.61167500	11.25405100
H	7.50562500	8.75092900	10.12578400
C	8.82732800	6.71876500	8.69321200
H	7.83924000	6.94574000	8.25517100
H	8.68212300	5.88165000	9.40617000
H	9.46816800	6.34774000	7.87356400
C	8.54221000	10.35923300	7.46727800
H	8.97645300	10.91559300	6.60713800
C	7.89690800	11.43133400	8.37807800
H	7.43589800	10.98436200	9.27907500
H	7.09432600	11.96669400	7.83274500
H	8.62390900	12.19070500	8.71498800
C	7.44972900	9.42014500	6.90444600
H	7.86346300	8.63368500	6.24609500
H	6.70673700	9.99234200	6.31510000
H	6.89656700	8.91509100	7.71830900
C	10.98496800	10.63171800	9.43352500
H	10.23380800	11.06409300	10.12993900
C	12.06926000	9.93994100	10.29126000
H	11.65381400	9.15587500	10.95031000
H	12.58511500	10.67527900	10.94176700
H	12.84666000	9.47066700	9.65859100
C	11.60459300	11.79942900	8.63613100
H	12.35741600	11.42985200	7.91074600
H	12.12876800	12.50955400	9.30771700
H	10.85785500	12.37350500	8.05958200
C	11.95489100	7.67842000	7.32132500
H	11.66399500	7.19725800	8.27643200
H	13.00739500	8.00557400	7.46847300
C	11.90599200	6.60272900	6.23138500
H	12.55259100	5.73078500	6.47890600
H	10.86750300	6.23849900	6.14595400

C	7.64149100	9.25116400	2.00511100
H	7.23848100	9.57636700	1.02137500
C	7.24759800	10.32132600	3.04574500
H	7.69600400	10.10471300	4.03346500
H	6.14777700	10.35269100	3.18541100
H	7.57333000	11.33612600	2.75574400
C	6.98090600	7.89656300	2.35082300
H	7.20604200	7.10926400	1.60661200
H	5.87763600	7.99551800	2.40048500
H	7.31541200	7.52850800	3.33918600
C	9.88273700	7.86694400	0.33334400
H	9.59265000	6.88061700	0.75646200
C	11.36337000	7.75429600	-0.09443400
H	11.69039900	8.65372200	-0.64811800
H	11.51837100	6.88685100	-0.76763300
H	12.04406600	7.63451000	0.76872700
C	8.98293000	8.08307000	-0.90661000
H	7.90814200	8.08754600	-0.65149500
H	9.14226600	7.27583800	-1.65016200
H	9.20745500	9.03859400	-1.41528100
C	10.19694800	10.91129800	1.42053600
H	9.90080800	11.48883200	2.32240600
C	11.72800300	11.05299500	1.28256100
H	12.29661000	10.57754700	2.10800500
H	12.02255200	12.12037800	1.26306000
H	12.09864600	10.59212500	0.34904900
C	9.50037300	11.58622400	0.21444600
H	9.79069000	11.11176600	-0.74177200
H	9.79008600	12.65370700	0.14794200
H	8.39821100	11.54909200	0.28426600
C	10.21343900	7.11703900	3.58113100
H	9.70262100	6.54815800	2.77834800
H	9.59147900	6.95963400	4.48983200
C	11.59597000	6.48791400	3.79359200
H	11.53403700	5.39437500	3.99349300
H	12.18976000	6.63155600	2.87448000
N	12.29611300	7.17962400	4.91382500

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Th(TRENTIPS)I

Th	11.46836900	9.84535700	4.94103900
I	10.37788600	12.81119700	4.91754900
Si	15.11429600	10.81629500	4.70019100
Si	10.01027200	9.38873500	8.33973800
Si	9.55660300	9.15021000	1.79476100
N	13.73132600	9.70549900	4.42951100
N	11.08984400	8.86559500	7.00745100
N	10.29604800	8.65925500	3.35237900
C	16.22766700	10.24497500	6.18496900
H	16.92832200	11.09528600	6.33585000
C	15.42771800	10.07385000	7.49290200
H	14.83383300	10.96941600	7.75141700
H	16.09731500	9.86220200	8.35109700
H	14.71986900	9.22721300	7.41487500
C	17.09441400	8.99149700	5.92645300
H	16.47511100	8.08743400	5.76920200
H	17.74888700	8.78011200	6.79658300
H	17.75073400	9.10337700	5.04442700
C	16.28327800	10.82316400	3.15104700
H	16.74891500	9.81365400	3.15229200
C	17.44530200	11.83616100	3.29306800
H	17.08204000	12.88031700	3.26979900
H	18.16596100	11.72720100	2.45726300
H	18.01185400	11.70226700	4.23318700
C	15.58070800	10.98346300	1.78472800
H	14.76295500	10.25324200	1.64922400
H	16.30144300	10.83646500	0.95466700
H	15.14441800	11.99067400	1.66326900
C	14.40766700	12.56258200	5.12378300
H	13.46198700	12.38503600	5.68692300
C	15.31441500	13.41820200	6.04212800
H	15.51524500	12.94023100	7.01672700
H	14.83402300	14.39515700	6.24762100
H	16.29056300	13.62987700	5.56677700
C	14.02602900	13.38908900	3.87258700
H	14.92885000	13.71424700	3.32230700
H	13.46924300	14.29966900	4.16604800
H	13.38287600	12.83102100	3.17131600
C	14.12552700	8.41295400	3.80056900
H	15.21707900	8.34053800	3.61873800
H	13.65721400	8.29844400	2.79815500

C	13.72759500	7.22622000	4.68468300
H	14.03685500	6.25437100	4.23832000
H	14.23774800	7.32683700	5.65856700
C	9.39616300	7.86752200	9.38114200
H	10.30989100	7.47139100	9.87486500
C	8.44295800	8.30822300	10.51870700
H	8.88232800	9.09654400	11.15658900
H	8.19487900	7.45101400	11.17685000
H	7.48747800	8.69608400	10.11951300
C	8.77049700	6.69792400	8.58898900
H	7.80545700	6.98347800	8.13518900
H	8.57507100	5.83328300	9.25554800
H	9.42245100	6.34277700	7.77115900
C	8.56684500	10.37926500	7.53555800
H	9.04445400	10.97115400	6.72227600
C	7.90183400	11.41964400	8.46846100
H	7.40803100	10.94199800	9.33575700
H	7.12304900	11.98482700	7.91901600
H	8.62415400	12.15824900	8.85765600
C	7.48363900	9.49444500	6.87544400
H	7.90984500	8.72255200	6.20765500
H	6.79166000	10.11314400	6.27101700
H	6.87033100	8.97473500	7.63527200
C	10.95899600	10.54168300	9.57259100
H	10.18811000	10.95104600	10.26131600
C	12.00934200	9.80538600	10.43632100
H	11.56776200	8.99937500	11.05097600
H	12.50978200	10.50964100	11.13167300
H	12.80339000	9.35510200	9.81015000
C	11.61617600	11.73454800	8.84604200
H	12.40345500	11.38545400	8.14840500
H	12.10601200	12.42117300	9.56591400
H	10.89792800	12.32926100	8.25357500
C	11.99911500	7.74022600	7.34709700
H	11.75234300	7.26579800	8.31803500
H	13.05042200	8.08574100	7.45142900
C	11.92595900	6.65729100	6.26706400
H	12.59378600	5.79587800	6.49229900
H	10.89101400	6.27791300	6.22201500
C	7.62811500	9.21214900	1.91809000
H	7.27690800	9.40995500	0.88203500

C	7.12594400	10.36941200	2.80929900
H	7.53456100	10.29998400	3.83493200
H	6.02030700	10.35067900	2.89419500
H	7.40840700	11.36068700	2.41284400
C	6.99236500	7.87687800	2.37155900
H	7.29920700	7.01878900	1.74332400
H	5.88586200	7.93435500	2.33018200
H	7.26301400	7.64035700	3.41774400
C	10.01580600	7.84311300	0.43155800
H	9.87846600	6.85587100	0.92384300
C	11.49008400	7.90963800	-0.02990700
H	11.67220000	8.80247700	-0.65631000
H	11.75382500	7.02544900	-0.64493700
H	12.19903800	7.95178100	0.81787600
C	9.07939600	7.84943200	-0.80109200
H	8.02142000	7.68696700	-0.52854500
H	9.36429400	7.04583100	-1.51018800
H	9.13736700	8.80464000	-1.35530400
C	10.15064800	10.93491100	1.39163000
H	9.74553700	11.54651700	2.22559800
C	11.67640800	11.16228000	1.37782900
H	12.19403300	10.79997900	2.29097400
H	11.90636200	12.24272400	1.29890300
H	12.16415700	10.65579200	0.52589900
C	9.53055300	11.49082800	0.08612000
H	9.93042500	10.97553300	-0.80779100
H	9.76738200	12.56733800	-0.02698700
H	8.42992000	11.39328200	0.06405000
C	10.12268700	7.22332400	3.70513000
H	9.53757100	6.65837700	2.95260100
H	9.55616600	7.11100100	4.65525000
C	11.49571900	6.55626900	3.84891000
H	11.41832700	5.46547400	4.05687000
H	12.04853200	6.68358700	2.90241800
N	12.25877700	7.23707900	4.93505100

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Pa(TREN^{TIPS})F

Pa	11.50856500	9.64863500	4.89036000
F	10.87370200	11.67575200	4.75453500

Si	10.07932900	9.61498100	8.27843000
Si	15.06465600	10.63494300	4.77427800
Si	9.51545400	8.88564100	1.89043400
N	11.10733200	8.89202400	7.00354300
N	13.75727700	9.44657100	4.53109600
N	10.36414700	8.36639000	3.37774100
N	12.27598800	7.03539700	5.08178400
C	8.96195700	8.21991800	9.03487200
H	9.68836700	7.50156300	9.47541200
C	8.13183400	7.43451100	7.99489600
H	7.29175200	8.04032100	7.60869100
H	7.69328000	6.52000400	8.44333000
H	8.74004200	7.12826900	7.12427000
C	8.05969200	8.69715200	10.19669400
H	8.62665700	9.22886000	10.98254900
H	7.55080000	7.83843000	10.67971400
H	7.26737700	9.37980100	9.83737200
C	9.10564800	11.08975200	7.49868500
H	9.88262700	11.69570800	6.98579400
C	8.43529600	12.02198700	8.53654200
H	7.64412600	11.50264600	9.10867900
H	7.95563300	12.88080700	8.02571200
H	9.15498900	12.43635300	9.26499700
C	8.07539900	10.67860900	6.42440700
H	8.49314600	9.98034300	5.67285300
H	7.70522500	11.56580300	5.87413300
H	7.19767400	10.17840100	6.87476800
C	11.12568800	10.35316500	9.73177100
H	10.37391000	10.82762000	10.39987900
C	12.08341500	11.46169000	9.24466700
H	12.83175700	11.05267200	8.53966600
H	12.63869500	11.91327000	10.09166700
H	11.55337600	12.27976400	8.72333200
C	11.89213400	9.31626500	10.58411600
H	11.23183100	8.51873800	10.97285800
H	12.36964400	9.80206400	11.45929000
H	12.70096200	8.83088100	10.00662100
C	11.88602600	7.70411700	7.44432600
H	11.52348900	7.28982200	8.40749500
H	12.95021100	7.97200300	7.61910900
C	11.80813800	6.56954800	6.41416300

H	12.39328600	5.68053200	6.74304700
H	10.75347100	6.25939900	6.31259800
C	14.24804100	12.30113600	5.32146000
H	13.37834600	12.00632600	5.95257600
C	13.69496900	13.14052200	4.14502600
H	14.51906400	13.54111100	3.52600500
H	13.11493400	14.00430300	4.52469600
H	13.02318400	12.56671100	3.48465000
C	15.15500700	13.19520100	6.20205100
H	15.47338800	12.69994200	7.13594400
H	14.61736000	14.12106800	6.48843900
H	16.06825300	13.50586900	5.66024200
C	16.32593200	10.10859800	6.15866500
H	16.94214500	11.02375100	6.29909100
C	15.65155200	9.79954800	7.51235300
H	14.96642000	10.60142800	7.84144800
H	16.40533100	9.65719300	8.31330500
H	15.05646900	8.86819300	7.45606100
C	17.30441700	8.96851900	5.79211500
H	16.78088100	7.99897500	5.68873600
H	18.06472800	8.83369600	6.58850600
H	17.84962200	9.15770800	4.84964800
C	16.11086300	10.78697300	3.14857500
H	16.62951500	9.80606400	3.07329700
C	17.21582400	11.86599500	3.23484200
H	16.78784200	12.88456200	3.29035600
H	17.86690400	11.83847300	2.33749000
H	17.86773000	11.73149900	4.11780900
C	15.28293700	10.94397100	1.85426300
H	14.49577100	10.17272800	1.77329900
H	15.93222400	10.85745100	0.95918100
H	14.78577000	11.92896000	1.80174300
C	14.21248600	8.13094300	4.00934000
H	15.31465700	8.06663900	3.90163700
H	13.81054700	7.94881200	2.98880700
C	13.75888100	7.00723400	4.95069900
H	14.09945400	6.00513200	4.60349600
H	14.19685100	7.18812200	5.94773500
C	7.61770400	8.48609000	1.94605400
H	7.21773600	9.01548800	1.05386400
C	6.92743600	9.08872900	3.18859800

H	7.27553600	8.59385900	4.11438200
H	5.82741400	8.95668900	3.13783400
H	7.12524300	10.17041500	3.30221000
C	7.22232600	6.99895500	1.79180200
H	7.67601200	6.52614100	0.90124500
H	6.12251700	6.89720400	1.69139800
H	7.51699500	6.40388500	2.67633300
C	9.68626200	10.80676400	1.73202200
H	9.51374900	11.19995100	2.75616400
C	8.61196600	11.46046900	0.82734100
H	8.68176200	11.10990300	-0.21937400
H	8.74541200	12.56067900	0.81107900
H	7.58338200	11.26155600	1.17735400
C	11.08912500	11.29005900	1.29522900
H	11.90666100	10.84769200	1.89774000
H	11.17057300	12.39046100	1.39329800
H	11.29258200	11.03808900	0.23736100
C	10.22915000	7.91137400	0.37229900
H	9.94703300	6.85459200	0.57465100
C	9.56399100	8.29766800	-0.97002200
H	8.46090200	8.23416500	-0.93249100
H	9.90505100	7.62983200	-1.78708200
H	9.82794700	9.32997500	-1.26737600
C	11.76728500	7.94227100	0.23764500
H	12.13010200	8.94109800	-0.06440700
H	12.11224100	7.22293000	-0.53276900
H	12.27015400	7.68663900	1.18789800
C	10.24671000	6.91012400	3.65081200
H	9.83758200	6.34319200	2.78880700
H	9.54032800	6.71969100	4.48831400
C	11.61631500	6.29899300	3.97124700
H	11.53487400	5.21540100	4.21660100
H	12.25583200	6.39240100	3.07687800

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Pa(TREN^{TIPS})Cl

Pa	11.48166800	9.69373800	4.94595600
Cl	10.58101000	12.18254500	4.94474700
Si	9.97557600	9.33758000	8.28388000
Si	15.05492800	10.72829700	4.79931800

Si	9.58395600	9.13051300	1.81997500
N	11.05640700	8.74800700	6.97254900
N	13.71189200	9.57315400	4.49473100
N	10.36726500	8.55329700	3.33072100
N	12.26516000	7.09637500	4.94804300
C	9.38025500	7.84788400	9.38408900
H	10.30191600	7.49142100	9.89340100
C	8.78086900	6.63290200	8.64034000
H	7.80249900	6.87207500	8.18767100
H	8.61824300	5.78754300	9.33970700
H	9.43359400	6.26800800	7.82754700
C	8.41834300	8.30951700	10.50566200
H	8.82927400	9.14726200	11.09755800
H	8.20903100	7.47841100	11.20920900
H	7.44543100	8.63683900	10.09486400
C	8.50231200	10.29838500	7.49015600
H	8.93940800	10.88240000	6.65243400
C	7.84371300	11.33189700	8.43675800
H	7.38059800	10.85136800	9.31896900
H	7.03996300	11.87932900	7.90507000
H	8.56229800	12.08501500	8.80444700
C	7.42000100	9.37187600	6.88942700
H	7.84527600	8.61650900	6.20278800
H	6.67510500	9.95987000	6.31830500
H	6.86683400	8.83290300	7.68131500
C	10.93619800	10.53155800	9.46545700
H	10.17802900	10.92971800	10.17490200
C	11.53742600	11.73168700	8.70232500
H	12.28879300	11.39292800	7.96161500
H	12.05191100	12.42801300	9.39559500
H	10.77982300	12.31178300	8.14609400
C	12.03141300	9.83219900	10.30282300
H	11.63089200	9.01586700	10.93151700
H	12.52803300	10.55473800	10.98195200
H	12.82186600	9.40398900	9.65753600
C	11.93633300	7.60960100	7.34705400
H	11.64106300	7.14330600	8.30748100
H	12.98769300	7.93904300	7.49065900
C	11.88459200	6.52374400	6.26781400
H	12.53592100	5.65643600	6.51788700
H	10.84734400	6.15523500	6.18950200

C	14.30316200	12.45891500	5.21146600
H	13.36801600	12.25356800	5.77843300
C	13.89306100	13.27131600	3.96023100
H	14.78289400	13.62423900	3.40528300
H	13.31098800	14.16583700	4.25516800
H	13.26546900	12.69305700	3.26129100
C	15.19462500	13.33594200	6.12426900
H	15.40848800	12.86158100	7.09781800
H	14.69255100	14.30159100	6.33237300
H	16.16427600	13.57085200	5.64667800
C	16.15329900	10.17343000	6.30140300
H	16.83589300	11.03505800	6.47021100
C	15.33110800	9.97902800	7.59198700
H	14.72919600	10.86790300	7.85339400
H	15.98646400	9.75448100	8.45803800
H	14.62607400	9.13350300	7.48408900
C	17.04685400	8.93695000	6.05234300
H	16.44637200	8.02271300	5.88175200
H	17.68953200	8.73416500	6.93323100
H	17.71646800	9.06363500	5.18236800
C	16.24986000	10.76121600	3.27075500
H	16.73809000	9.76249300	3.27992500
C	17.38620100	11.80040000	3.43324400
H	17.00006100	12.83609500	3.39943500
H	18.12469400	11.70528100	2.61144200
H	17.93783600	11.68180700	4.38425100
C	15.57119500	10.90794300	1.89117100
H	14.78422600	10.14983400	1.73078900
H	16.31517400	10.79505400	1.07632300
H	15.10047200	11.89934700	1.76820800
C	14.14855000	8.29131200	3.87247600
H	15.24695400	8.24076400	3.73163800
H	13.71518400	8.17541800	2.85547600
C	13.73926800	7.09757100	4.74299500
H	14.07059200	6.12993900	4.30337300
H	14.21886600	7.20139000	5.73204600
C	7.66819800	9.25353200	2.04453600
H	7.27700400	9.58012700	1.05646900
C	7.27333200	10.32850200	3.08004700
H	7.70711000	10.10503800	4.07214800
H	6.17199200	10.37464100	3.20320000

H	7.61702900	11.33857400	2.79403000
C	6.99118900	7.90586100	2.38443500
H	7.21800000	7.11488800	1.64460500
H	5.88841900	8.01613300	2.41884800
H	7.30813500	7.53737100	3.37814100
C	10.22481100	10.90570600	1.43786800
H	9.97383000	11.48426900	2.35166200
C	9.48267500	11.58615700	0.26174500
H	9.72607300	11.10833800	-0.70575300
H	9.78423500	12.64949100	0.18164200
H	8.38401700	11.56481800	0.37763900
C	11.75003100	11.02829300	1.23369800
H	12.33111300	10.55034100	2.04704500
H	12.05428300	12.09297500	1.19633900
H	12.07567800	10.56304900	0.28537400
C	9.91051800	7.84736200	0.39573400
H	9.58720100	6.87267400	0.82095500
C	9.03931100	8.07462600	-0.86269400
H	7.96061500	8.11335800	-0.62748700
H	9.18850300	7.25406700	-1.59364900
H	9.30146400	9.01663800	-1.37830000
C	11.39463800	7.69079600	-0.00527200
H	11.75262100	8.57037600	-0.57061200
H	11.53907800	6.80604800	-0.65800300
H	12.05845900	7.57372600	0.87108900
C	10.17441300	7.10964800	3.64159400
H	9.62886200	6.56565700	2.84541800
H	9.56184200	6.97683500	4.55971900
C	11.53611800	6.43115900	3.83247900
H	11.43981700	5.33992900	4.02961100
H	12.12572600	6.55850400	2.90867800

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Pa(TREN^{TIPS})Br

Pa	11.47300000	9.72026300	4.94818300
Br	10.50833500	12.36794800	4.91715000
Si	9.96706400	9.34534800	8.27947600
Si	15.05534700	10.72493800	4.80075500
Si	9.59004700	9.12452500	1.82328800
N	11.05697000	8.76508600	6.96928900

N	13.70060900	9.58011700	4.49680500
N	10.35967200	8.56482100	3.35007500
N	12.25817900	7.10191200	4.95393400
C	9.38306100	7.85397300	9.38347900
H	10.30663600	7.50597400	9.89515400
C	8.79258500	6.63103700	8.64573300
H	7.81316200	6.86064400	8.19032100
H	8.63459500	5.78889900	9.35000300
H	9.44910500	6.26532600	7.83652100
C	8.41681700	8.31401600	10.50210700
H	8.81953200	9.15962300	11.08837900
H	8.21528900	7.48564400	11.21106900
H	7.44097600	8.62921800	10.08885200
C	8.48524400	10.28833700	7.48020300
H	8.91731400	10.87814000	6.64356900
C	7.81341900	11.31637200	8.42290100
H	7.35017200	10.83253500	9.30318300
H	7.00801400	11.85728300	7.88718000
H	8.52462900	12.07508700	8.79341400
C	7.41662700	9.34957800	6.87456000
H	7.85490600	8.59719300	6.19271100
H	6.67020700	9.92865700	6.29639700
H	6.86346200	8.80648700	7.66360700
C	10.91930200	10.54776200	9.46019400
H	10.15839600	10.94499800	10.16712700
C	11.51882900	11.74886200	8.69786300
H	12.26921700	11.41272700	7.95450500
H	12.03557000	12.44325500	9.39139900
H	10.76052600	12.33071700	8.14472200
C	12.01473200	9.85337100	10.30157200
H	11.61539700	9.03700600	10.93083400
H	12.50713400	10.57896600	10.98046500
H	12.80826000	9.42659900	9.65911100
C	11.94207600	7.63118400	7.34887700
H	11.65600800	7.17379500	8.31631400
H	12.99296900	7.96577600	7.48125900
C	11.88747900	6.53684100	6.27872500
H	12.54277800	5.67368200	6.53329300
H	10.85139500	6.16339300	6.20985500
C	14.31961900	12.46157100	5.21658300
H	13.37448600	12.26595600	5.77114600

C	13.93485800	13.28627200	3.96540600
H	14.83567200	13.63063300	3.42322200
H	13.36036500	14.18615600	4.25866800
H	13.30738100	12.72041800	3.25641300
C	15.20993400	13.32310800	6.14516800
H	15.40323600	12.84344800	7.12041900
H	14.71811000	14.29497900	6.34849500
H	16.18953000	13.54587300	5.68219200
C	16.15239600	10.16103900	6.29988500
H	16.83903300	11.01977400	6.46702000
C	15.33358600	9.97023600	7.59308700
H	14.72688400	10.85704500	7.85066700
H	15.99177100	9.75456600	8.45918700
H	14.63403700	9.11954800	7.49209700
C	17.04013800	8.92096800	6.04807000
H	16.43551900	8.00969800	5.87636300
H	17.68282400	8.71390600	6.92794000
H	17.70939400	9.04628200	5.17765100
C	16.24889300	10.75138000	3.27098500
H	16.72855000	9.74854600	3.27696400
C	17.39489000	11.77965200	3.43600500
H	17.01859900	12.81907300	3.40712800
H	18.13117700	11.68093700	2.61266100
H	17.94694700	11.65199200	4.38558500
C	15.57046300	10.90775000	1.89238200
H	14.77320400	10.16019600	1.73318900
H	16.31164800	10.78516900	1.07644300
H	15.11287000	11.90538000	1.77060800
C	14.13206100	8.29871200	3.86740200
H	15.22894300	8.24878300	3.71547500
H	13.68907500	8.18686000	2.85411700
C	13.72939400	7.10238600	4.73682500
H	14.05891600	6.13691300	4.29076100
H	14.21765700	7.20237000	5.72205200
C	7.67332900	9.24662100	2.03386100
H	7.28917000	9.54620700	1.03456800
C	7.26696400	10.34660600	3.03833600
H	7.70437000	10.15914300	4.03637900
H	6.16524200	10.38256100	3.16104400
H	7.59797500	11.35189600	2.72247800
C	6.99828600	7.90569800	2.40333000

H	7.24051200	7.09431700	1.69083800
H	5.89458400	8.01063000	2.41791200
H	7.30208400	7.56865700	3.41213500
C	10.22591200	10.89642100	1.42463600
H	9.93835300	11.49129000	2.31704200
C	9.51284100	11.53962100	0.21012300
H	9.78846100	11.04054300	-0.73797400
H	9.80646700	12.60367500	0.11218900
H	8.41151500	11.51009600	0.29517400
C	11.75451300	11.03783700	1.26729600
H	12.31851100	10.58096100	2.10457700
H	12.04481600	12.10601300	1.22317800
H	12.11684800	10.56155400	0.33831600
C	9.94015100	7.82851900	0.41630200
H	9.67765000	6.84660100	0.86662900
C	9.03082700	7.98790200	-0.82596800
H	7.95650100	7.96451600	-0.57001900
H	9.21494100	7.16832900	-1.55003800
H	9.22480600	8.93724000	-1.35872800
C	11.42055100	7.74036500	-0.02034900
H	11.71416700	8.62214900	-0.61886000
H	11.59448800	6.84761800	-0.65468800
H	12.11442200	7.68250100	0.83876500
C	10.15668000	7.12456800	3.67264900
H	9.58947000	6.58212300	2.89084000
H	9.55910500	7.00568700	4.60224900
C	11.51600100	6.43729100	3.84756500
H	11.41499000	5.34669800	4.04665100
H	12.09559400	6.55995500	2.91659200

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Pa(TREN^{TIPS})I

Pa	11.44596200	9.78763700	4.97352100
I	10.37940200	12.69214700	4.93531900
Si	9.96207000	9.34898500	8.34059700
Si	15.06109200	10.73151900	4.75781000
Si	9.57499200	9.11583000	1.82190100
N	11.05534100	8.84281400	7.00271300
N	13.65978600	9.63973900	4.45929400
N	10.30217500	8.64275800	3.40117600

N	12.21928800	7.17476100	4.97101900
C	9.36295800	7.80700900	9.36258500
H	10.28129100	7.40501500	9.84258700
C	8.73085200	6.64777200	8.56068000
H	7.76535700	6.94098600	8.11309600
H	8.53544700	5.77690200	9.21909400
H	9.37874300	6.29874500	7.73726600
C	8.41913400	8.22752300	10.51588000
H	8.86193800	9.00634100	11.16293100
H	8.18010800	7.35858700	11.16186000
H	7.45878700	8.61863000	10.13213300
C	8.50389600	10.34352800	7.57253200
H	8.97074400	10.94838300	6.76530300
C	7.84355100	11.35853000	8.53687000
H	7.36847300	10.86136300	9.40353100
H	7.04985200	11.92439900	8.00973900
H	8.56384000	12.09848000	8.92760000
C	7.41979500	9.46532700	6.90615600
H	7.84700100	8.71698800	6.21302900
H	6.71620300	10.09342000	6.32512900
H	6.81933900	8.92162300	7.65953200
C	10.91459100	10.48230200	9.58891100
H	10.13986500	10.87039600	10.28575400
C	11.56149900	11.69557700	8.88760300
H	12.34026600	11.36739600	8.17131700
H	12.05306100	12.36508400	9.62236100
H	10.83493200	12.30115800	8.31693400
C	11.97062700	9.73946000	10.44000100
H	11.53722400	8.91510700	11.03609100
H	12.45952900	10.43509100	11.15195400
H	12.77257500	9.31295400	9.80761500
C	11.99129300	7.74220200	7.36188100
H	11.77083400	7.30116700	8.35387600
H	13.03585100	8.11107500	7.42961700
C	11.91342900	6.62436400	6.31894800
H	12.59619100	5.77921500	6.55891900
H	10.88352700	6.23011400	6.29962500
C	14.38283600	12.47573300	5.22840300
H	13.43486900	12.29129600	5.78324400
C	14.01468600	13.33825000	3.99826200
H	14.91993500	13.65069200	3.44504200

H	13.48572700	14.25726800	4.31658100
H	13.34770500	12.81264300	3.29399000
C	15.30077300	13.29166100	6.17135900
H	15.48904200	12.78582900	7.13479000
H	14.83486400	14.27049100	6.40026800
H	16.28269000	13.50115700	5.70665500
C	16.20040400	10.11743700	6.20543900
H	16.88898500	10.97768700	6.35567600
C	15.44898300	9.90031000	7.53537800
H	14.77717100	10.73849400	7.79471400
H	16.15658500	9.76634000	8.37851300
H	14.82704600	8.98693800	7.48944100
C	17.08500800	8.88783500	5.89673600
H	16.47934500	7.97616400	5.72921200
H	17.76064700	8.66712400	6.74821700
H	17.72163700	9.03373800	5.00560000
C	16.21666800	10.76360000	3.19636900
H	16.67420500	9.75071700	3.16918600
C	17.39012400	11.76142600	3.35673800
H	17.03841800	12.80962400	3.36404100
H	18.10185800	11.66668900	2.51158800
H	17.96435400	11.59725700	4.28733000
C	15.51186200	10.96323700	1.83703100
H	14.69505600	10.23640200	1.68216000
H	16.23222400	10.83948500	1.00285200
H	15.07421100	11.97272500	1.74324800
C	14.04300400	8.35950800	3.79629700
H	15.12863500	8.30194500	3.58113500
H	13.54232400	8.25799800	2.80935900
C	13.67841400	7.16305000	4.68102100
H	13.97544900	6.19560500	4.21783100
H	14.21647200	7.25696000	5.64054900
C	7.64821900	9.21447200	1.95455500
H	7.30846800	9.42250000	0.91653300
C	7.16884100	10.38303800	2.84393100
H	7.54487800	10.28482500	3.87906500
H	6.06125200	10.40855800	2.89583300
H	7.50403000	11.36636100	2.46920100
C	6.97282000	7.89647400	2.40055400
H	7.27107400	7.02905100	1.78120900
H	5.86908500	7.98057700	2.33742200

H	7.21606500	7.65825000	3.45295500
C	10.20088800	10.87161600	1.35340300
H	9.88624200	11.49675900	2.21582900
C	9.50508400	11.45320400	0.09815000
H	9.81325200	10.92360700	-0.82337900
H	9.78099000	12.51815600	-0.03456200
H	8.40291600	11.40548600	0.15845300
C	11.72991700	11.03298600	1.22377700
H	12.28278900	10.60544800	2.08319200
H	12.00369600	12.10470100	1.16314100
H	12.11803400	10.54295100	0.31271300
C	9.99813300	7.74923900	0.50377700
H	9.79263700	6.78302900	1.01430800
C	9.08850400	7.77825700	-0.74903800
H	8.01732400	7.68143400	-0.49769400
H	9.34327400	6.94349200	-1.43309100
H	9.21244200	8.71522300	-1.32303700
C	11.48206100	7.72012900	0.06876300
H	11.71916200	8.56948600	-0.59792100
H	11.71106700	6.79369000	-0.49586100
H	12.17988100	7.77281300	0.92508900
C	10.07113700	7.21896600	3.77965000
H	9.45003900	6.67560400	3.04179800
H	9.51573700	7.14570200	4.73891200
C	11.41869700	6.50098600	3.91036300
H	11.30428600	5.41822000	4.13973800
H	11.96036000	6.59088900	2.95342700

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U(TREN^{TIPS})F

U	11.53169400	9.58908500	4.88055100
F	11.02444100	11.63534700	4.95461900
Si	10.04015600	9.61986400	8.26045100
Si	15.09593000	10.64323200	4.74159700
Si	9.49603700	8.86329400	1.94064100
N	11.07388400	8.89505000	6.99523300
N	13.77880200	9.46465200	4.49919000
N	10.34918400	8.29573400	3.39919800
N	12.27994000	7.04903100	5.06883500
C	8.94472800	8.21640200	9.03505300

H	9.68348700	7.49794100	9.45412800
C	8.09798100	7.43711700	8.00381600
H	7.24585400	8.04224600	7.64267600
H	7.67399100	6.51450400	8.44975200
H	8.68985800	7.14562600	7.11689800
C	8.06455800	8.67621300	10.22039000
H	8.64569900	9.20099200	11.00044100
H	7.56907800	7.80972400	10.70369800
H	7.26279300	9.36018800	9.88625000
C	9.04824300	11.06542300	7.45682200
H	9.82818200	11.70561200	6.99583000
C	8.28522000	11.95012100	8.47131700
H	7.47513500	11.39409500	8.97876700
H	7.81303100	12.80892400	7.95303000
H	8.94472800	12.36569100	9.25482200
C	8.09809900	10.63338800	6.31950500
H	8.58118000	9.96681700	5.57827400
H	7.72118300	11.51533200	5.76489100
H	7.21833500	10.08699500	6.70779700
C	11.07724000	10.39056200	9.70385300
H	10.32095400	10.84979600	10.37744200
C	12.00612400	11.52007700	9.20862400
H	12.75776100	11.12989700	8.49638300
H	12.55885800	11.98235100	10.05155200
H	11.45270700	12.32624000	8.69360500
C	11.87311800	9.37047400	10.54962200
H	11.23387300	8.55983500	10.94685000
H	12.35106500	9.86674300	11.41871500
H	12.68466400	8.90098600	9.96281900
C	11.86044000	7.71277400	7.43329700
H	11.49809000	7.28919600	8.39276300
H	12.92167800	7.98885900	7.61810100
C	11.80175800	6.58029300	6.40030000
H	12.39178800	5.69562000	6.73210400
H	10.75088600	6.26181700	6.28675700
C	14.31057500	12.33120500	5.26222500
H	13.44948400	12.06992500	5.91525400
C	13.74648000	13.14399300	4.07273700
H	14.56308200	13.52115200	3.42900100
H	13.17990600	14.02283800	4.43816900
H	13.05949400	12.55692500	3.44095800

C	15.25014400	13.23608500	6.09671600
H	15.57991300	12.76409600	7.03879400
H	14.73185100	14.17786900	6.36695300
H	16.15699200	13.51744800	5.52897900
C	16.33163700	10.11517800	6.14786300
H	16.97481900	11.01451200	6.26727700
C	15.63392400	9.86775400	7.50269500
H	14.97797300	10.70396000	7.80509800
H	16.37440200	9.71695700	8.31444300
H	15.00369300	8.95864200	7.46462900
C	17.27587800	8.93491000	5.82312700
H	16.72351100	7.97894200	5.74722700
H	18.02852300	8.80187100	6.62708700
H	17.83044100	9.07791300	4.87791800
C	16.16031500	10.75758500	3.12273000
H	16.66997900	9.77058300	3.06744600
C	17.27589100	11.82623500	3.19900500
H	16.85861100	12.85024900	3.22841900
H	17.93617000	11.77288800	2.30948800
H	17.91708900	11.70318000	4.09146500
C	15.34493400	10.90203100	1.81884200
H	14.55614800	10.13225200	1.73927000
H	16.00207400	10.80219700	0.93085400
H	14.85181900	11.88821900	1.74957300
C	14.22842000	8.13837500	4.00120200
H	15.33047200	8.06445200	3.89551800
H	13.82740100	7.94002700	2.98315500
C	13.76796400	7.03138300	4.95957200
H	14.11928200	6.02357900	4.64066800
H	14.18960600	7.23707800	5.95887900
C	7.59604400	8.47196700	1.96885900
H	7.19750100	9.02890100	1.09248000
C	6.89286800	9.02588700	3.22655000
H	7.23744000	8.50284100	4.13798200
H	5.79436500	8.88711200	3.16237900
H	7.08041400	10.10467700	3.37755700
C	7.21307700	6.98749400	1.76345300
H	7.66165300	6.55250200	0.85160800
H	6.11328000	6.87864900	1.67107900
H	7.52398500	6.36343200	2.62221400
C	9.70344300	10.78566400	1.89358800

H	9.54803500	11.12216500	2.94229600
C	8.63900600	11.51912100	1.04135900
H	8.69924300	11.23344600	-0.02544500
H	8.79199200	12.61556700	1.09429600
H	7.60885900	11.31519400	1.38301500
C	11.11386500	11.26173000	1.47194400
H	11.93253900	10.76322800	2.02876400
H	11.22552400	12.35076300	1.63863600
H	11.29860500	11.07181300	0.39799600
C	10.19862900	7.95473700	0.37645000
H	9.90605800	6.89306500	0.53456200
C	9.53561300	8.40507400	-0.94701600
H	8.43233000	8.34384200	-0.91291600
H	9.87442400	7.77457900	-1.79415100
H	9.80313300	9.44918600	-1.19664300
C	11.73689900	7.97280300	0.23965200
H	12.11211400	8.97600100	-0.03197000
H	12.07236500	7.27477600	-0.55412300
H	12.23826900	7.67971200	1.17987200
C	10.26815100	6.83508400	3.62737300
H	9.89595600	6.27040700	2.74573500
H	9.55368700	6.60126300	4.44730200
C	11.65421300	6.27411100	3.96120400
H	11.61592800	5.19116500	4.21996200
H	12.29735500	6.38329200	3.07130100

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U(TREN^{TIPS})Cl

U	11.48948600	9.66547800	4.95327200
Cl	10.51465100	12.11537500	4.93658400
Si	9.97647400	9.37650200	8.31147900
Si	15.04610200	10.66798500	4.78370600
Si	9.57799800	9.13982000	1.80588000
N	11.05766300	8.79333900	7.00097600
N	13.70964300	9.51594200	4.46499600
N	10.34378400	8.58807700	3.32769700
N	12.24395900	7.11423800	4.94947900
C	9.41818900	7.89593400	9.44130900
H	10.35210200	7.55734300	9.94100600
C	8.82108300	6.66370400	8.72465200

H	7.83421400	6.88564500	8.28115800
H	8.67567600	5.82815600	9.43944000
H	9.46731100	6.29178300	7.90997200
C	8.46646500	8.36391000	10.56884100
H	8.87359900	9.21799600	11.13945300
H	8.27807100	7.54298400	11.28999600
H	7.48385300	8.67074400	10.16531600
C	8.49077900	10.29852000	7.49825400
H	8.93503000	10.89059400	6.67038300
C	7.79259200	11.31824100	8.43026300
H	7.30980300	10.82760800	9.29628200
H	6.99828500	11.86027000	7.87920100
H	8.49212100	12.07671700	8.82313500
C	7.44219100	9.34863200	6.87519600
H	7.89897200	8.59365500	6.20827900
H	6.70383100	9.91782500	6.27701100
H	6.87575300	8.80678900	7.65586000
C	10.92594900	10.60738300	9.46486200
H	10.16648000	11.01250100	10.16876700
C	11.51094800	11.79742300	8.67493600
H	12.27886100	11.45421400	7.95329300
H	12.00562800	12.52238400	9.35287000
H	10.74925100	12.34660400	8.09354200
C	12.03099500	9.93555400	10.31123500
H	11.63915200	9.13172000	10.96088100
H	12.52752100	10.67663700	10.97013600
H	12.81975900	9.49642500	9.67091600
C	11.94415200	7.65255800	7.35335700
H	11.67956600	7.19125000	8.32569100
H	12.99842800	7.98425400	7.46195900
C	11.86217300	6.56061300	6.28074300
H	12.49697600	5.68134100	6.53169200
H	10.81701400	6.21241700	6.21538900
C	14.26987200	12.36727800	5.28246300
H	13.33005400	12.12677000	5.82953400
C	13.86327500	13.24054200	4.07186100
H	14.75525000	13.61186200	3.53284700
H	13.28738900	14.12371600	4.40974200
H	13.23075700	12.69918700	3.34956700
C	15.14274800	13.20817700	6.24608900
H	15.36073400	12.68986200	7.19617400

H	14.62621900	14.15518700	6.49935400
H	16.11057200	13.48058100	5.78406400
C	16.19766700	10.08755800	6.23860200
H	16.84622100	10.97210100	6.42203000
C	15.43052700	9.80542900	7.54750100
H	14.73071400	10.61567000	7.82235300
H	16.12701700	9.66515500	8.39894100
H	14.83624500	8.87634200	7.46051100
C	17.13825100	8.90266200	5.92066500
H	16.57269000	7.96930700	5.73495500
H	17.81531300	8.69869100	6.77531000
H	17.77575800	9.08852900	5.03746900
C	16.20803600	10.78181400	3.23489200
H	16.69652900	9.78379900	3.19260100
C	17.34597500	11.81596300	3.41579900
H	16.95712800	12.85087800	3.44410300
H	18.06101700	11.76398000	2.56968200
H	17.92532500	11.65339300	4.34361500
C	15.49997600	10.98020800	1.87688300
H	14.70625800	10.23081800	1.70947600
H	16.22547300	10.89222200	1.04256200
H	15.03194100	11.97749400	1.79765200
C	14.14975000	8.23672100	3.84890400
H	15.24915700	8.17161500	3.71110100
H	13.71722100	8.12163000	2.83147200
C	13.71630600	7.05948300	4.72760900
H	14.00843600	6.07755500	4.29153400
H	14.21046100	7.15213800	5.71061200
C	7.65513800	9.24193600	1.97230000
H	7.29818100	9.52415100	0.95784100
C	7.20031300	10.34816300	2.94878300
H	7.60481300	10.18094900	3.96397200
H	6.09450800	10.37044100	3.03264000
H	7.52726800	11.35354100	2.62911700
C	6.98617200	7.89644900	2.33726500
H	7.26463000	7.07816800	1.64621800
H	5.88121000	7.98541600	2.31187800
H	7.25911000	7.57826700	3.36091900
C	10.20833400	10.91888400	1.44105700
H	9.84455100	11.51359000	2.30452000
C	9.58516900	11.53719600	0.16670100

H	9.94501300	11.03320400	-0.75024700
H	9.86399200	12.60620500	0.07855400
H	8.48100200	11.48566400	0.16503400
C	11.74209500	11.07520800	1.40502300
H	12.24854600	10.65024300	2.29608400
H	12.02680700	12.14455900	1.35503400
H	12.18635600	10.57523600	0.52556300
C	9.96541300	7.85819000	0.39502900
H	9.74770100	6.86630600	0.84883800
C	9.04972700	7.97533500	-0.84755800
H	7.97769000	7.89161300	-0.59435800
H	9.27923000	7.17126300	-1.57616000
H	9.19261400	8.93711500	-1.37453900
C	11.44729700	7.83476700	-0.04592100
H	11.69998000	8.73291700	-0.63954100
H	11.65684300	6.95517200	-0.68800800
H	12.14600500	7.79976200	0.81075300
C	10.13267300	7.15512600	3.67141600
H	9.55572800	6.60571400	2.90063700
H	9.53594400	7.05109100	4.60472500
C	11.48443400	6.45341600	3.84799600
H	11.37248600	5.36488900	4.05331300
H	12.06242800	6.56635100	2.91494800

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U(TREN^{TIPS})Br

U	11.48528200	9.68143900	4.96181400
Br	10.44383900	12.28444400	4.92165000
Si	9.96253100	9.36732100	8.31721500
Si	15.04377700	10.68138100	4.77922500
Si	9.59023000	9.14282500	1.80134600
N	11.05547000	8.80429100	7.00546300
N	13.70049800	9.53267100	4.46439100
N	10.34816800	8.60587100	3.33494700
N	12.24252500	7.12879000	4.95681000
C	9.41777300	7.87432900	9.43812100
H	10.35365600	7.53820200	9.93576100
C	8.82760100	6.64171300	8.71637700
H	7.84014900	6.85987300	8.27244000
H	8.68564000	5.80325100	9.42843900

H	9.47669500	6.27499700	7.90160900
C	8.46395800	8.33033700	10.56891300
H	8.86817200	9.18115600	11.14638000
H	8.27857100	7.50300400	11.28347200
H	7.48030700	8.63686000	10.16775300
C	8.46662300	10.27493500	7.50743600
H	8.90452900	10.87400400	6.68082500
C	7.76083400	11.28657100	8.44211900
H	7.28177600	10.78995800	9.30678300
H	6.96276100	11.82434600	7.89248100
H	8.45510400	12.04877400	8.83700400
C	7.42684100	9.31853200	6.88012100
H	7.89099800	8.56955200	6.21147700
H	6.68597800	9.88421600	6.28173200
H	6.86282200	8.76966500	7.65762100
C	10.90265900	10.59751400	9.47979000
H	10.14059000	10.99132900	10.18719000
C	11.48139500	11.79880800	8.70275200
H	12.23612200	11.46719600	7.96194000
H	11.98963200	12.50823700	9.38715500
H	10.71347500	12.36264300	8.14441600
C	12.01139800	9.92390200	10.32026300
H	11.62424300	9.11208400	10.96270500
H	12.50327200	10.66204400	10.98585100
H	12.80299700	9.49525700	9.67635800
C	11.95205800	7.67131400	7.35839300
H	11.69821600	7.21396400	8.33531000
H	13.00446100	8.01112900	7.45795000
C	11.87093100	6.57510400	6.29078200
H	12.51263600	5.70065500	6.54064900
H	10.82788100	6.21990100	6.23171600
C	14.28036200	12.39147400	5.25787900
H	13.33338400	12.16654900	5.79956600
C	13.89091200	13.25648200	4.03584100
H	14.78963000	13.61303700	3.49814200
H	13.32205000	14.14882300	4.36128300
H	13.25521100	12.71462700	3.31639700
C	15.15384500	13.23195900	6.22112000
H	15.35544900	12.72043500	7.17844200
H	14.64580200	14.18736100	6.45941600
H	16.12966800	13.48822900	5.76687000

C	16.18480000	10.10430500	6.24353400
H	16.84003100	10.98513400	6.42090200
C	15.41082800	9.84111800	7.55231600
H	14.71394900	10.65774100	7.81551700
H	16.10308400	9.70654900	8.40810400
H	14.81262900	8.91398000	7.47303100
C	17.11640200	8.90866900	5.93997800
H	16.54379400	7.97911800	5.75646800
H	17.78573000	8.70440400	6.80058700
H	17.76148800	9.08291300	5.05998200
C	16.21523000	10.77196900	3.23561500
H	16.69938300	9.77147500	3.20631300
C	17.35766100	11.80174600	3.41457600
H	16.97500700	12.83920700	3.42742800
H	18.07941600	11.73552500	2.57520400
H	17.92814800	11.64663200	4.34908800
C	15.51826800	10.96115400	1.87065700
H	14.72504900	10.21152300	1.70216200
H	16.25038100	10.86590100	1.04294800
H	15.05207500	11.95830100	1.78037200
C	14.13956100	8.25389600	3.84560100
H	15.23824800	8.19110300	3.70252100
H	13.70184100	8.13881600	2.83052300
C	13.71316300	7.07584000	4.72583800
H	14.00421300	6.09471000	4.28745500
H	14.21290100	7.16861200	5.70596700
C	7.67002000	9.27021200	1.97771900
H	7.30918200	9.54462600	0.96249700
C	7.23796900	10.39391200	2.94472200
H	7.65063200	10.23438600	3.95792900
H	6.13334400	10.43069200	3.03801300
H	7.57527300	11.39125300	2.61100100
C	6.98725700	7.93795200	2.36462600
H	7.25507700	7.10621400	1.68548000
H	5.88330400	8.03867100	2.34079500
H	7.25929600	7.63299100	3.39253600
C	10.24326700	10.90527300	1.40566200
H	9.88782500	11.51709600	2.26048900
C	9.62756100	11.51458000	0.12364800
H	9.97744800	10.99313900	-0.78742000
H	9.92261400	12.57789700	0.02079700

H	8.52267100	11.48018900	0.12556700
C	11.77907900	11.03899600	1.36944100
H	12.27853500	10.61054100	2.26251000
H	12.07964800	12.10359900	1.31246800
H	12.21496200	10.52705400	0.49267900
C	9.96070700	7.83467200	0.40964400
H	9.74341300	6.85010000	0.87909800
C	9.03294900	7.93939800	-0.82522300
H	7.96328800	7.86310300	-0.56009800
H	9.25220300	7.12530700	-1.54577900
H	9.17423900	8.89400800	-1.36549800
C	11.43784000	7.79853100	-0.04654400
H	11.68714700	8.68467000	-0.65938900
H	11.63736200	6.90661100	-0.67463700
H	12.14596200	7.77673000	0.80277000
C	10.12691100	7.17718600	3.69151700
H	9.53656900	6.62871600	2.93067300
H	9.53850600	7.08557600	4.63142100
C	11.47493800	6.46698100	3.86146200
H	11.35817400	5.38004600	4.07168300
H	12.04836000	6.57328800	2.92485600

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U(TREN^{TIPS})I

U	11.43158800	9.71804500	4.95834200
I	10.38736200	12.63281300	4.86343300
Si	10.01947700	9.31601900	8.32703900
Si	15.04663200	10.76800700	4.81107300
Si	9.53381100	9.10919300	1.80159300
N	11.10707000	8.77468700	6.99853700
N	13.65689100	9.66444100	4.51084600
N	10.25652200	8.62940700	3.37837600
N	12.20665000	7.17049000	4.94125300
C	9.39464500	7.80125400	9.37386700
H	10.30382400	7.40199700	9.87287700
C	8.76279700	6.63190400	8.58626600
H	7.80291300	6.92314700	8.12528300
H	8.55617900	5.77352000	9.25750900
H	9.41612000	6.26521600	7.77471900
C	8.44072800	8.25356200	10.50636200

H	8.88175700	9.04414800	11.14014700
H	8.18862300	7.40121800	11.16929400
H	7.48739800	8.64204900	10.10299300
C	8.57678200	10.31319200	7.53228700
H	9.05344900	10.90270000	6.71814600
C	7.92020300	11.35277500	8.47256600
H	7.42699000	10.87554200	9.34038600
H	7.14200300	11.92281100	7.92725500
H	8.64677100	12.08756000	8.86113000
C	7.48585400	9.43684000	6.87382100
H	7.90479700	8.66757300	6.19851600
H	6.79493200	10.06294600	6.27582500
H	6.87282900	8.91550700	7.63283300
C	10.97920100	10.46315800	9.55549800
H	10.21116500	10.86619400	10.25119600
C	11.62628300	11.66130600	8.82902200
H	12.39971700	11.31764200	8.11420500
H	12.12757600	12.34091800	9.54770600
H	10.89812500	12.26112300	8.25418700
C	12.03671500	9.72489100	10.40836000
H	11.60124100	8.91419900	11.02124900
H	12.53866300	10.42708700	11.10465400
H	12.82851300	9.28070500	9.77534800
C	11.98482100	7.63205600	7.35688200
H	11.71068000	7.15678200	8.32026400
H	13.03891500	7.95901800	7.47942800
C	11.89928600	6.56351100	6.26635400
H	12.57268000	5.70011800	6.46565500
H	10.86505100	6.18114700	6.23004800
C	14.35963600	12.50902500	5.28137700
H	13.40800000	12.32472300	5.82872300
C	13.99714200	13.37451500	4.05149100
H	14.90412200	13.68250200	3.49851400
H	13.47406800	14.29649000	4.37124100
H	13.32402400	12.85402700	3.34997300
C	15.27464300	13.32511800	6.22742300
H	15.46352500	12.81940300	7.19069800
H	14.80673600	14.30295000	6.45670000
H	16.25656500	13.53714700	5.76396300
C	16.16719700	10.14675200	6.26954300
H	16.86829600	10.99360100	6.43658800

C	15.38322200	9.93817600	7.58133500
H	14.78419600	10.82153300	7.86705900
H	16.06504700	9.71206100	8.42611500
H	14.68198500	9.08776500	7.49090600
C	17.03315700	8.90270100	5.96633900
H	16.41417900	8.00256500	5.78622100
H	17.69434300	8.66602000	6.82479900
H	17.68292000	9.04229000	5.08350100
C	16.21028100	10.80597700	3.25631500
H	16.66561100	9.79204300	3.22675600
C	17.38532800	11.80023100	3.42607800
H	17.03607900	12.84925300	3.43640900
H	18.10062800	11.70742700	2.58368800
H	17.95485100	11.63042300	4.35859900
C	15.51069100	11.01398400	1.89528400
H	14.68922700	10.29318600	1.73623100
H	16.23227800	10.88810300	1.06246400
H	15.08002100	12.02667500	1.80386900
C	14.04047400	8.39899100	3.81838100
H	15.12647200	8.34390900	3.60384100
H	13.54631700	8.32418800	2.82452000
C	13.67110800	7.17691400	4.66479500
H	13.97922900	6.22465500	4.17766500
H	14.19806000	7.24679200	5.63202200
C	7.60897100	9.22262200	1.94048600
H	7.25645500	9.40033800	0.90125800
C	7.14642000	10.41750800	2.80337100
H	7.55940200	10.36135100	3.82803200
H	6.04109500	10.43388300	2.89223200
H	7.45755200	11.38946900	2.38122600
C	6.94131000	7.91922200	2.43761900
H	7.22771100	7.03294800	1.83977600
H	5.83664000	8.00211200	2.39316900
H	7.20552900	7.71356000	3.49189700
C	10.18087400	10.85602100	1.33219100
H	9.77434200	11.51163700	2.12974600
C	9.60565800	11.36514700	-0.01196900
H	10.01299200	10.80043800	-0.87216000
H	9.87259000	12.42922300	-0.16769000
H	8.50331400	11.29415800	-0.05629500
C	11.71269700	11.03555100	1.35195500

H	12.18289700	10.70405000	2.30054000
H	11.98099700	12.10313200	1.22807200
H	12.20692600	10.47284500	0.53980400
C	9.95542600	7.74856500	0.47562200
H	9.82023500	6.77619600	0.99682300
C	8.99260900	7.72901200	-0.73670800
H	7.94071800	7.57295200	-0.43822000
H	9.26271100	6.91000000	-1.43380600
H	9.03853600	8.67200100	-1.31194900
C	11.41960700	7.79041500	-0.02008700
H	11.59617600	8.66591800	-0.67191100
H	11.66086400	6.88873900	-0.61871200
H	12.14860100	7.84683600	0.80965200
C	10.06020800	7.19769400	3.74287200
H	9.44064100	6.64661300	3.00862400
H	9.51611000	7.10459000	4.70743100
C	11.42438700	6.50785500	3.85615600
H	11.33714500	5.41597700	4.05293500
H	11.96597000	6.63878500	2.90366400

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Np(TREN^{TIPS})F

Np	8.01525100	6.05822400	5.09525300
F	8.67764700	4.05475800	5.25797800
Si	4.50177200	4.95529000	5.26421500
Si	9.98778500	6.66608800	8.19679500
Si	9.33758800	5.98610300	1.68804900
N	7.26842500	8.56480400	4.94174900
N	5.77948000	6.17908500	5.48192800
N	9.13633600	7.20002100	6.72209000
N	8.34081200	6.76427000	2.95509400
C	5.78086500	8.60811000	5.03946200
H	5.36770000	8.43359900	4.03105400
H	5.44694000	9.61551500	5.37749400
C	5.29043100	7.49142700	5.96906000
H	5.64412700	7.68252700	7.00596900
H	4.18393000	7.55751800	6.02436900
C	7.90443100	9.27490200	6.08788400
H	7.23979600	9.16849100	6.96191000
H	7.99578200	10.36149100	5.86164400

C	9.26270700	8.65335100	6.43935700
H	9.98949400	8.84309900	5.61733000
H	9.65666800	9.22463000	7.30607000
C	7.76312800	9.08187600	3.63484600
H	8.82805300	9.34430200	3.76286900
H	7.21616300	10.01127200	3.35585600
C	7.65133900	8.00883300	2.54407000
H	6.57960900	7.80744400	2.32897100
H	8.05945100	8.45391600	1.61191200
C	3.21593100	5.44970800	3.88676200
H	2.64104200	4.51062300	3.72966800
C	3.88066800	5.80852700	2.54070600
H	3.12341000	5.94235300	1.74150700
H	4.59073300	5.03516600	2.19680300
H	4.44684000	6.75625600	2.61698100
C	2.18453300	6.53783800	4.26586000
H	2.65921400	7.53106500	4.37926400
H	1.64962900	6.31289000	5.20631300
H	1.41838300	6.64307700	3.47055600
C	3.47036100	4.78611500	6.89718800
H	2.93067500	5.75583100	6.97065600
C	4.30715300	4.65210600	8.18800100
H	3.65829200	4.71624000	9.08530300
H	5.06929300	5.44801500	8.26872000
H	4.83544400	3.68339000	8.23641100
C	2.39175000	3.68025400	6.81841300
H	2.84547600	2.67285100	6.76297100
H	1.73286700	3.79599600	5.93796500
H	1.74429000	3.69367000	7.71873800
C	5.35900100	3.31248000	4.71086400
H	6.22614400	3.62884700	4.08779600
C	4.47688600	2.40594600	3.81800100
H	5.03620300	1.49437700	3.52733100
H	4.15349800	2.90225800	2.88645100
H	3.56742400	2.07086000	4.35190900
C	5.92636300	2.47509400	5.88233100
H	5.10964300	2.04685400	6.49278200
H	6.58186500	3.05851900	6.54927800
H	6.52900400	1.62999500	5.49587600
C	9.78234900	4.75220300	8.33382100
H	9.97366900	4.37415600	7.30798100

C	8.35475200	4.29844100	8.71719600
H	8.24793700	3.20236500	8.59679800
H	7.56923500	4.77219800	8.09846600
H	8.12373500	4.53608100	9.77295200
C	10.81162600	4.06517600	9.26383400
H	10.70560200	4.39424900	10.31459100
H	11.85583700	4.25736100	8.95875100
H	10.66432500	2.96651000	9.25171500
C	9.28922400	7.65018100	9.71677400
H	9.58772700	8.70273000	9.51535100
C	9.94498500	7.25440100	11.06064100
H	9.61104100	7.92687100	11.87698900
H	11.04899500	7.30289900	11.02605100
H	9.66638700	6.22573400	11.35721600
C	7.75012800	7.64139500	9.84560400
H	7.37230000	6.64749100	10.14591100
H	7.25486300	7.90326400	8.89298600
H	7.41209700	8.36536700	10.61482000
C	11.89203800	7.03554900	8.13871800
H	12.28710100	6.51017600	9.03558300
C	12.30733100	8.51892100	8.27468500
H	13.40943300	8.60932000	8.36099400
H	11.86994000	9.00535600	9.16620900
H	12.00869500	9.10967200	7.38835200
C	12.57074700	6.40916900	6.90125500
H	12.23364800	6.90427600	5.97136400
H	12.35059600	5.33104000	6.79584000
H	13.67318500	6.51981000	6.95089800
C	8.26399400	5.19678400	0.28396400
H	9.00009500	4.74720000	-0.41805200
C	7.36792600	4.05524500	0.81084700
H	6.64119400	4.43248300	1.55479800
H	7.94929000	3.25136900	1.29769300
H	6.78568400	3.59180200	-0.01128900
C	7.42312900	6.21059300	-0.52525400
H	6.90013500	5.70819400	-1.36434300
H	8.03835200	7.01965200	-0.96164000
H	6.64399300	6.68202300	0.10246800
C	10.45346800	7.33585100	0.84715500
H	9.72920300	8.01773100	0.35028900
C	11.27595500	8.19299100	1.83470300

H	12.07680200	7.60094700	2.31402600
H	10.65161800	8.61123100	2.64474200
H	11.76484300	9.04084200	1.31306800
C	11.36940700	6.78310600	-0.27009100
H	11.86454000	7.61118000	-0.81687300
H	10.81739700	6.18072500	-1.01426400
H	12.17339700	6.14695100	0.14460000
C	10.32465100	4.54821200	2.51371300
H	9.55774100	3.95773700	3.05721300
C	10.99598200	3.58269300	1.50750600
H	11.78624100	4.08470000	0.91946500
H	10.27788600	3.14414700	0.79161500
H	11.47578600	2.74099700	2.04594700
C	11.36038000	5.00676000	3.56377000
H	11.72656900	4.14703200	4.15754800
H	10.95417400	5.74478200	4.28279000
H	12.23921600	5.47843200	3.08556100

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Np(TREN^{TIPS})Cl

Np	8.11120800	5.96432600	5.06041600
Cl	9.07676900	3.52681700	5.29714500
Si	4.57654700	4.86536700	5.22697400
Si	9.92953300	6.52988900	8.30558000
Si	9.37840100	6.16639600	1.61924100
N	7.32084300	8.47875800	5.04637500
N	5.89817200	6.03915700	5.53171000
N	9.19380900	7.00687800	6.74188600
N	8.36052200	6.80277400	2.95888700
C	5.84875700	8.50100100	5.27590800
H	5.35147300	8.40609100	4.29520700
H	5.54023800	9.47354800	5.72112500
C	5.43997800	7.31071300	6.14978800
H	5.87254600	7.42844700	7.16667200
H	4.34034200	7.35743000	6.29116000
C	8.07818400	9.13955800	6.15004300
H	7.49631000	9.03935500	7.08192000
H	8.20212000	10.22483600	5.93652300
C	9.42107400	8.42110700	6.33761500
H	10.00770300	8.48267000	5.39196100

H	10.02360900	8.98714200	7.07532800
C	7.68859700	9.05801300	3.72326300
H	8.74342200	9.37853300	3.77916100
H	7.07304000	9.96112700	3.51040100
C	7.55902700	8.00353400	2.62017900
H	6.48988200	7.73626700	2.48347000
H	7.86703800	8.48192600	1.66836600
C	3.37889000	5.45565900	3.81221000
H	2.75534000	4.55521200	3.61975700
C	4.10728100	5.79538500	2.49605700
H	3.38762600	5.95220500	1.66707200
H	4.81157000	5.00578500	2.17887800
H	4.69260400	6.72830300	2.59967700
C	2.40601800	6.59996400	4.17905000
H	2.94214700	7.55158300	4.35837000
H	1.80451700	6.37989600	5.07941800
H	1.69456900	6.78947500	3.34934000
C	3.44368700	4.70493700	6.79389900
H	2.94317200	5.69529200	6.86458400
C	4.17163800	4.48736600	8.13764200
H	3.45302000	4.53438200	8.98122400
H	4.94732500	5.25222500	8.31650500
H	4.66658900	3.50142100	8.18516600
C	2.31682900	3.65963800	6.60568000
H	2.71965000	2.63193300	6.53975100
H	1.71599400	3.84015500	5.69500300
H	1.61911000	3.67765600	7.46749900
C	5.37053700	3.18982200	4.68040800
H	6.30363800	3.45733000	4.13460000
C	4.50076200	2.36243500	3.70196600
H	5.02715300	1.42814300	3.42304800
H	4.26943800	2.89940300	2.76529300
H	3.53974300	2.06655600	4.16411500
C	5.79392100	2.29057700	5.86625800
H	4.91017600	1.91216800	6.41347600
H	6.44666600	2.81275900	6.58435900
H	6.35851300	1.41175300	5.49887100
C	9.33610600	4.75354200	8.73353100
H	9.73990500	4.13831600	7.90326900
C	7.80772100	4.55165000	8.72786800
H	7.55420100	3.47445300	8.78020900

H	7.32585500	4.95309600	7.81534200
H	7.32317500	5.04484800	9.58999700
C	9.94048300	4.20650000	10.04881400
H	9.53732500	4.73342000	10.93460200
H	11.04203100	4.29381300	10.08055900
H	9.69223400	3.13328300	10.17144300
C	9.45440500	7.87046400	9.63287100
H	9.62595900	8.84581500	9.12631500
C	10.35236400	7.86968000	10.89340100
H	10.06015100	8.68933400	11.58106000
H	11.42084000	8.00983800	10.65106900
H	10.26120200	6.92460900	11.46031300
C	7.96575400	7.83693600	10.04940400
H	7.75044400	6.96002100	10.68760700
H	7.28313800	7.78605400	9.18090900
H	7.69712300	8.73787700	10.63763600
C	11.86348900	6.47728500	8.22192200
H	12.17884900	6.29571400	9.27294400
C	12.51569800	7.80628200	7.77426700
H	13.61972500	7.75154800	7.86249700
H	12.18216700	8.67333800	8.37601300
H	12.28985500	8.02646600	6.71385700
C	12.40349800	5.30783100	7.36959900
H	12.05723000	5.37426800	6.32211800
H	12.08597700	4.32322200	7.75602300
H	13.51261800	5.31418700	7.35200900
C	8.32977000	5.11031700	0.38601000
H	9.05824000	4.73431100	-0.36446500
C	7.69231600	3.88508600	1.07435400
H	6.96711600	4.20094100	1.84872500
H	8.43840400	3.23747400	1.56932100
H	7.13910600	3.25967000	0.34487600
C	7.25780800	5.92225600	-0.37516800
H	6.71299800	5.27961200	-1.09622700
H	7.69158400	6.76188600	-0.94960100
H	6.50327600	6.34299600	0.31600100
C	10.11968000	7.63946100	0.59198200
H	9.23472300	8.14038000	0.14294900
C	10.87703700	8.70707400	1.41290500
H	11.82085600	8.30681500	1.82542500
H	10.28399300	9.08465200	2.26490500

H	11.14202900	9.57803100	0.77948600
C	10.99571900	7.16346800	-0.59178400
H	11.27716600	8.01959300	-1.23792000
H	10.48094300	6.42383800	-1.23119600
H	11.93705300	6.70289200	-0.23939000
C	10.70384100	5.00902000	2.39835600
H	10.12059500	4.32613100	3.05226000
C	11.44832000	4.09866900	1.39008900
H	12.10507900	4.67703900	0.71374900
H	10.76106400	3.50541300	0.76013000
H	12.09467200	3.38086000	1.93316400
C	11.72515200	5.72932400	3.30741900
H	12.32533500	4.99470600	3.87861100
H	11.24396200	6.40337900	4.04289200
H	12.43167800	6.34283700	2.71789600

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Np(TREN^{TIPS})Br

Np	8.09296000	5.94389200	5.02549200
Br	9.12983700	3.35276700	5.21648700
Si	4.54908400	4.86028900	5.22462400
Si	9.92476300	6.44999700	8.27989500
Si	9.40002000	6.23460200	1.62439600
N	7.32178600	8.46550400	5.06227500
N	5.88675800	6.02303600	5.52289000
N	9.18803400	6.93863400	6.71917800
N	8.33803600	6.83444400	2.94664400
C	5.85373700	8.49313500	5.31123000
H	5.34467100	8.42322900	4.33442800
H	5.55706800	9.45792300	5.78061200
C	5.44425700	7.28916300	6.16460100
H	5.88475100	7.38542900	7.18033700
H	4.34609000	7.34209000	6.31275600
C	8.10383600	9.09628400	6.16639700
H	7.53529600	8.98904400	7.10561100
H	8.24250400	10.18268500	5.96922400
C	9.43614200	8.34955200	6.31443600
H	9.99309200	8.40137600	5.34977600
H	10.07606900	8.89650800	7.03419100
C	7.67221400	9.07121900	3.74621100

H	8.72793400	9.39039000	3.79330900
H	7.05344700	9.97765500	3.55897900
C	7.52776500	8.03352800	2.63018400
H	6.45718600	7.76449100	2.50823100
H	7.81818800	8.52241100	1.67887500
C	3.41062400	5.43577600	3.75811800
H	2.74089500	4.56415000	3.58929100
C	4.19201100	5.67293100	2.44982600
H	3.50541500	5.87303900	1.60221700
H	4.82514500	4.81318100	2.16674800
H	4.86047800	6.54893100	2.54366000
C	2.50035400	6.64943300	4.05409600
H	3.08828500	7.57186700	4.22425300
H	1.85731600	6.49502500	4.93934900
H	1.82975600	6.85500100	3.19484900
C	3.37556300	4.77996300	6.76853500
H	2.88690400	5.77836500	6.78955900
C	4.06729300	4.60162300	8.13740500
H	3.33017300	4.69485400	8.96092800
H	4.85421600	5.35732900	8.30711900
H	4.54056000	3.60857900	8.23399200
C	2.23745500	3.74467200	6.59256200
H	2.62379200	2.70860000	6.58890300
H	1.66930400	3.89114300	5.65528700
H	1.51305000	3.81477100	7.42933700
C	5.31326700	3.14839900	4.76043600
H	6.25844600	3.37216700	4.21604800
C	4.43875100	2.29747600	3.80731100
H	4.94808000	1.34087600	3.57649500
H	4.23356700	2.79942300	2.84578900
H	3.46468600	2.04324800	4.26617600
C	5.70311700	2.29673100	5.99184700
H	4.80358400	1.93353300	6.52392400
H	6.32652600	2.85037600	6.71292700
H	6.28412100	1.40830700	5.67735900
C	9.27596500	4.70322600	8.74153300
H	9.67424100	4.05566400	7.93358300
C	7.74270100	4.54615700	8.71918700
H	7.45672600	3.48012100	8.81584900
H	7.28729000	4.92026000	7.78155600
H	7.25997500	5.09194900	9.54991500

C	9.84871600	4.17585900	10.07870100
H	9.45165500	4.73890200	10.94482500
H	10.95209000	4.23190500	10.12044700
H	9.56787300	3.11412200	10.22770700
C	9.50503800	7.81735300	9.60034300
H	9.67183700	8.78498600	9.07810300
C	10.43800300	7.82314800	10.83528700
H	10.16571100	8.64776800	11.52510200
H	11.49951000	7.96040900	10.56251400
H	10.36155600	6.88185200	11.41030200
C	8.02847300	7.80416600	10.05975800
H	7.82340800	6.93888700	10.71716600
H	7.32046800	7.74695600	9.21218000
H	7.78563500	8.71614700	10.64215000
C	11.85457400	6.33220600	8.17179400
H	12.17851300	6.17654700	9.22423600
C	12.53926400	7.62482300	7.67019500
H	13.64231100	7.54098600	7.74647600
H	12.23870100	8.52134100	8.24552900
H	12.30528000	7.81404700	6.60563900
C	12.34722700	5.11848500	7.35253300
H	11.98790100	5.15819600	6.30809900
H	12.00648100	4.15722100	7.77624000
H	13.45571100	5.09187500	7.32109000
C	8.42220700	5.04696100	0.45519000
H	9.16079600	4.67105700	-0.28604900
C	7.86528800	3.82635600	1.21875200
H	7.14539300	4.14135300	1.99936800
H	8.65415900	3.23973700	1.72273500
H	7.32427900	3.14133200	0.53477500
C	7.29445800	5.75605600	-0.32877800
H	6.77448900	5.04534100	-1.00269900
H	7.67136000	6.58508800	-0.95600400
H	6.52906000	6.17209200	0.35343500
C	10.01811000	7.71855500	0.53140300
H	9.09020700	8.16962700	0.11783600
C	10.76726000	8.83738600	1.28923000
H	11.75273500	8.49196200	1.64940700
H	10.20799500	9.20071800	2.17004700
H	10.94922600	9.70854000	0.62761700
C	10.85065200	7.25229200	-0.68704700

H	11.08325800	8.10953400	-1.35093500
H	10.32284000	6.49755600	-1.29769800
H	11.81637800	6.81374300	-0.37593300
C	10.82040100	5.22718400	2.44386700
H	10.29517700	4.52186100	3.12414200
C	11.63138700	4.34275700	1.46605500
H	12.25545900	4.94654900	0.78068700
H	10.98586900	3.69439900	0.84734800
H	12.31795800	3.68038300	2.02971500
C	11.78325200	6.05584000	3.32510800
H	12.44079400	5.38831400	3.91518900
H	11.25386000	6.71254800	4.04293300
H	12.44090300	6.70316800	2.71534700

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Np(TREN^{TIPS})I

Np	8.12924500	5.89901500	5.00405500
I	9.26300500	3.04294700	5.25442800
Si	4.56777600	4.82690800	5.22771000
Si	9.92447300	6.45307200	8.29619600
Si	9.39231700	6.25213600	1.58543400
N	7.34319600	8.42368400	5.06416100
N	5.92858900	5.96982400	5.52513800
N	9.20922900	6.88767200	6.70535900
N	8.33784500	6.81455500	2.93237900
C	5.88072000	8.44186300	5.34122200
H	5.35288100	8.37684100	4.37409000
H	5.58777400	9.40071200	5.82462600
C	5.49654700	7.22839000	6.19120600
H	5.96080500	7.31494000	7.19690800
H	4.40223900	7.27522200	6.36536600
C	8.14539700	9.05171200	6.15501800
H	7.59406500	8.94890500	7.10480600
H	8.28868200	10.13664300	5.95449100
C	9.47087100	8.28935600	6.27318700
H	9.99384900	8.31739300	5.28819300
H	10.14680100	8.83315200	6.96099400
C	7.66463300	9.04186800	3.74713100
H	8.71690100	9.37357400	3.77922500
H	7.03231100	9.94182000	3.57589900

C	7.51397400	8.00833200	2.62933000
H	6.44490200	7.72998800	2.51945000
H	7.78907800	8.50205800	1.67578200
C	3.42607300	5.42687800	3.77358200
H	2.74844400	4.56075100	3.60835200
C	4.19330300	5.66316100	2.45722400
H	3.49760700	5.86083300	1.61657900
H	4.82517700	4.80436700	2.16898800
H	4.86075300	6.54063900	2.54211500
C	2.52676300	6.64522100	4.08382200
H	3.12183500	7.56291000	4.25493800
H	1.88935000	6.48997300	4.97288700
H	1.85104100	6.86030800	3.23096700
C	3.39699700	4.75800700	6.77615000
H	2.92481300	5.76395900	6.80543300
C	4.08527300	4.55802600	8.14348800
H	3.34982700	4.65987500	8.96745900
H	4.88547400	5.29843300	8.31731800
H	4.54055600	3.55620000	8.23436000
C	2.23971600	3.74491300	6.59340000
H	2.60567600	2.70166700	6.58150800
H	1.67263100	3.90897200	5.65843500
H	1.51825700	3.82281800	7.43201300
C	5.29513500	3.10216200	4.75483400
H	6.25295600	3.30436800	4.22305000
C	4.40984600	2.27758800	3.78807500
H	4.89867800	1.31009900	3.55885700
H	4.22677900	2.78757400	2.82615300
H	3.42509100	2.04467800	4.23538800
C	5.64920100	2.23310200	5.98512900
H	4.73599700	1.90333000	6.51483700
H	6.29581400	2.75895900	6.70721600
H	6.19612700	1.32413400	5.66838500
C	9.26493100	4.73073100	8.82958400
H	9.68455800	4.03994500	8.06955700
C	7.73298500	4.56942700	8.77230500
H	7.44640800	3.50731600	8.90420700
H	7.30464200	4.90144600	7.80667600
H	7.22694200	5.14839200	9.56584600
C	9.80276400	4.27855900	10.20808300
H	9.38576100	4.88954200	11.03125800

H	10.90492900	4.33578800	10.27340900
H	9.51600500	3.22701000	10.40849800
C	9.48854300	7.86893900	9.56148100
H	9.64227100	8.81878100	9.00439200
C	10.42477700	7.92996700	10.79282900
H	10.13913600	8.77037900	11.45777600
H	11.48264100	8.07844400	10.51270300
H	10.36793500	7.00563200	11.39657000
C	8.01413400	7.85558100	10.02787000
H	7.81874500	7.00887100	10.71180400
H	7.30207900	7.76755100	9.18631200
H	7.76591900	8.78264200	10.58357200
C	11.85703300	6.33655900	8.21949700
H	12.15937800	6.20801200	9.28231700
C	12.55346500	7.61600000	7.70010700
H	13.65405100	7.53535700	7.80806600
H	12.23780600	8.52832800	8.24131200
H	12.34868300	7.77418100	6.62448500
C	12.37186600	5.10455500	7.44271200
H	12.05648600	5.12958400	6.38371600
H	12.00607700	4.15269300	7.86653200
H	13.48042500	5.06945800	7.45725800
C	8.39707300	5.12049300	0.37641900
H	9.13573600	4.75613900	-0.37018400
C	7.81319700	3.88634900	1.09707500
H	7.07737800	4.18964300	1.86715300
H	8.58466500	3.27952900	1.60463200
H	7.28262400	3.22317700	0.38417700
C	7.28659300	5.87043000	-0.39466900
H	6.75788200	5.18629800	-1.08887400
H	7.68110800	6.70817000	-0.99916900
H	6.52479800	6.28269600	0.29399800
C	10.03471000	7.76295100	0.54567500
H	9.12008800	8.22713000	0.11770500
C	10.76904200	8.86006500	1.34822800
H	11.73159500	8.49360600	1.74757600
H	10.17792400	9.22480500	2.20717200
H	10.99402400	9.73522200	0.70532500
C	10.90027800	7.32022200	-0.65868400
H	11.14655500	8.18957100	-1.30136800
H	10.39200600	6.57394900	-1.29547000

H	11.85932800	6.88019200	-0.32933800
C	10.79583300	5.20136600	2.37227800
H	10.25622300	4.49536700	3.04212400
C	11.58164000	4.30895400	1.38087200
H	12.21089900	4.90617600	0.69471300
H	10.92012500	3.67580000	0.76323900
H	12.25911600	3.63015300	1.93556500
C	11.78202600	5.98886500	3.26574200
H	12.41104400	5.29306400	3.85434500
H	11.27346100	6.65971300	3.98600900
H	12.46466000	6.61664900	2.66297800

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Pu(TREN^{TIPS})F

Pu	7.98147700	6.02369100	5.14749700
F	8.60291600	4.00519800	5.22517200
Si	4.46303600	4.94616100	5.27755700
Si	10.02408600	6.64848500	8.16377200
Si	9.41937100	5.94642800	1.76993900
N	7.27455000	8.53800600	4.98431600
N	5.73946200	6.17141200	5.50537000
N	9.13653000	7.23097300	6.72571400
N	8.42687600	6.74431500	3.03016300
C	5.78485100	8.58419300	5.00342900
H	5.42295800	8.38685900	3.97967000
H	5.43746400	9.60078000	5.29825000
C	5.23613200	7.49564100	5.93334700
H	5.53334600	7.70919600	6.98326000
H	4.12925900	7.57480500	5.92417600
C	7.84061300	9.26265000	6.15546200
H	7.15288600	9.11690800	7.00565400
H	7.88846900	10.35517700	5.94341000
C	9.21026300	8.69645500	6.54089100
H	9.96232000	8.95693400	5.76296900
H	9.53463800	9.24253300	7.45270700
C	7.83086400	9.05910900	3.70550800
H	8.88836900	9.32054800	3.88408400
H	7.29780700	9.99054400	3.40652100
C	7.76968200	7.99766300	2.60113000
H	6.70984000	7.80817900	2.32290500

H	8.23108600	8.45206400	1.69881800
C	3.20363200	5.43067700	3.87195600
H	2.63138000	4.48998700	3.71538600
C	3.89866500	5.76962900	2.53585100
H	3.15941200	5.89362000	1.71847500
H	4.61383100	4.98945600	2.21888200
H	4.46568200	6.71701800	2.61097500
C	2.16384000	6.52326700	4.21321800
H	2.63271100	7.52110500	4.30792500
H	1.61768100	6.31909500	5.15203900
H	1.40755300	6.60578000	3.40595000
C	3.41162500	4.81341100	6.90241700
H	2.88548500	5.79192700	6.95515000
C	4.23295200	4.68646700	8.20409200
H	3.57723700	4.78664100	9.09302300
H	5.01509200	5.46380100	8.27541600
H	4.73479500	3.70542900	8.27902300
C	2.31901600	3.72152500	6.82617600
H	2.75893100	2.70713400	6.79360300
H	1.67397200	3.83194000	5.93489900
H	1.65951400	3.75879800	7.71706100
C	5.31213700	3.28571300	4.76601100
H	6.19174700	3.57838800	4.15087700
C	4.43085500	2.37342900	3.87838400
H	4.98411400	1.45125700	3.61058800
H	4.12633300	2.85770000	2.93430800
H	3.51037400	2.05711400	4.40482400
C	5.85157300	2.46683400	5.96284700
H	5.02113400	2.06383700	6.57223200
H	6.50646500	3.05671300	6.62486700
H	6.44771500	1.60560200	5.60310400
C	9.85169200	4.72682000	8.22536300
H	9.98622200	4.38908000	7.17657400
C	8.45462100	4.23742100	8.67387200
H	8.35544900	3.14549300	8.51701700
H	7.62692500	4.72165700	8.12107300
H	8.28387400	4.43260000	9.74944800
C	10.94348700	4.01690100	9.06261100
H	10.90262100	4.30664200	10.12937900
H	11.96392400	4.23194900	8.69811500
H	10.80499400	2.91800800	9.01886000

C	9.32615900	7.54925700	9.73618700
H	9.62474600	8.61105300	9.59359000
C	9.98508700	7.07735100	11.05385300
H	9.64924300	7.69934100	11.90852900
H	11.08893100	7.13279400	11.02136600
H	9.71121900	6.03182300	11.28957900
C	7.78701600	7.53478100	9.86693300
H	7.40812600	6.52912300	10.12351000
H	7.28992100	7.83980200	8.92819700
H	7.45147600	8.22353800	10.66882500
C	11.91775400	7.07085000	8.09841500
H	12.34002900	6.50823700	8.95973200
C	12.28770400	8.55672200	8.31143900
H	13.38813200	8.67818600	8.37770800
H	11.85663000	8.97495700	9.23941500
H	11.94740700	9.18709200	7.46853100
C	12.59565600	6.53583800	6.81902800
H	12.22846200	7.06933400	5.92247900
H	12.40841700	5.45853400	6.65808900
H	13.69471800	6.67891200	6.85984200
C	8.34977700	5.18329700	0.34676200
H	9.09154100	4.72207500	-0.34173400
C	7.42467900	4.05627000	0.85412400
H	6.68172600	4.44787300	1.57397600
H	7.98135700	3.24892200	1.36337500
H	6.86054800	3.59495300	0.01827900
C	7.54310500	6.21220100	-0.47730000
H	7.03065000	5.72064700	-1.32927200
H	8.18086200	7.01213300	-0.89767100
H	6.75783900	6.69524100	0.13388200
C	10.56428400	7.28630300	0.94978600
H	9.85913500	7.96967900	0.42797800
C	11.36288300	8.14431100	1.95618000
H	12.14984300	7.55168100	2.45719400
H	10.71894600	8.56443900	2.74969500
H	11.86670300	8.98994300	1.44513900
C	11.50789600	6.72175700	-0.13782200
H	12.02085200	7.54428000	-0.67666000
H	10.97319700	6.11688400	-0.89264800
H	12.29810900	6.08526200	0.30239100
C	10.37866400	4.48719800	2.58754500

H	9.59894000	3.90777500	3.12375200
C	11.04169300	3.51874100	1.57906600
H	11.84104100	4.01217900	0.99615900
H	10.32094200	3.09218800	0.85850900
H	11.50814700	2.66849600	2.11598100
C	11.41181900	4.92660500	3.64775900
H	11.76783200	4.05620400	4.23300400
H	11.00341700	5.65896100	4.36977000
H	12.29852800	5.39540800	3.18069100

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Pu(TREN^{TIPS})Cl

Pu	8.03965000	5.93199000	5.14162100
Cl	8.95424200	3.46553900	5.15229000
Si	4.49110000	4.84179300	5.23645600
Si	9.94396100	6.47129900	8.26900700
Si	9.52935600	6.17270800	1.76757200
N	7.27598100	8.45847600	5.10761200
N	5.81147300	6.01495400	5.56658200
N	9.13378900	7.07777700	6.78489400
N	8.47983600	6.81583200	3.08038900
C	5.79042100	8.46203300	5.22566100
H	5.36806400	8.31957800	4.21569600
H	5.43749900	9.44746100	5.60598000
C	5.32936700	7.30526600	6.11782900
H	5.70972900	7.45300300	7.15160400
H	4.22489600	7.36304900	6.19988200
C	7.91514500	9.14994300	6.26175600
H	7.27887900	8.99886800	7.15024100
H	7.97702600	10.24452000	6.06847700
C	9.28685800	8.53036400	6.53665900
H	9.96104500	8.71392800	5.67199200
H	9.74262000	9.08098200	7.38435800
C	7.72549700	9.04980800	3.81719400
H	8.77165200	9.37790100	3.94516600
H	7.11541000	9.94842600	3.57114200
C	7.67776400	8.00300900	2.70347200
H	6.62172100	7.72029700	2.50039900
H	8.02774800	8.49308000	1.77336800
C	3.39609800	5.40296900	3.73061800

H	2.74199900	4.52407800	3.53912500
C	4.22807500	5.64291900	2.45376900
H	3.57553500	5.84905700	1.58112900
H	4.86818200	4.78158600	2.19139000
H	4.89607600	6.51605600	2.57826500
C	2.46136300	6.60752800	3.98439800
H	3.03012400	7.54128700	4.15662600
H	1.79598700	6.45611600	4.85354200
H	1.81267800	6.78968900	3.10344000
C	3.28749100	4.78587600	6.75763800
H	2.79650500	5.78317600	6.75204300
C	3.95989400	4.63206900	8.13934000
H	3.21050500	4.73489200	8.95051300
H	4.74181400	5.39338200	8.30933300
H	4.43498200	3.64218100	8.25743700
C	2.15810300	3.74215000	6.57859900
H	2.54968700	2.70829600	6.60259100
H	1.60914200	3.86817300	5.62696500
H	1.41624200	3.82455300	7.39875300
C	5.27109600	3.12794300	4.81250200
H	6.21870700	3.34820500	4.27342300
C	4.40836800	2.25898900	3.86522400
H	4.92528800	1.30300100	3.64954200
H	4.20869300	2.74931100	2.89652400
H	3.43193600	2.00447200	4.31885200
C	5.65902800	2.29915400	6.06029300
H	4.76008500	1.93366100	6.59197400
H	6.27108500	2.87065100	6.77768800
H	6.25180400	1.41252800	5.76337300
C	9.31391100	4.68542900	8.60774500
H	9.58780100	4.12703400	7.68842900
C	7.78428600	4.55464400	8.76890400
H	7.48383400	3.48858300	8.78915600
H	7.22101500	5.03665300	7.94579300
H	7.43006000	5.01202000	9.71094400
C	10.03086800	3.98616900	9.78721200
H	9.75248100	4.43532500	10.75888400
H	11.13215200	4.02705900	9.70385200
H	9.74445900	2.91655200	9.83144700
C	9.62642000	7.71758400	9.72999000
H	9.97000000	8.69949500	9.33945700

C	10.48162500	7.43598200	10.98794900
H	10.34505000	8.23965000	11.73986800
H	11.56099300	7.37949300	10.75916300
H	10.19393100	6.48649000	11.47456900
C	8.14043900	7.88419000	10.11901900
H	7.75822400	6.98608400	10.63770000
H	7.49177500	8.05550700	9.24031100
H	8.00384200	8.74024400	10.81060200
C	11.86158700	6.36963800	8.02977600
H	12.25647700	6.02667600	9.01103900
C	12.52232600	7.73154400	7.71692800
H	13.62558200	7.63157900	7.66846500
H	12.29693200	8.50200100	8.47830600
H	12.19192900	8.12233000	6.73606800
C	12.26624900	5.31929900	6.97344100
H	11.83969200	5.56091500	5.98275400
H	11.92640400	4.30161100	7.23538500
H	13.36859800	5.28181900	6.85640600
C	8.52033900	4.99331500	0.61237500
H	9.25919800	4.55686000	-0.09468000
C	7.88850200	3.82878100	1.40474500
H	7.15396100	4.20518100	2.14317500
H	8.63262600	3.23841500	1.96787700
H	7.34669100	3.13451400	0.73053600
C	7.44335400	5.71885600	-0.22537800
H	6.89626200	5.00121000	-0.87013300
H	7.87073900	6.49343600	-0.88833100
H	6.69115800	6.20821400	0.42207200
C	10.16093100	7.62838500	0.64074500
H	9.24424400	8.01272200	0.14348200
C	10.82041300	8.82548600	1.36318400
H	11.80280500	8.55385900	1.78754100
H	10.20487700	9.21375600	2.19423000
H	10.99109400	9.66306700	0.65644900
C	11.08518400	7.11987900	-0.49258600
H	11.32186700	7.93900900	-1.20172300
H	10.62790200	6.30074700	-1.07664800
H	12.04819300	6.74886200	-0.09575300
C	10.98024200	5.17558400	2.55519600
H	10.53177300	4.63154400	3.41259800
C	11.58391200	4.09417200	1.62564800

H	12.04672200	4.53299700	0.72155700
H	10.83424400	3.35505100	1.29322800
H	12.37851100	3.53443400	2.15846600
C	12.11096300	6.06976200	3.11574600
H	12.83427200	5.46412900	3.69641700
H	11.73248800	6.86657300	3.78220300
H	12.68048900	6.55797100	2.30269300

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Pu(TREN^{TIPS})Br

Pu	8.04181800	5.91591100	5.14057000
Br	9.02385800	3.29682600	5.15316100
Si	4.48573200	4.83944500	5.24197700
Si	9.94247300	6.45967700	8.26924600
Si	9.53753400	6.18075700	1.76844600
N	7.27966400	8.44538600	5.11100600
N	5.81722900	6.00201600	5.57552600
N	9.13586600	7.06160000	6.77927700
N	8.47786600	6.80697100	3.08308100
C	5.79504000	8.44944200	5.23905300
H	5.36617400	8.30802800	4.23173400
H	5.44479500	9.43452100	5.62253700
C	5.33975000	7.29204000	6.13259200
H	5.72766100	7.43739300	7.16374200
H	4.23598400	7.35026400	6.22211700
C	7.92692400	9.13759200	6.26008600
H	7.29604200	8.99000400	7.15296900
H	7.99112800	10.23149600	6.06438900
C	9.29753200	8.51247600	6.52554700
H	9.96481300	8.68840500	5.65409000
H	9.76422900	9.06261000	7.36739000
C	7.71872300	9.03823000	3.81769700
H	8.76437600	9.37048000	3.93846600
H	7.10358900	9.93419900	3.57484300
C	7.66733400	7.98899800	2.70719700
H	6.61131200	7.70053200	2.51356100
H	8.00789900	8.47660600	1.77263500
C	3.40271000	5.40738600	3.73097100
H	2.74015600	4.53439100	3.54147700
C	4.24142300	5.63185900	2.45577200

H	3.59392900	5.83623800	1.57899200
H	4.87663500	4.76419300	2.20223700
H	4.91476300	6.50124400	2.57645900
C	2.47974900	6.62251700	3.97677200
H	3.05729300	7.55066500	4.15023500
H	1.80817500	6.47996300	4.84264700
H	1.83782800	6.80956300	3.09192600
C	3.27605700	4.79943200	6.75900500
H	2.79268600	5.80030300	6.74935800
C	3.94191900	4.64293800	8.14356100
H	3.19069900	4.75502900	8.95177000
H	4.73057500	5.39709000	8.31439700
H	4.40712000	3.64892200	8.26555700
C	2.13887200	3.76446600	6.57750300
H	2.52162100	2.72742800	6.60508400
H	1.59466500	3.89316400	5.62349700
H	1.39456700	3.85483400	7.39457300
C	5.24810800	3.11726600	4.82476500
H	6.20163600	3.32692400	4.29125300
C	4.38310700	2.25550100	3.87319000
H	4.89038900	1.29250500	3.66618100
H	4.19869800	2.74431700	2.90067600
H	3.39939800	2.01477000	4.31847900
C	5.61981100	2.28785700	6.07693700
H	4.71401900	1.93271800	6.60386200
H	6.23365000	2.85538700	6.79619000
H	6.20615300	1.39494700	5.78630000
C	9.30341100	4.68145000	8.62412000
H	9.58935800	4.11154800	7.71541300
C	7.77165800	4.55283400	8.76394300
H	7.47055400	3.48711000	8.78729600
H	7.21931500	5.02929700	7.93017500
H	7.40415600	5.01741800	9.69735300
C	10.00368700	3.99523900	9.82098300
H	9.71317100	4.45435900	10.78449800
H	11.10599600	4.03449600	9.75110100
H	9.71595900	2.92631800	9.87256700
C	9.63139200	7.71674800	9.72217500
H	9.96362000	8.69869300	9.32248500
C	10.50134200	7.44972400	10.97318400
H	10.36513700	8.25658800	11.72174300

H	11.57875800	7.40168800	10.73367000
H	10.22751500	6.50053700	11.46822100
C	8.14781800	7.87364000	10.12421900
H	7.77711300	6.97478000	10.64999800
H	7.48994700	8.03668300	9.25068600
H	8.01104100	8.73149000	10.81351600
C	11.85813700	6.34624200	8.02204500
H	12.25500700	6.00351600	9.00268900
C	12.52512600	7.70362300	7.70306300
H	13.62778700	7.59794500	7.65375600
H	12.30427000	8.47815900	8.46166000
H	12.19573900	8.09199300	6.72094100
C	12.25122500	5.29080400	6.96639200
H	11.81918400	5.53085800	5.97756400
H	11.90767100	4.27557400	7.23266400
H	13.35268500	5.24818900	6.84324700
C	8.54257500	4.98685100	0.61425000
H	9.28647100	4.56377600	-0.09571000
C	7.92670500	3.80945400	1.39948800
H	7.19546100	4.17004600	2.14938300
H	8.68006900	3.21840400	1.94905500
H	7.38454700	3.11905600	0.72147900
C	7.45528400	5.70103600	-0.22019100
H	6.92192900	4.97881600	-0.87128200
H	7.87072200	6.48740200	-0.87664200
H	6.69314000	6.17264900	0.42883700
C	10.14054700	7.64425400	0.63497400
H	9.21669100	8.01192200	0.13815000
C	10.78335200	8.85637400	1.34741600
H	11.77170300	8.60436600	1.77016700
H	10.16452000	9.24091600	2.17769500
H	10.93793700	9.69172700	0.63434000
C	11.06956300	7.14456600	-0.49838300
H	11.28616100	7.96187500	-1.21594700
H	10.62674700	6.31075300	-1.07254800
H	12.04165800	6.79725100	-0.10247500
C	11.01273600	5.21616700	2.55114200
H	10.58107900	4.66575900	3.41322600
C	11.62921600	4.14255300	1.62148800
H	12.07821700	4.58585600	0.71261500
H	10.88953400	3.38981300	1.29733300

H	12.43674900	3.59825000	2.15077200
C	12.12874100	6.13339900	3.10363800
H	12.86736100	5.54237500	3.68008300
H	11.73818200	6.92190100	3.77317100
H	12.68306900	6.63337100	2.28724600

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Pu(TREN^{TIPS})I

Pu	8.11458900	5.90330100	5.00864200
I	9.17507100	3.03309100	5.21239800
Si	4.52706600	4.79229400	5.25344400
Si	9.94068100	6.34275300	8.33067000
Si	9.48303400	6.30339600	1.62053800
N	7.33990100	8.39118700	5.08242100
N	5.88607000	5.93881400	5.51955800
N	9.21989300	6.78566800	6.75017800
N	8.36897300	6.83219700	2.92595900
C	5.87677200	8.42382100	5.35030200
H	5.35873100	8.38536600	4.37652500
H	5.59372900	9.37846300	5.84793200
C	5.46039000	7.20330900	6.17573800
H	5.89953800	7.27949500	7.19459400
H	4.36315300	7.26997200	6.32536500
C	8.15752000	8.96607800	6.19332800
H	7.60292600	8.84640700	7.13904500
H	8.32468300	10.05322400	6.02634200
C	9.47443100	8.17645900	6.28780700
H	9.95887000	8.18031300	5.28046600
H	10.18671800	8.72326100	6.93558000
C	7.67684300	9.03242200	3.77916600
H	8.72919300	9.36229800	3.82666600
H	7.04699500	9.93570200	3.61846900
C	7.53576300	8.01796700	2.63839100
H	6.46811400	7.73200400	2.52771300
H	7.80473500	8.53159000	1.69293900
C	3.43672400	5.37491500	3.75163800
H	2.72804100	4.53306600	3.59169700
C	4.26273600	5.53387300	2.45936400
H	3.61883400	5.80802100	1.59887700
H	4.80394300	4.61040800	2.18596600

H	5.02293800	6.32881800	2.57283300
C	2.58300000	6.63899800	3.99764600
H	3.21126100	7.53632300	4.15709000
H	1.91655100	6.53845600	4.87350000
H	1.93975300	6.85432600	3.11998500
C	3.32651900	4.78713300	6.78043200
H	2.86250500	5.79718800	6.77342600
C	3.99786600	4.61890000	8.16085000
H	3.25597200	4.75048500	8.97488700
H	4.80537900	5.35438500	8.32310700
H	4.44150800	3.61508100	8.28205400
C	2.16578500	3.77652000	6.61094800
H	2.52659900	2.73168300	6.63853200
H	1.61745200	3.91410300	5.66059600
H	1.42954800	3.88487000	7.43329500
C	5.22200600	3.04241600	4.83381100
H	6.17115500	3.22146900	4.28143300
C	4.31076000	2.19847300	3.90842200
H	4.78519000	1.21853700	3.70214100
H	4.11870400	2.67980900	2.93356400
H	3.33036000	1.99087600	4.37691300
C	5.58873100	2.20609000	6.08276700
H	4.68226700	1.89669500	6.63631000
H	6.25086000	2.74675700	6.77909000
H	6.12408300	1.28424700	5.78320100
C	9.23507900	4.64703500	8.88751200
H	9.62504900	3.93390300	8.13201300
C	7.69715300	4.53866200	8.84677800
H	7.37555300	3.49226800	9.01784200
H	7.27694700	4.85196100	7.87219200
H	7.21848300	5.16077400	9.62451300
C	9.77311600	4.19569500	10.26643500
H	9.38629900	4.83129700	11.08571600
H	10.87745300	4.21532500	10.31937500
H	9.45280100	3.15748900	10.48443300
C	9.57671000	7.78594000	9.58731900
H	9.75374700	8.72044900	9.01118600
C	10.53699200	7.83204400	10.80065300
H	10.29355300	8.69294700	11.45599600
H	11.59463500	7.93710200	10.50015400
H	10.45674200	6.92024300	11.42054500

C	8.11127000	7.83147200	10.08014700
H	7.89857400	7.00169400	10.77966500
H	7.38010400	7.75723100	9.25379100
H	7.90736900	8.77424900	10.62739100
C	11.86559700	6.17247400	8.19634500
H	12.19698000	6.02105200	9.24702700
C	12.57860900	7.43782900	7.66686300
H	13.67931200	7.33163200	7.74739400
H	12.29653000	8.35424600	8.21942400
H	12.35168000	7.60448300	6.59704100
C	12.30915700	4.93576300	7.38423400
H	11.94565900	4.98307300	6.34091500
H	11.93192600	3.99042100	7.81292600
H	13.41558400	4.86653500	7.34954000
C	8.55052700	5.10030500	0.42509900
H	9.32398400	4.72206800	-0.27867300
C	7.96198300	3.88656100	1.17482600
H	7.18004200	4.20649700	1.88983500
H	8.71836100	3.32602800	1.75297100
H	7.48715400	3.17624500	0.46799800
C	7.45422900	5.79688500	-0.41223100
H	6.96694900	5.07455400	-1.09801100
H	7.85115000	6.62044100	-1.03383000
H	6.65764400	6.21373100	0.23313900
C	10.07447100	7.81050400	0.54467200
H	9.14932700	8.19600500	0.06354600
C	10.71235100	8.99251600	1.30930500
H	11.68652000	8.71495100	1.74878600
H	10.07550100	9.36118300	2.13321400
H	10.89435300	9.84719400	0.62646700
C	11.00960700	7.36010800	-0.60392300
H	11.23838900	8.21024000	-1.27796600
H	10.56513200	6.55982700	-1.22253900
H	11.97542900	6.98579000	-0.21709700
C	10.93090900	5.35473100	2.46520200
H	10.44274200	4.74247800	3.25718600
C	11.65642200	4.34433400	1.54516600
H	12.18620000	4.84715500	0.71406700
H	10.96390000	3.60668300	1.10386700
H	12.41437600	3.77704600	2.12057200
C	11.96357200	6.26369600	3.17067300

H	12.63139400	5.66439800	3.81983200
H	11.49035700	7.03638600	3.80594700
H	12.60715200	6.78660000	2.43868300