

Supporting Information

A Porphyrin-Based Molecular Cage Guided by Designed Local-Electric Field Is Highly Selective and Efficient

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Table of Contents:

	Pages
Figure S1. Primary altered cage for HM1 entrapment.....	S3
Figure S2. Modifications for <i>modeled cage</i>	S3
Text S1	S4
Text S2	S5
Text S3	S6
Text S4 with Figure S3 & S4	S6-S8
Figure S5. Tetralin (TLN) docked in the active site.....	S9
Figure S6. RMSD during 100 ns MD simulation.....	S9
Figure S7. A representative MD snapshot highlighting the substitutions for substrate entrapment.....	S9
Figure S8. Evolution of pro-R(H) and pro-S(H) distances for replica simulation.....	S10
Figure S9. QM/MM TS1(R) and TS2(R) optimized structures.....	S10

Figure S10. QM/MM optimized structures for (R)-PES scan in sextet spin state.....	S10
Figure S11. QM/MM (S)-PES scan profile & Comparative rate constant data.....	S11
Figure S12. QM/MM optimized structures for (S)-PES scan in sextet spin state.....	S12
Figure S13. Single-point gas-phase profile for RS, TS1(S) and TS1(R) doppelgangers, in absence and presence of OEEF.....	S12
Table S1. Mulliken spin and charges for both the R- and S- reaction profiles.....	S13
Table S2. Mulliken spin and charges for RS doppelganger species.....	S13
Figure S14. Modifications for generating mod1 and mod2.....,,.....	S14
Figure S15. Distance analysis for pi-pi interactions.....	S14
Table S3. QM/MM energy values for all the systems	S15
References.	S16
QM region for QM/MM optimized geometries.....	S17-S62

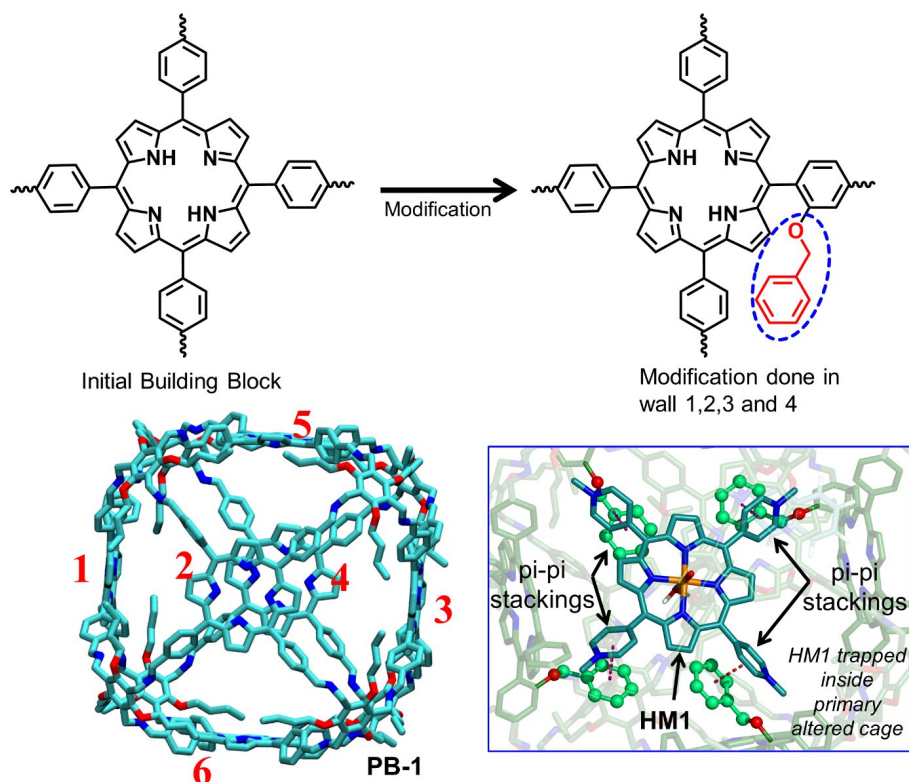


Figure S1. Modification done for primary altered cage for HM1 entrapment through pi-pi stacking interactions.

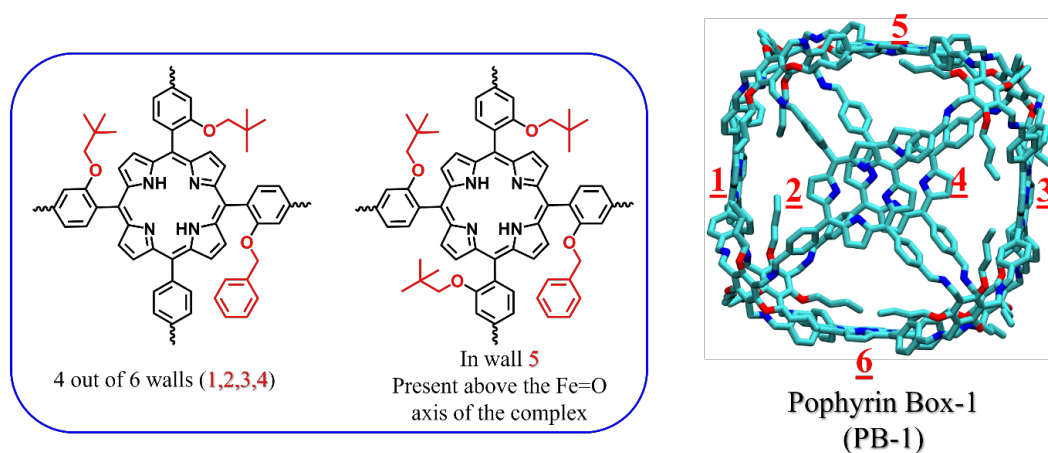
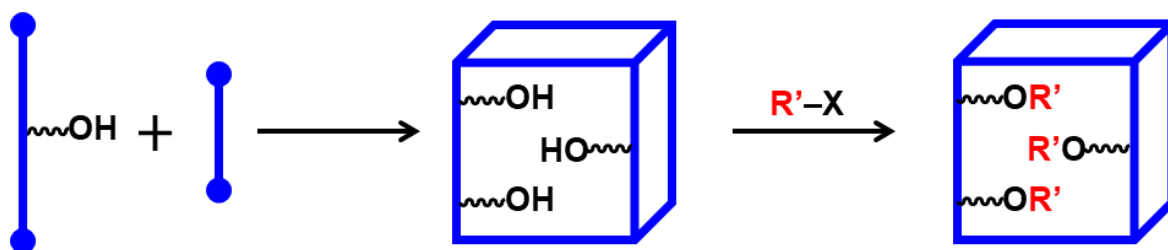


Figure S2. Modifications made in the porphyrin box-1 (PB-1) skeleton for computationally designing the ‘modeled cage’ with a local electric field (LEF) aligned along the Fe=O axis of active oxidant HM1. The right-hand side figure shows the structure of PB-1 synthesized by K. Kim et al.², H’s are omitted for clarity. Numbers 1, 2, 3, 4, 5, and 6 represent the six faces of the box. The left-hand side figure shows the modifications made in red to the faces/walls of the PB-1 skeleton.

Text S1. The structural modification/functionalization for the phenyl, alkyl or other substitutions in the PB-1 can be done through pre-synthetic approach as well as some post synthetic modifications which has been extensively discussed by Yusran et al.¹ For both the approaches, the scaffold should be quite stable towards the modifications and as discussed by K. Kim et al., the PB-1 possesses the applicability and exceptional chemical stability² and it has been already subjected to various modifications.^{3,4} We have utilized the concept of covalent linkage modification which can be done using functionalizing the already existing pendant groups in the skeleton via triazole linkages, ester linkages, ether linkages, amide linkages etc.¹ These pendant groups can be added with the pre-synthetic approaches in the building block. Herein, we have applied the ether covalent linkage as a source of inspiration for the post synthetic modification that can be generated by the coupling of the hydroxyl (–OH) pendant group (which can be pre-functionalized in the building block meso-porphyrins) and the alkyl or aryl-halide (Scheme S1). Subsequently, the desired porous organic cages were modeled computationally.



Scheme S1. Structural modification strategy of the cage using post synthetic modifications.

By encasing the guest in the host in the manner of a "ship-in-a-bottle," porphyrin or metalloporphyrin derivatives can be effectively encapsulated inside the cage. One of the most often used strategies to capture a moiety with dimensions larger than the host's aperture size is the ship-in-a-bottle technique.⁵

Text S2. Spin-state Selectivity Calculation:

To calculate the percentage of each spin state (doublet and sextet) for Fe, we can use the Boltzmann population formula:

$$P(D) / P(S) = \exp[-((\Delta G(D) - \Delta G(S)) / kT)]$$

where $P(D)$ and $P(S)$ are the populations of the doublet and sextet states, $\Delta G(D)$ and $\Delta G(S)$ are the energy differences between the doublet and sextet states, k is the Boltzmann constant ($8.617333262145 \times 10^{-5}$ eV/K), and T is the temperature in K.

The calculated transition state energy barriers: $\Delta G(D) = 4.8$ kcal/mol and $\Delta G(S) = 7.3$ kcal/mol, it is needed to convert to the corresponding energy units (eV) for consistent calculations. Assuming the temperature of 298 K:

$$\Delta G(D) = 4.8 \text{ kcal/mol} \times 4.184 \text{ eV/kcal} = 20.07 \text{ eV}$$

$$\Delta G(S) = 7.3 \text{ kcal/mol} \times 4.184 \text{ eV/kcal} = 30.49 \text{ eV}$$

Now, we can calculate the population ratio:

$$\begin{aligned} P(D) / P(S) &= \exp[-(\Delta G(D) - \Delta G(S)) / kT] \\ &= \exp[-(20.07 - 30.49) / (8.617333262145 \times 10^{-5} \times 298)] \end{aligned}$$

$$P(D) / P(S) \approx \exp(114.78)$$

Taking the natural logarithm of both sides:

$$\ln(P(D) / P(S)) \approx 114.78$$

Taking the exponential (antilog) of both sides:

$$P(D) / P(S) \approx e^{114.78} \approx 3.22 \times 10^{49}$$

Therefore, the population ratio of the doublet state to the sextet state is estimated to be approximately 3.22×10^{49} .

To estimate the spin selectivity, we can use the following formula:

$$\text{Spin Selectivity} = (P(D) / (P(D) + P(S))) \times 100$$

Plugging in the population ratio:

$$\text{Spin Selectivity} \approx (3.22 \times 10^{49} / (3.22 \times 10^{49} + 1)) \times 100 \approx 99.99\%$$

Based on these calculations, the estimated spin selectivity is >99.9% for the doublet state.

Text S3. Consistency in local electric field calculations in TITAN and TUPA codes:

The TITAN-code and TUPA both are used to calculate the magnitude and direction of electric fields (EFs) imposed by surrounding charged groups (point charges). These calculations are mainly based on Coulomb's law for both the codes. Coulomb's law describes the electrostatic interaction between charged particles, and it is a fundamental principle used to calculate electric fields. The specification of the point charges is exactly the same in both cases. Therefore, it is reasonable to expect that the calculation of electric field between both the two codes should be consistent with each other.

However, factors such as numerical approximations and computational precision can still introduce some discrepancies. Therefore, we selected 5 most representative MD snapshots from the clustering analysis and subjected it to LEF calculations by both TITAN and TUPA code. The LEF values from both the codes were exactly matching to one another. Therefore, it is evident that the electric field results are consistent between the two codes. The LEF values are summarized in the adjoining table:

MD Snapshot	LEF along Fe–O axis (in a.u.)		LEF along Fe–O axis (in V/Å)	
	TITAN	TUPA	TITAN	TUPA
1	0.0056877579	0.0056640796	0.29235075606	0.2911336948
2	0.0056483091	0.0058617523	0.29032308774	0.3012940692
3	0.0053655644	0.0054019565	0.27579001016	0.2776605670
4	0.0052873262	0.0051657775	0.27176856668	0.2655209680
5	0.0050722410	0.0049986949	0.26071318740	0.2569329225

Text S4. Entry/Exit of the Substrate/Product

To investigate the process of substrate/product binding and unbinding, we employed adaptive steered molecular dynamics (ASMD) simulation and calculated the potential of mean

force (PMF) using the Jarzynski average.⁶ Previous studies has shown that the PMF values qualitatively fit with the theoretical and experimental binding free energy calculations.⁷ The results of this calculation are illustrated in Figure 11a, with PMF values of ~15.5 and ~15.9 kcal/mol for the substrate (tetralin) and the hydroxylated product (*R*-1-tetralol), respectively. The smaller values of free energies as observed by the PMF plot show a feasible substrate entry and exit from the supramolecular cage.

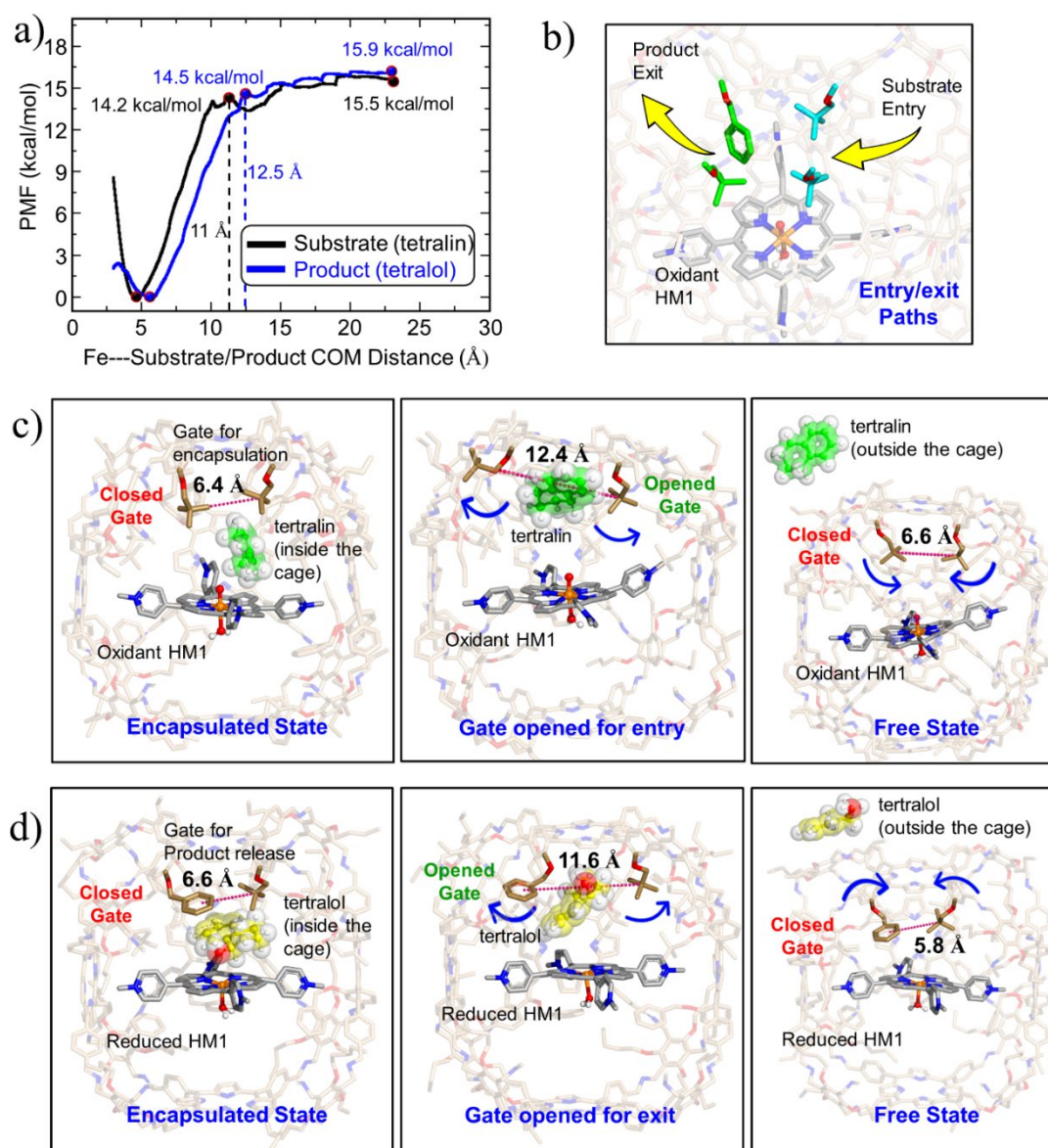


Figure S3. (a) ASMD derived PMF along the reaction coordinate for both, substrate & hydroxylated product. (b) Obtained paths for substrate entry and product exit from the cage. (c,d) Representative states for unbinding/binding process for substrate and product, respectively. The distances for the movement of crucial groups are in Figure S4.

During the exit, we observe a sharp increase in the PMF, i.e., free energy for both substrate and product as they dissociate from the active site. The rise in PMF is mainly due to the force against the hydrophobic interactions (Figure S7) between substrate and cage-substituents when substrate/product moves from 3 to 10-12 Å from the reactive center, i.e., Fe=O for **HMI**. Interestingly, we observed that both t-butyl groups and the phenyl substitution of the cage act as *doorways which can easily be shuttles from open to close conformation to allow the substrate entry and the product exit* (Figure S3b-d). Interestingly, once substrate enters or product exists the cage, the two t-butyl groups and the phenyl groups, restore their previous orientations, indicating an important dynamics during the entry/exit of the substrate/product. As can be seen, the PMF becomes linear after the substrate/product dissociates the cage at 23 Å indicating no further force is applied. *The total work (PMF) implies that the substrate can easily access the active oxidant inside the modeled cage, while the hydroxylated product can escape and leave the space.* These findings shed light on the energetics and dynamics of the substrate/product dissociation process and have important implications for the design and optimization of supramolecular cages for catalytic applications.

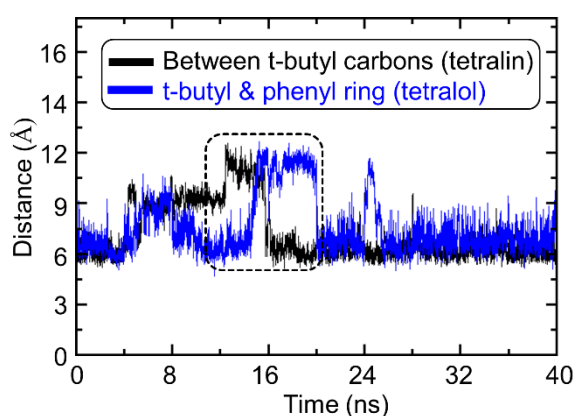


Figure S4. The mutual distance for the gatekeeper groups observed during ASMD simulations.

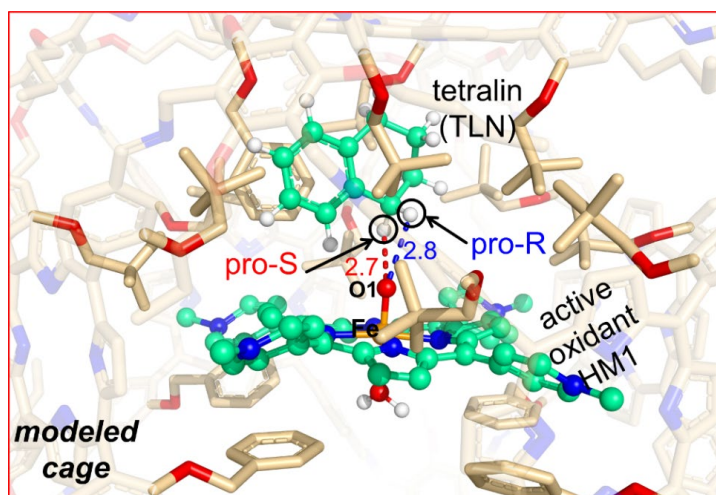


Figure S5. The substrate tetralin (TLN) docked into the so-created active site speculating the initial distances of pro-R(H) and pro-S(H) from reactive O1 atom of active oxidant HM1.

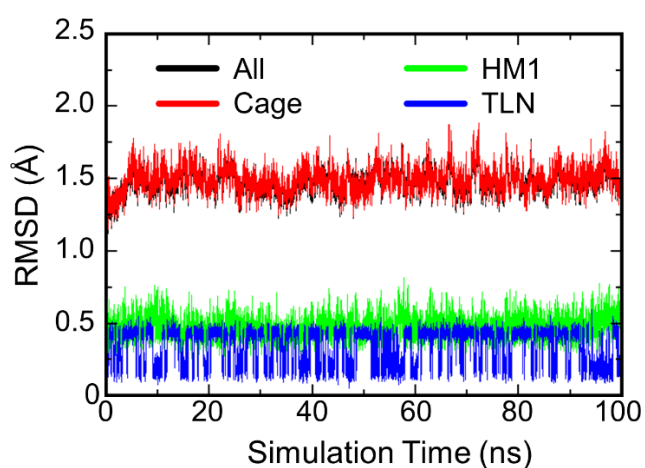


Figure S6. Root mean square deviation (RMSD) during 100 ns MD simulation for modeled cage.

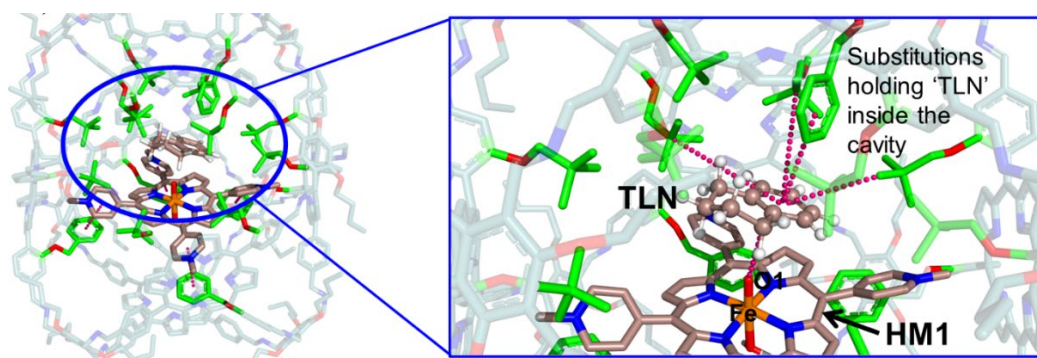


Figure S7. A representative MD snapshot highlighting the substitutions for substrate entrapment.

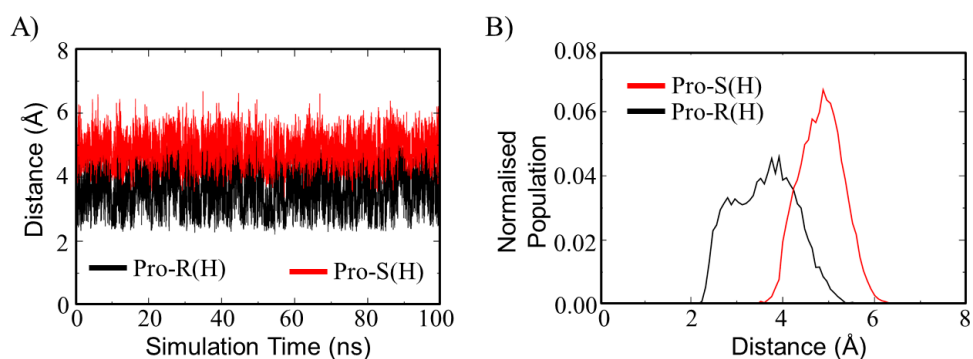


Figure S8. (A) Evolution of pro-R(H) and pro-S(H) distances from O1 atom of the active oxidant HM1 for 100 ns replica simulation. (B) The Boltzmann population distribution plot corresponds to distance plots between the pro-R and pro-S hydrogens with the reactive oxygen (N1) over the 100 ns simulation.

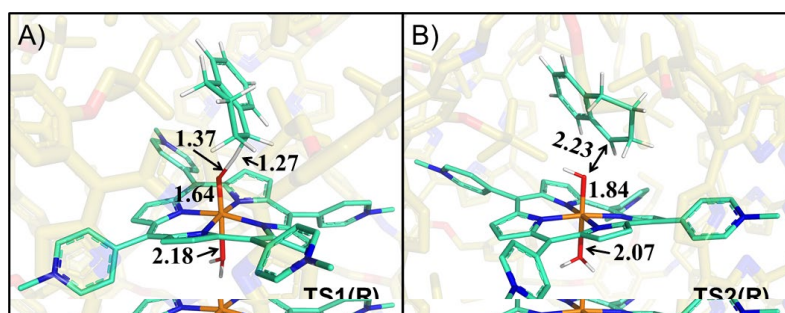


Figure S9. QM/MM optimized transition state structures for R-selective hydroxylation with critical geometric data in doublet spin state. TS1(R) and TS2(R) represent the transition state for H-abstraction and cation transfer steps, respectively. Bond lengths are in Å unit.

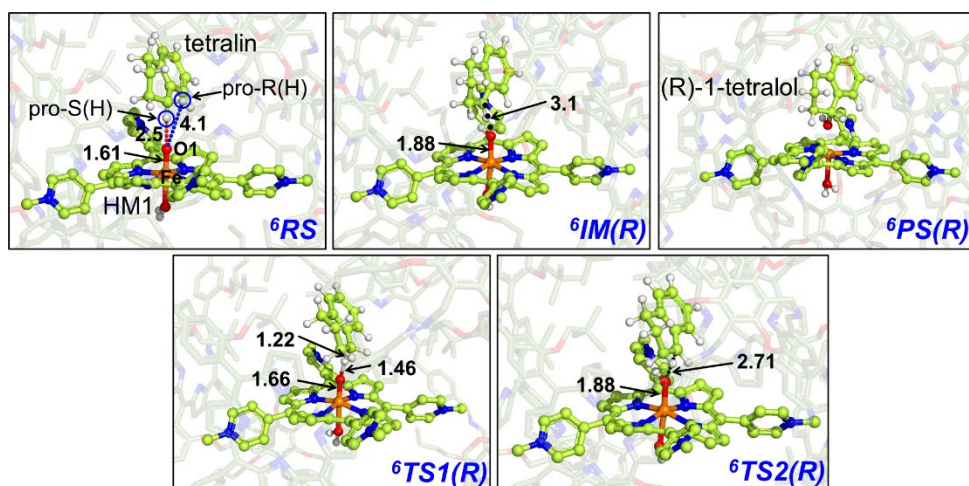


Figure S10. QM/MM optimized structures with critical geometric data for R-selective hydroxylation in sextet spin state, obtained during PES scan. ${}^6\text{TS1(R)}$ and ${}^6\text{TS2(R)}$ represent the transition states for H-abstraction and cation transfer steps, respectively. Bond lengths are in Å unit.

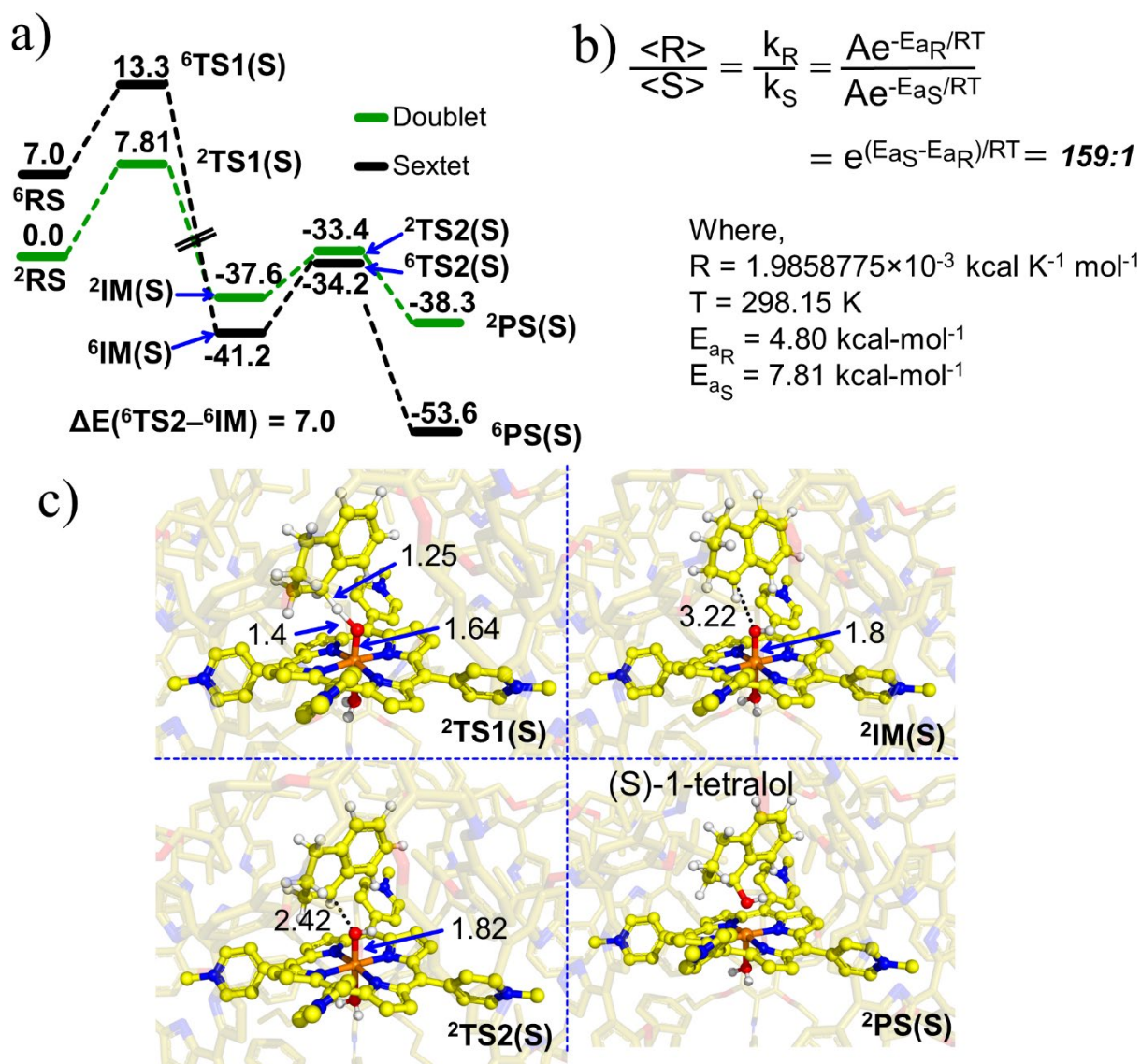


Figure S11. (A) ZPE corrected QM/MM/UB3LYP/def2-TZVP reaction profile diagram for the S-enantioselective C-H hydroxylation of tetralin into S-(1)-tetralol by active oxidant HM1 entrapped inside the modeled cage. (B) Comparative rate constant data for R- and S-selective hydroxylation calculated using the Arrhenius equation. (C) QM/MM optimized structures for S-selective hydroxylation with critical geometric data.

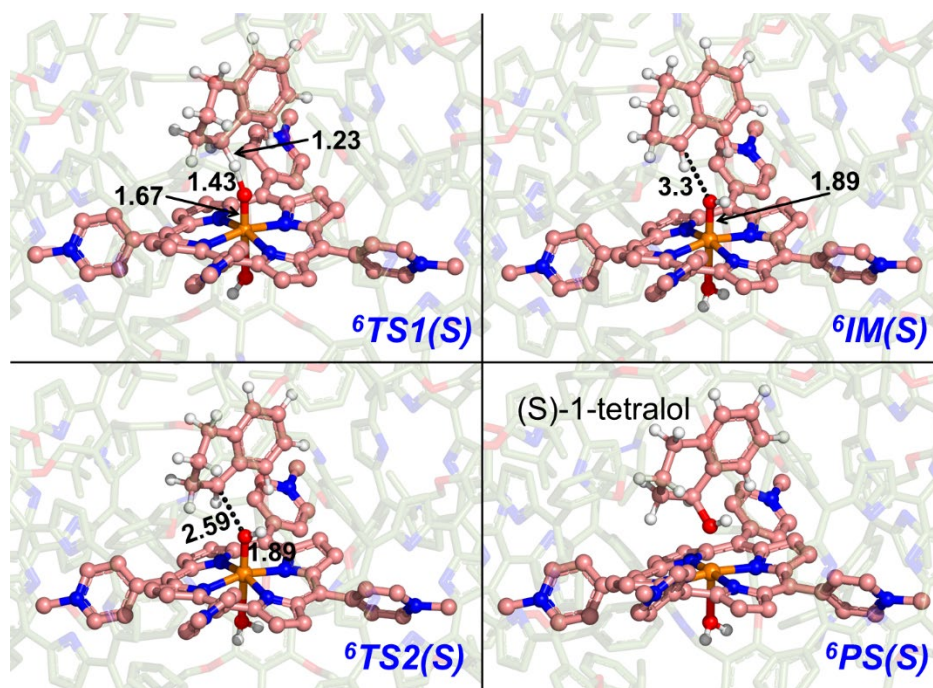


Figure S12. QM/MM optimized structures with critical geometric data for S-selective hydroxylation in sextet spin state, obtained during PES scan. ${}^6\text{TS1(S)}$ and ${}^6\text{TS2(S)}$ represent the transition states for H-abstraction and cation transfer steps, respectively. Bond lengths are in Å unit.

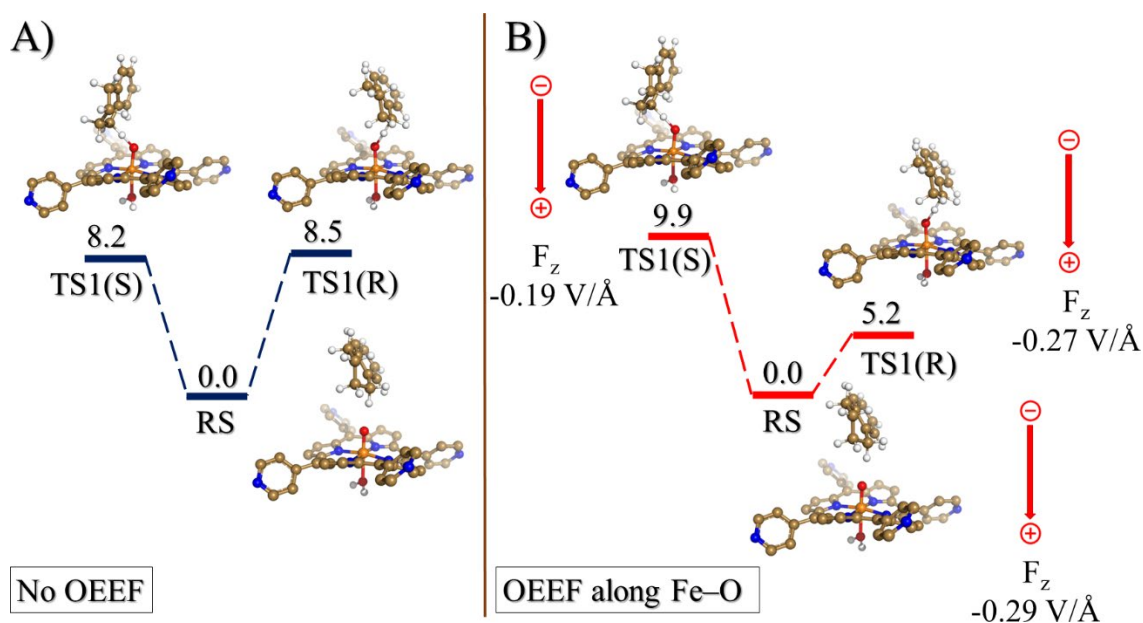


Figure S13. The zero-point corrected UB3LYP/def2-TZVP single-point gas-phase energy profile diagram for RS, TS1(S) and TS1(R) doppelgangers, in (A) the absence of EF and (B) presence of OEEF along Fe–O axis (negative z axis). For electric field vectors, gaussian convention is used.

Table S1. Mulliken spin and charges of RS, IM, and PS species for both the R- and S- reaction profiles (modeled cage).

<u>Mulliken Spin</u>										
	² RS	² IM(R)	² PS(R)	² IM(S)	² PS(S)	⁶ RS	⁶ IM(R)	⁶ PS(R)	⁶ IM(S)	⁶ PS(S)
Fe-O1	2.07	1.07	1.06	1.07	1.05	3.74	4.54	4.29	4.54	4.36
Rest of Complex	- 0.13	-0.07	-0.06	-0.07	-0.05	0.40	0.34	0.56	0.36	0.56
Substrate	- 0.86	0.00	0.00	0.00	0.00	0.81	0.00	0.00	0.00	0.00
<u>Mulliken Charge</u>										
	RS	IM(R)	PS(R)	IM(S)	PS(S)	⁶ RS	⁶ IM(R)	⁶ PS(R)	⁶ IM(S)	⁶ PS(S)
Fe-O1	0.32	0.24	0.33	0.24	0.32	0.47	0.46	0.59	0.47	0.57
Rest of Complex	3.85	3.86	4.00	3.86	4.00	3.86	3.46	4.00	3.47	4.00
Substrate	0.83	0.90	0.34	0.90	0.34	0.80	1.07	0.27	1.05	0.27

Table S2. Mulliken spin and charges of N-methyl stripped RS doppelganger species at the oriented external electric field (OEEF) = 0 and -0.29 V/Å along the Fe=O1 axis.

	<u>Mulliken Spin</u>		<u>Mulliken Charge</u>	
	0.0 V/Å	-0.29 V/Å	0.0 V/Å	-0.29 V/Å
Fe-O1	2.06	2.06	0.32	0.31
Rest of Complex	-1.06	-0.07	0.70	-0.28
Substrate	0.00	-1.00	-0.02	0.97

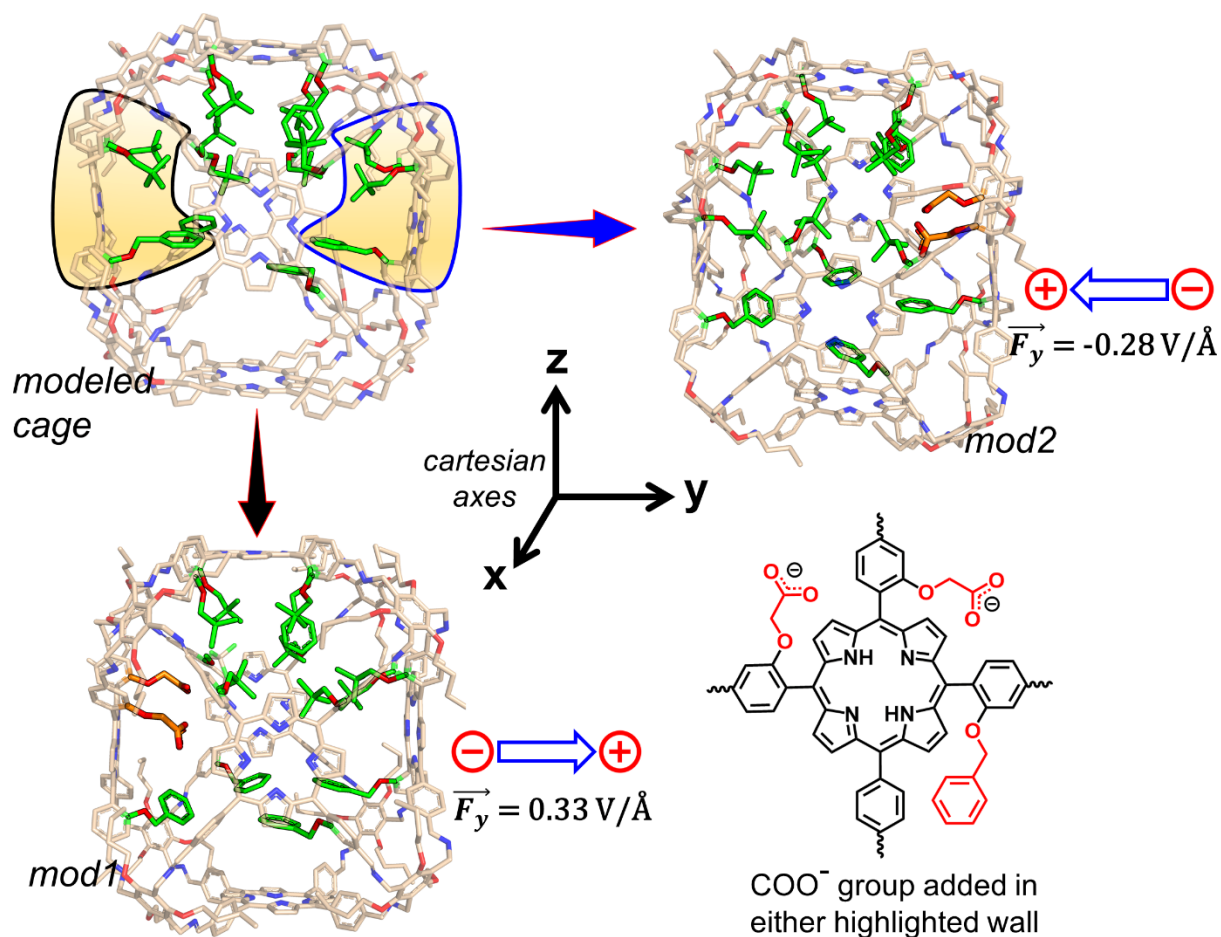


Figure S14. Modification done in either highlighted wall of modeled cage for generating mod1 and mod2. Local electric field (LEF) along y-axis due to modification is also shown.

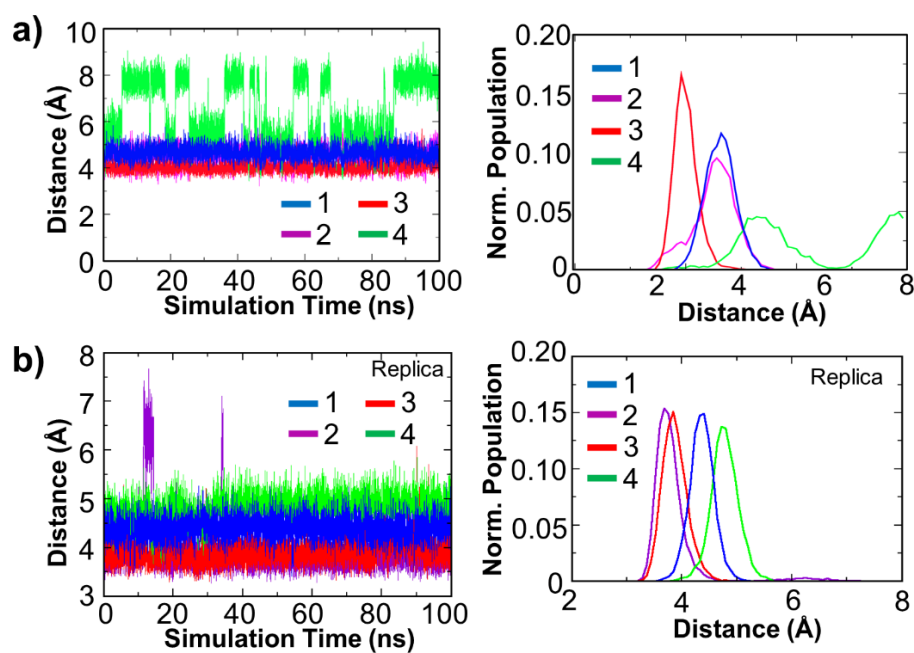


Figure S15. Characterization of pi-pi interactions present between HM1 and cage to stabilize the HM1 inside the cage. The mutual distance between rings of the HM1 and the phenyl rings of the modeled supramolecular cage, (a) for MD simulations, (b) for another replica simulation.

Table S3. QM/MM energy values for all the systems. Energy units are in a.u. B1, B2 and D3 stand for def2-SVP, def2-TZVP and Grimme's Dispersion respectively.

	B1	B2	B2+D3	ZPE
²RS	-3936.253600	-3939.2999	-3939.4429	0.963369031
²TS1(R)	-3936.243468	-3939.2868	-3939.4374	0.957975041
²IM(R)	-3936.3388	-3939.3788	-3939.524	0.972140886
²TS2(R)	-3936.3291	-3939.3706	-3939.5265	0.96922187
²PS(R)	-3936.3457	-3939.3805	-3939.5398	0.970948112
²TS1(S)	-3936.2472	-3939.2897	-3939.4427	0.957905446
²IM(S)	-3936.3321	-3939.3763	-3939.5215	0.972140924
²TS2(S)	-3936.3165	-3939.3673	-3939.5127	0.970201639
²PS(S)	-3936.3370	-3939.3820	-3939.5344	0.976732388
⁶RS	-3936.2423	-3939.2882	-3939.4342	0.96293547
⁶TS1(R)	-3936.2376	-3939.2833	-3939.433	0.95858311
⁶IM(R)	-3936.3286	-3939.3759	-3939.5224	0.97358339
⁶TS2(R)	-3936.3245	-3939.3734	-3939.5215	0.9727141
⁶PS(R)	-3936.3576	-3939.3959	-3939.5537	0.97449413
⁶TS1(S)	-3936.2274	-3939.2714	-3939.4231	0.95616875
⁶IM(S)	-3936.3281	-3939.3744	-3939.5209	0.97227416
⁶TS2(S)	-3936.3164	-3939.3629	-3939.5141	0.97182621
⁶PS(S)	-3936.3556	-3939.3938	-3939.5533	0.97189892
²RS_{mod1}	-3936.8143	-3939.863	-3939.0438	0.96484176
²TS1-R_{mod1}	-3936.7995	-3939.8452	-3939.998099	0.95821706
²TS1-S_{mod1}	-3936.7738	-3939.8182	-3939.969374	0.95855375
²RS_{mod2}	-3936.8369	-3939.8853	-3940.038961	0.96675416
²TS1-R_{mod2}	-3936.8111	-3939.856	-3940.020040	0.96106259
²TS1-S_{mod2}	-3936.8191	-3939.8643	-3940.028253	0.96104858

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QM region for QM/MM optimized geometries:

For *modeled cage*:

² RS				H	23.4347942	26.6360093	22.1566833
N	26.9476408	29.9956137	23.9125132	H	23.9149059	24.7351028	23.9501802
N	25.8465862	27.4397354	24.3478479	H	31.6682363	31.5622222	24.8034019
N	28.1412405	26.7405672	25.8981098	H	32.6425290	29.2420779	25.6722453
N	29.3131899	29.2393443	25.2962543	C	24.0145411	29.3612048	21.6253857
C	25.8176145	30.1294860	23.1557746	C	29.3677174	32.9073634	24.3280394
C	27.5032922	31.2535479	24.0143636	C	31.8088799	26.8462491	26.8774889
C	27.3233466	25.6997550	26.2877451	C	25.2587294	24.2425906	26.2566985
C	29.3552120	26.5330956	26.5016708	C	24.4716504	29.9913522	20.4479573
C	25.0240264	27.7906525	23.2980338	C	23.5923786	30.2883895	19.4244233
C	25.4568606	26.1907186	24.7427133	N	22.2818352	29.9641687	19.5093091
C	29.6722712	30.5118883	24.9393723	C	22.6435107	29.0426525	21.6794215
C	30.4632940	28.6062402	25.7108993	C	21.8065474	29.3397848	20.6117629
C	25.5886184	31.5272152	22.8593416	H	25.5217566	30.2565896	20.3217702
C	26.6146580	32.2258460	23.4178951	H	23.9133132	30.7933334	18.5145342
C	28.0198547	24.8612940	27.2334494	H	22.1980355	28.5899421	22.5628845
C	29.2789566	25.3628631	27.3552596	H	20.7421571	29.0951165	20.6226952
C	24.1506533	26.6831567	22.9708405	C	23.9573143	24.4474575	26.7606929
C	24.3889389	25.7111351	23.8920548	C	23.1622960	23.3795886	27.1357301
C	31.1033263	30.6710839	25.0623469	N	23.6134770	22.1089406	27.0275384
C	31.5980416	29.4838185	25.5062301	C	25.7066507	22.9094500	26.2009460
C	24.9748021	29.0726458	22.7277396	C	24.8696905	21.8689858	26.5910818
C	28.8045233	31.5225153	24.4680674	H	23.5482057	25.4504713	26.8637946
C	30.5076846	27.3447582	26.3391839	H	22.1477597	23.5088723	27.5199204
C	26.0470705	25.4216376	25.7716118	H	26.6963037	22.6564933	25.8187470
H	24.7275804	31.9307808	22.3352022	H	25.1804123	20.8229617	26.5474896
H	26.7442343	33.3039744	23.4285401	C	32.6785892	27.6468452	27.6471791
H	27.5953679	24.0029061	27.7432903	C	33.8858720	27.1410436	28.1096454
H	30.0662015	24.9844678	28.0007346	N	34.2454967	25.8603839	27.8641232

C	32.2348710	25.5232887	26.6333218	H	35.4651061	24.2561901	28.4923731
C	33.4344905	25.0573420	27.1401316	H	36.3349341	25.5961806	27.6543077
H	32.4211771	28.6679855	27.9213963	H	35.7495023	25.8060605	29.3392438
H	34.5860058	27.7455518	28.6890935	H	26.9221909	28.6558336	27.4046511
H	31.6284986	24.8384219	26.0459079	Fe	27.6271235	28.3027446	24.7380043
H	33.7756984	24.0333796	26.9779936	C	30.2450193	26.4538725	20.1136485
C	29.4990358	33.5304284	23.0723467	C	30.7764720	25.2977155	19.3953400
C	30.0989453	34.7786727	22.9587190	C	32.1428696	24.9766190	19.5241410
N	30.5751147	35.4265631	24.0455112	C	32.9870015	25.7910858	20.2539383
C	29.8356928	33.6346807	25.4433540	C	32.4777635	26.9639269	20.9046102
C	30.4290899	34.8791952	25.2773086	C	31.1286561	27.2730011	20.8396948
H	29.1586955	33.0379853	22.1604006	H	32.5318321	24.1032291	18.9972774
H	30.2239718	35.2816244	21.9972610	H	34.0507642	25.5599566	20.3289150
H	29.7339849	33.2411091	26.4562970	H	33.1678305	27.6055543	21.4587274
H	30.8029506	35.4643834	26.1216443	H	30.7314224	28.1409737	21.3705391
O	28.2874250	27.7393090	23.3806880	C	29.8855317	24.4557589	18.5422585
O	26.7600615	29.1087730	26.5643731	H	29.7810603	23.4820459	19.0647325
H	25.8252122	29.3654175	26.5677572	H	30.4218936	24.1833740	17.6163345
C	31.3121109	36.7081736	23.8792664	C	28.7844670	26.7778078	20.0541593
H	31.0438204	37.1575970	22.9154598	H	28.6886112	27.6576657	19.3797021
H	31.0390748	37.3962842	24.6881781	H	28.4622109	27.1407676	21.0470000
H	32.3918730	36.5016212	23.9114139	C	28.5014792	25.0418063	18.2595222
C	21.3776963	30.2784908	18.3798885	H	27.8501639	24.2584183	17.8485883
H	20.3741354	30.4728735	18.7753267	H	28.5845997	25.8207918	17.4823879
H	21.7486397	31.1696315	17.8594144	C	27.9002666	25.6423213	19.5285068
H	21.3487469	29.4225510	17.6892096	H	26.8850687	26.0233019	19.3390427
C	22.6887329	20.9975965	27.3543253	H	27.7998034	24.8592974	20.2992831
H	21.9193873	20.9357069	26.5734672				
H	23.2537178	20.0615071	27.4074056	²TS1(R)			
H	22.2154516	21.1960155	28.3230308	N	27.1254323	29.8833185	23.6124582
C	35.5376155	25.3425839	28.3686209	N	25.9710955	27.3933735	24.1768278

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C	25.9536022	30.0278476	22.9115636	C	25.3089428	24.2970263	26.2331344
C	27.6549752	31.1525646	23.7513135	C	24.4916133	29.9235103	20.2704980
C	27.3823325	25.7454951	26.2426135	C	23.5672378	30.2546112	19.2985400
C	29.4340330	26.5467810	26.4346864	N	22.2567949	29.9564594	19.4466511
C	25.1429937	27.7132307	23.1181461	C	22.7130944	28.9751066	21.5716178
C	25.5600991	26.1628882	24.6294774	C	21.8280858	29.3108459	20.5548827
C	29.8118921	30.4330715	24.6965657	H	25.5370683	30.1799994	20.0964634
C	30.5843955	28.5337815	25.5197794	H	23.8508819	30.7693492	18.3824805
C	25.6933397	31.4272863	22.6761985	H	22.3016437	28.5099005	22.4645115
C	26.7295905	32.1235962	23.2232847	H	20.7620813	29.0830035	20.6152615
C	28.0407311	24.9658233	27.2598503	C	23.9978822	24.5307657	26.6994038
C	29.3107519	25.4462200	27.3687565	C	23.1925013	23.4814137	27.1065854
C	24.2529135	26.6112465	22.8447121	N	23.6421334	22.2057237	27.0655030
C	24.4839264	25.6712684	23.8029011	C	25.7545030	22.9627561	26.2472059
C	31.2410017	30.5740993	24.8103061	C	24.9058803	21.9425607	26.6665239
C	31.7240803	29.3879731	25.2768748	H	23.5879657	25.5394753	26.7425997
C	25.0891540	28.9814929	22.5169558	H	22.1702391	23.6288460	27.4636264
C	28.9513077	31.4390383	24.2122138	H	26.7509370	22.6912110	25.8962598
C	30.6090357	27.3089160	26.2209901	H	25.2138945	20.8947701	26.6762074
C	26.1171209	25.4457758	25.7064888	C	32.8118856	27.6413499	27.4790426
H	24.8035597	31.8330483	22.2040485	C	33.9988015	27.1316451	27.9870725
H	26.8373548	33.2029254	23.2762688	N	34.3050000	25.8210087	27.8568910
H	27.5857968	24.1567388	27.8218738	C	32.2702353	25.4559767	26.6707224
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H	23.5307500	26.5461049	22.0372541	H	32.6064433	28.6931591	27.6605776
H	23.9923962	24.7072933	23.9026301	H	34.7208439	27.7582931	28.5158319
H	31.8139063	31.4526722	24.5269525	H	31.6332638	24.7435459	26.1520348
H	32.7666909	29.1349088	25.4352112	H	33.7567341	23.9438763	27.1372495
C	24.0827953	29.2803599	21.4584577	C	29.5508767	33.5197360	22.8718364

C	30.1233157	34.7840992	22.7905998
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C	30.0089171	33.5150342	25.2235940
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H	25.9002580	29.1992148	26.3408984
C	31.3548504	36.6876535	23.7456207
H	31.0497666	37.1695143	22.8088939
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C	22.7071691	21.1116352	27.4251178
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H	23.2586709	20.1674534	27.4764065
H	22.2569268	21.3293094	28.4009902
C	35.5809535	25.3010081	28.4004378
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H	36.3899258	25.5066384	27.6837484
H	35.7917229	25.8046194	29.3515235
H	27.1886333	28.9212118	27.1601567
Fe	27.7645608	28.2241713	24.5268062
C	30.2240609	27.0761215	20.5702673
C	30.4874283	25.7953431	19.9498695

C	31.7986792	25.3261269	19.9206601
C	32.8493303	26.0810665	20.4638086
C	32.6061471	27.3479765	21.0514221
C	31.3188711	27.8313283	21.1050570
H	32.0211495	24.3715806	19.4359971
H	33.8707843	25.6977003	20.4143318
H	33.4386990	27.9326113	21.4473736
H	31.1118506	28.8024016	21.5626798
C	29.3607967	25.0465281	19.2862159
H	28.9238005	24.3317458	20.0079021
H	29.7571834	24.4345619	18.4614687
C	28.8776468	27.5986751	20.6676308
H	28.8455441	28.6996133	20.5880807
H	28.6595923	27.5833331	21.9219651
C	28.2507376	25.9830606	18.8066270
H	27.4235994	25.3890872	18.3900489
H	28.6268864	26.6304651	17.9953734
C	27.7453950	26.8443586	19.9724632
H	26.9794295	27.5582918	19.6318803
H	27.2428519	26.1843735	20.7041235

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N	25.8708422	27.4303237	24.4703476
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C	25.7838365	30.0516763	23.1697209
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C	27.3488071	25.8477375	26.5579487
C	29.3885798	26.6777443	26.7099209
C	25.0571817	27.7033915	23.3923162

C	25.5203694	26.1841463	24.9182298	C	21.6985350	29.0487990	20.7907145
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C	30.5044413	28.6414126	25.6959102	H	23.5574170	30.8282301	18.7147807
C	25.4972474	31.4491362	22.9154453	H	22.2416988	28.2032154	22.6529615
C	26.5411120	32.1650665	23.4178989	H	20.6647447	28.7012118	20.8299905
C	28.0086825	25.1398592	27.6283521	C	23.9860754	24.5184231	26.9566444
C	29.2764242	25.6349693	27.7097608	C	23.2074267	23.4365068	27.3250967
C	24.2425354	26.5472664	23.0942901	N	23.7050177	22.1789990	27.2998428
C	24.4972145	25.6246729	24.0638987	C	25.8247514	23.0209433	26.5975896
C	31.1266902	30.6428021	24.8602789	C	24.9989456	21.9667180	26.9729249
C	31.6340533	29.4803886	25.3598945	H	23.5380739	25.5116501	26.9927401
C	24.9553148	28.9695085	22.7808537	H	22.1662009	23.5376502	27.6346622
C	28.8068521	31.4924566	24.3465914	H	26.8497814	22.7916453	26.3040307
C	30.5540257	27.4369396	26.4341504	H	25.3465357	20.9316994	26.9994198
C	26.0963881	25.5033349	26.0146454	C	32.8155937	27.7888164	27.5653404
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H	26.6394697	33.2464658	23.4469601	N	34.3218328	25.9695715	27.8905547
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H	30.0456474	25.3392122	28.4184702	C	33.4296168	25.1268753	27.3251784
H	23.5565518	26.4315029	22.2617132	H	32.6167934	28.8453519	27.7315359
H	24.0615081	24.6327339	24.1502762	H	34.7884488	27.9196664	28.4725369
H	31.6857243	31.5029975	24.5028689	H	31.5369544	24.8585512	26.3941992
H	32.6847366	29.2385221	25.4822842	H	33.7269334	24.0797449	27.2623248
C	23.9402740	29.2147493	21.7199593	C	29.3607552	33.5314338	22.9270585
C	29.3555826	32.8754315	24.1730012	C	29.9419630	34.7860971	22.7872695
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C	24.2819908	29.9508583	20.5622989	C	30.5057036	34.8282395	25.0609666
C	23.3295634	30.2381032	19.6025151	H	28.9364475	33.0587360	22.0402891
N	22.0554796	29.7992164	19.7249150	H	29.9690738	35.3158728	21.8329255
C	22.6096738	28.7575374	21.7946420	H	29.9293800	33.1621366	26.2605694

H	30.9607105	35.3948081	25.8772880
O	28.3653065	27.5518322	23.3869215
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C	31.2347393	36.6989879	23.6360246
H	30.9021635	37.1530640	22.6949596
H	31.0055253	37.3764956	24.4680663
H	32.3158694	36.5030501	23.5983488
C	21.0586939	30.1388156	18.6859290
H	20.0635266	30.1533009	19.1455863
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C	22.7855591	21.0523001	27.5853465
H	22.0450256	20.9916259	26.7768457
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H	22.2757140	21.2324330	28.5398951
C	35.6245885	25.4555723	28.3700105
H	35.5659791	24.3659112	28.4700901
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H	26.9562382	28.8654664	27.3991942
Fe	27.6272459	28.3298990	24.8530858
C	30.2211456	26.2618039	20.3169829
C	30.8640752	25.4158901	19.3336918
C	32.2548212	25.3992901	19.2991189
C	32.9988455	26.2453670	20.1330319
C	32.3808526	27.1157784	21.0610607
C	31.0084415	27.1102524	21.1724077
H	32.7655584	24.7453950	18.5897795
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C	30.0376613	24.5480062	18.4261959
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H	28.4104685	26.7400968	21.3477181
H	28.9878715	26.8861188	23.7186569
C	28.5944500	25.0371047	18.2787375
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C	27.9677757	25.3717975	19.6358653
H	26.9800573	25.8564441	19.5423439
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C	27.4715485	25.7353877	26.3024866
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C	29.7528576	30.4652700	24.6862748
C	30.5859960	28.6009214	25.5300623
C	25.5249507	31.4158421	22.8368590
C	26.5768976	32.1253310	23.3344225
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C	29.4067869	25.5083812	27.4362413

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C	24.5448225	25.5836782	23.9005811	C	25.8779888	22.9149538	26.2791164
C	31.1828147	30.6382909	24.7663520	C	25.0472420	21.8787492	26.6942889
C	31.7019913	29.4753084	25.2535495	H	23.7480560	25.4750002	26.9917208
C	24.9842022	28.9424260	22.6537876	H	22.3634578	23.5310694	27.6994354
C	28.8586137	31.4553520	24.2181804	H	26.8594973	22.6603177	25.8762115
C	30.6509945	27.3805297	26.2398147	H	25.3499758	20.8305005	26.6438952
C	26.2056847	25.4104283	25.7851478	C	32.8626152	27.7503957	27.4701505
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H	30.1814598	25.1986427	28.1320876	C	33.5369867	25.1055501	27.1813339
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C	23.9310417	29.2083165	21.6331101	C	29.3944482	33.5301635	22.8433897
C	29.3887274	32.8513416	24.0766914	C	29.9652979	34.7927331	22.7287640
C	31.9557461	26.9093035	26.7914677	N	30.5363494	35.4004135	23.7918899
C	25.4297401	24.2478722	26.3300472	C	29.9494071	33.5425738	25.1734044
C	24.2279292	29.9696164	20.4798413	C	30.5113190	34.8002058	25.0068983
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N	21.9792343	29.8075189	19.7090062	H	29.9933168	35.3394296	21.7836459
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C	21.6633850	29.0352447	20.7711176	H	30.9552446	35.3566452	25.8363034
H	25.2339842	30.3468024	20.2965770	O	28.4585247	27.5105369	23.1511588
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H	22.2698084	28.1684096	22.6027020	H	25.9041595	29.2561821	26.3347919
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C	23.3635894	23.4011119	27.2819435	H	31.0115197	37.3572227	24.4622689

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C	20.9477941	30.1566119	18.7072551
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H	22.1170105	20.9538936	26.6840184
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C	35.6681763	25.4345729	28.3474784
H	35.5924378	24.3505959	28.4896396
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H	35.8706569	25.9168147	29.3113050
H	27.0826484	28.7273233	27.2058874
Fe	27.7124308	28.2655292	24.6592967
C	30.3470764	27.5412866	20.9176522
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C	31.7318217	25.7990982	19.9378787
C	32.8694090	26.4321317	20.4539196
C	32.7666198	27.6139927	21.2135502
C	31.5189454	28.1578654	21.4509843
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H	33.8558236	26.0078426	20.2522679
H	33.6666222	28.0970311	21.5953021
H	31.4171114	29.0749063	22.0372932
C	29.2149313	25.7087468	19.5737317
H	28.7622525	25.0533855	20.3426526
H	29.4721145	25.0549786	18.7273086
C	29.0820834	28.1445407	21.1060803
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C	28.1951350	26.7749143	19.1651954
H	27.2679457	26.2975076	18.8184291
H	28.5895700	27.3641851	18.3202621
C	27.8759225	27.7004368	20.3473569
H	27.3076488	28.5908509	20.0292950
H	27.2298311	27.1793178	21.0765205

²PS(R)

N	27.0367866	29.8459784	23.7610440
N	25.9535400	27.3440814	24.3663039
N	28.2920968	26.7106610	25.9144166
N	29.4138146	29.1657873	25.1973072
C	25.8369108	29.9773947	23.0993145
C	27.5624460	31.1201515	23.8679107
C	27.4701109	25.7018794	26.3819994
C	29.5066389	26.5501631	26.5529647
C	25.0665987	27.6547089	23.3503297
C	25.5791000	26.1065647	24.8401349
C	29.7529972	30.4345135	24.7799861
C	30.5842840	28.5718516	25.6366492
C	25.5615868	31.3728800	22.8583541
C	26.6139091	32.0804217	23.3589508
C	28.1581449	24.9422790	27.3923358
C	29.4185149	25.4533512	27.4888140
C	24.1817041	26.5396813	23.1228040
C	24.4677987	25.6049512	24.0713634
C	31.1775792	30.6142293	24.8870509
C	31.6956690	29.4549031	25.3817499
C	24.9755239	28.9166701	22.7341061
C	28.8706729	31.4191226	24.2877249
C	30.6550679	27.3454284	26.3303096

C	26.1955105	25.3880860	25.8827315	C	32.8715294	27.6943748	27.5603718
H	24.6539510	31.7689386	22.4124396	C	34.0918568	27.1973921	27.9994876
H	26.7180018	33.1611425	23.3952301	N	34.4315620	25.9044183	27.7920572
H	27.7257532	24.1252168	27.9617334	C	32.3639934	25.5270975	26.6707166
H	30.2022949	25.1264124	28.1663900	C	33.5832251	25.0755723	27.1461127
H	23.4287303	26.4559053	22.3468547	H	32.6349107	28.7303589	27.7959101
H	23.9910199	24.6365328	24.1965316	H	34.8175637	27.8193034	28.5288721
H	31.7266158	31.4986727	24.5779326	H	31.7247594	24.8192858	26.1458876
H	32.7452335	29.2375531	25.5472559	H	33.9133167	24.0438973	27.0165211
C	23.9500678	29.1783226	21.6827271	C	29.4547269	33.4499605	22.8715287
C	29.4058442	32.8130034	24.1254735	C	30.0237420	34.7119824	22.7394650
C	31.9679448	26.8665749	26.8619712	N	30.5540541	35.3547950	23.8029199
C	25.4263825	24.2173197	26.4266718	C	29.9252791	33.5375749	25.2197822
C	24.3166948	29.8566286	20.4989579	C	30.4898345	34.7922399	25.0339579
C	23.3698620	30.1500787	19.5347834	H	29.0752188	32.9611489	21.9729988
N	22.0804364	29.7699010	19.6820312	H	30.0826936	35.2297708	21.7798466
C	22.6030949	28.7844779	21.7874515	H	29.8840060	33.1350580	26.2330462
C	21.6988334	29.0748010	20.7752034	H	30.9045576	35.3744933	25.8608276
H	25.3465478	30.1663515	20.3194379	O	28.5771298	27.3703656	23.2178674
H	23.6154102	30.6983946	18.6253438	O	26.8717597	29.0763637	26.3950388
H	22.2167973	28.2785373	22.6677057	H	25.9047150	29.1699812	26.4008499
H	20.6535692	28.7664314	20.8282700	C	31.2620715	36.6494729	23.6097665
C	24.1888632	24.4353922	27.0638733	H	30.9210442	37.1118978	22.6756018
C	23.3965166	23.3643848	27.4437521	H	31.0387497	37.3172491	24.4509639
N	23.7896175	22.0919984	27.2103217	H	32.3430487	36.4536212	23.5609576
C	25.8371879	22.8810048	26.2711412	C	21.0918527	30.1189684	18.6370198
C	25.0014226	21.8413960	26.6673242	H	20.0948762	30.1386983	19.0915893
H	23.8230750	25.4438802	27.2624022	H	21.3359638	31.1095830	18.2350594
H	22.4233587	23.4924759	27.9207976	H	21.1295248	29.3675289	17.8341209
H	26.7881734	22.6272328	25.8001900	C	22.8400237	20.9882789	27.4942977
H	25.2712247	20.7912963	26.5346896	H	22.1035688	20.9431187	26.6801589

H	23.3923613	20.0453221	27.5605179	² TS1(S)		
H	22.3297504	21.1849944	28.4442946	N	26.8160401	30.0443277 23.9244974
C	35.7457983	25.4005018	28.2544670	N	25.7639872	27.4745520 24.3217947
H	35.7085483	24.3075783	28.3179493	N	28.0595198	26.7778002 25.8374874
H	36.5242198	25.7156004	27.5438895	N	29.2027131	29.2889172 25.2725903
H	35.9545119	25.8178165	29.2465866	C	25.6998587	30.1648888 23.1381910
H	27.1358360	28.7175227	27.2579905	C	27.3726371	31.3017152 24.0171592
Fe	27.7000360	28.2422787	24.7594039	C	27.2266726	25.7701271 26.2907939
C	30.0444549	27.2135308	21.2764922	C	29.2715931	26.5936170 26.4664898
C	30.3070603	26.3228705	20.2098675	C	24.9156054	27.8278306 23.2915836
C	31.6452603	26.0078502	19.9199208	C	25.3516884	26.2376972 24.7592068
C	32.7050478	26.6094305	20.5958508	C	29.5500988	30.5689905 24.9177612
C	32.4425179	27.5495327	21.5991624	C	30.3650803	28.6589030 25.6624362
C	31.1222218	27.8380083	21.9389344	C	25.4800447	31.5577727 22.8224495
H	31.8601484	25.2758120	19.1381299	C	26.4943813	32.2640340 23.3955119
H	33.7333305	26.3607185	20.3247642	C	27.9089591	24.9838539 27.2850886
H	33.2667283	28.0514487	22.1102322	C	29.1763349	25.4769278 27.3804122
H	30.9199307	28.5679187	22.7255706	C	24.0078403	26.7400982 23.0165067
C	29.1965805	25.7497488	19.3487610	C	24.2478768	25.7785521 23.9525166
H	29.0986552	24.6655240	19.5271950	C	30.9795913	30.7333260 25.0232427
H	29.4840866	25.8402262	18.2890594	C	31.4886257	29.5453326 25.4492939
C	28.6233681	27.4980898	21.7248459	C	24.8696749	29.1059173 22.7072523
H	28.3511418	28.5521184	21.5585704	C	28.6766457	31.5754945 24.4629182
H	29.2763824	26.7514952	23.4884366	C	30.4242414	27.3962218 26.2887062
C	27.8462468	26.4235137	19.5961331	C	25.9440421	25.4856778 25.7931491
H	27.0365486	25.8355268	19.1380537	H	24.6315621	31.9555534 22.2735584
H	27.8227666	27.4204651	19.1190107	H	26.6270596	33.3422182 23.3928681
C	27.5966377	26.5598585	21.1003932	H	27.4755429	24.1616056 27.8470781
H	26.5798235	26.9208029	21.3077404	H	29.9586174	25.1253194 28.0476939
H	27.6906020	25.5674936	21.5752175	H	23.2601852	26.6994154 22.2311592
				H	23.7429356	24.8213245 24.0503317

H	31.5330146	31.6302905	24.7612791	H	31.4882455	24.8661002	26.0430096
H	32.5373075	29.3094221	25.5960371	H	33.6739335	24.0654232	26.8902200
C	23.9331520	29.3824161	21.5798211	C	29.4152804	33.5510436	23.0452060
C	29.2426155	32.9596191	24.3102315	C	30.0266104	34.7932477	22.9224314
C	31.7285585	26.8924737	26.8159745	N	30.4744426	35.4618449	24.0083526
C	25.1597740	24.3207557	26.3200790	C	29.6801328	33.7077316	25.4231243
C	24.4398972	29.9663716	20.3992392	C	30.2881690	34.9441784	25.2470503
C	23.5961616	30.2676175	19.3478649	H	29.1003569	33.0393055	22.1344773
N	22.2732350	29.9938402	19.4117134	H	30.1834584	35.2737165	21.9541626
C	22.5535632	29.1004231	21.6071155	H	29.5471421	33.3359696	26.4409207
C	21.7523697	29.4049830	20.5131013	H	30.6441535	35.5445577	26.0883025
H	25.5013578	30.1930141	20.2932206	O	28.2215649	27.9223706	23.2697242
H	23.9561302	30.7367319	18.4335669	O	26.6714772	29.1141209	26.5314597
H	22.0726172	28.6735734	22.4860823	H	25.7373767	29.3745330	26.5256455
H	20.6802636	29.1963995	20.5027691	C	31.2267334	36.7338297	23.8342865
C	23.8775386	24.5316175	26.8692142	H	30.9724340	37.1743255	22.8624990
C	23.0920630	23.4600478	27.2583577	H	30.9536495	37.4340986	24.6326022
N	23.5370100	22.1885011	27.1302574	H	32.3033014	36.5143822	23.8803842
C	25.6085656	22.9889550	26.2563257	C	21.4073219	30.3303526	18.2586096
C	24.7829334	21.9476533	26.6674526	H	20.3954828	30.5342505	18.6256128
H	23.4757488	25.5366697	26.9997768	H	21.8041068	31.2237567	17.7619822
H	22.0870091	23.5863315	27.6671575	H	21.3903400	29.4827566	17.5574758
H	26.5902406	22.7364659	25.8535582	C	22.6167820	21.0742686	27.4637398
H	25.0934838	20.9018317	26.6172076	H	21.8194019	21.0363105	26.7100299
C	32.6257619	27.6941954	27.5529755	H	23.1763424	20.1331710	27.4734796
C	33.8439050	27.1840609	27.9814498	H	22.1815972	21.2511648	28.4539194
N	34.1897383	25.9002945	27.7292627	C	35.5033558	25.3859053	28.1824968
C	32.1267679	25.5586733	26.5874918	H	35.4712250	24.2910988	28.2058564
C	33.3444875	25.0926468	27.0519159	H	36.2873884	25.7308289	27.4920714
H	32.3822112	28.7189141	27.8271363	H	35.7035386	25.7673985	29.1908703
H	34.5647318	27.7880330	28.5368778	H	26.8156522	28.6293629	27.3582681

Fe	27.5273258	28.3473723	24.6933221	C	27.2826184	25.8145143	26.3862081
C	29.5698968	25.8122174	21.1752525	C	29.3129995	26.6496436	26.5585264
C	29.5867597	25.3098161	19.8212521	C	25.0224444	27.8373952	23.3342260
C	30.8093532	25.2592754	19.1554312	C	25.4344926	26.2610679	24.8129177
C	31.9706092	25.7920564	19.7323713	C	29.6182872	30.6440288	24.9997779
C	31.9335964	26.3974703	21.0130328	C	30.4117806	28.7337316	25.7651283
C	30.7553162	26.4000266	21.7235530	C	25.5715388	31.5739572	22.8138282
H	30.8557571	24.7871594	18.1711751	C	26.5848922	32.2956313	23.3713409
H	32.9143116	25.7617871	19.1853330	C	27.9762693	25.0115444	27.3645040
H	32.8440472	26.8365050	21.4274400	C	29.2384599	25.5113722	27.4580944
H	30.7036736	26.8329167	22.7248623	C	24.1551779	26.7233022	23.0155179
C	28.3319669	24.7533369	19.1994017	C	24.3798691	25.7666852	23.9588662
H	28.3880231	23.6478144	19.2357695	C	31.0412909	30.8181548	25.1652716
H	28.3140981	25.0020445	18.1258921	C	31.5395141	29.6290398	25.6005201
C	28.3965185	25.6361982	22.0120390	C	24.9732430	29.1131971	22.7373820
H	28.1608730	26.7657134	22.4849126	C	28.7565620	31.6388176	24.4931948
H	28.6669952	25.2781531	23.0180233	C	30.4606993	27.4604426	26.3767134
C	27.0628501	25.2265491	19.9089733	C	26.0099505	25.5199349	25.8679781
H	26.1855718	24.7102725	19.4954314	H	24.7160275	31.9627445	22.2697269
H	26.9137785	26.3066505	19.7270648	H	26.7057880	33.3748914	23.3562839
C	27.1729671	24.9680134	21.4118651	H	27.5493054	24.1747309	27.9074763
H	26.2640868	25.2956282	21.9405022	H	30.0285595	25.1549357	28.1131151
H	27.2430373	23.8778813	21.5932014	H	23.4493333	26.6587437	22.1938412
²IM(S)				H	23.9008838	24.7939010	24.0313392
N	26.9346521	30.0789967	23.9160000	H	31.5995380	31.7213020	24.9401568
N	25.8317082	27.5040285	24.3970221	H	32.5835208	29.4051673	25.7900974
N	28.1001281	26.8355032	25.9497519	C	24.0079998	29.3760975	21.6334749
N	29.2643483	29.3600708	25.3335761	C	29.3112453	33.0253803	24.3459687
C	25.8054425	30.1856711	23.1423999	C	31.7643774	26.9320738	26.8753901
C	27.4693105	31.3482047	24.0041612	C	25.2226519	24.3518359	26.3784940
				C	24.4497072	30.0085507	20.4504050

C	23.5623302	30.2931095	19.4306596	H	29.1880523	33.1090448	22.1694352
N	22.2565411	29.9519246	19.5218036	H	30.2539445	35.3517576	22.0011181
C	22.6416777	29.0344266	21.6895488	H	29.5820040	33.4075863	26.4786041
C	21.7964756	29.3189374	20.6258815	H	30.6636832	35.6264179	26.1400587
H	25.4950349	30.2883114	20.3173519	O	28.3239870	27.7779029	23.3099404
H	23.8720825	30.8023748	18.5191448	O	26.7155782	29.1528030	26.5920643
H	22.2047406	28.5735229	22.5727842	H	25.9994892	29.7980959	26.4817402
H	20.7360688	29.0584282	20.6418266	C	31.2586333	36.8234046	23.8958430
C	23.9234004	24.5578248	26.8895960	H	31.0413696	37.2428886	22.9060893
C	23.1314815	23.4855797	27.2612717	H	30.9376522	37.5330423	24.6676552
N	23.5848428	22.2152142	27.1514641	H	32.3352634	36.6245782	23.9959597
C	25.6787621	23.0210833	26.3364174	C	21.3419041	30.2566619	18.3992124
C	24.8455739	21.9783778	26.7270278	H	20.3379373	30.4349013	18.8010395
H	23.5143968	25.5616442	27.0040837	H	21.6971078	31.1550410	17.8807220
H	22.1149793	23.6097527	27.6416350	H	21.3218421	29.4037411	17.7046896
H	26.6732266	22.7727159	25.9634298	C	22.6583581	21.1000148	27.4615256
H	25.1608495	20.9334743	26.6904580	H	21.8725317	21.0687560	26.6953816
C	32.6787521	27.6923822	27.6347024	H	23.2161619	20.1578846	27.4731452
C	33.8854311	27.1437606	28.0463726	H	22.2079044	21.2693488	28.4463920
N	34.2047558	25.8615139	27.7547391	C	35.4999849	25.3002721	28.2005871
C	32.1415594	25.6007309	26.5936943	H	35.4256719	24.2077823	28.2303490
C	33.3473657	25.0954192	27.0443096	H	36.2928777	25.6130871	27.5052953
H	32.4531986	28.71113874	27.9437192	H	35.7203817	25.6750657	29.2068356
H	34.6180429	27.7128523	28.6217719	H	26.4028045	28.5066776	27.2443631
H	31.4884372	24.9432620	26.0224712	Fe	27.5713019	28.4157853	24.8367048
H	33.6599997	24.0690366	26.8491217	C	30.2110093	25.9311892	20.5647806
C	29.4906942	33.6217783	23.0834707	C	30.8214385	25.1494269	19.5103489
C	30.0913761	34.8692227	22.9672547	C	32.2101368	25.1087864	19.4526722
N	30.5207490	35.5422825	24.0581642	C	32.9831368	25.8911463	20.3204692
C	29.7282544	33.7798422	25.4631981	C	32.3972428	26.7023420	21.3198084
C	30.3253258	35.0218224	25.2946353	C	31.0283191	26.6997757	21.4664270

H	32.6998179	24.4869521	18.7009797	C	26.5677079	32.3025751	23.3639848
H	34.0708904	25.8732144	20.2209727	C	27.9276063	25.0156389	27.3607756
H	33.0345015	27.2966021	21.9772837	C	29.1927182	25.5119131	27.4470107
H	30.5261197	27.2524184	22.2654207	C	24.0639818	26.7611263	23.0522963
C	29.9618598	24.3623905	18.5611014	C	24.2905698	25.7982314	23.9898273
H	29.9722331	23.3092736	18.8971460	C	31.0191877	30.7951798	25.1424509
H	30.4308581	24.3360174	17.5665891	C	31.5130281	29.6014276	25.5681590
C	28.8382357	25.8717512	20.7646171	C	24.9224504	29.1335000	22.7550003
H	28.5218904	28.5594755	22.7701102	C	28.7376713	31.6299459	24.4791263
H	28.4288741	26.3829751	21.6523372	C	30.4288225	27.4354821	26.3402825
C	28.5274695	24.8887500	18.4750067	C	25.9539578	25.5186731	25.8687874
H	27.8959679	24.1915735	17.9091922	H	24.6981226	31.9784371	22.2601110
H	28.5243425	25.8422768	17.9202187	H	26.7030503	33.3798312	23.3359244
C	27.9304090	25.1299048	19.8653897	H	27.4983549	24.1947407	27.9270426
H	26.9482018	25.6324751	19.8282068	H	29.9792666	25.1640230	28.1110880
H	27.7096342	24.1673913	20.3834422	H	23.3406453	26.7118017	22.2450285
²TS2(S)				H	23.7961121	24.8339116	24.0696265
N	26.8903611	30.0892421	23.9331679	H	31.5809314	31.7002209	24.9341949
N	25.7745032	27.5124792	24.4071895	H	32.5551907	29.3742377	25.7615044
N	28.0645285	26.8097878	25.9073711	C	23.9776442	29.3970561	21.6317013
N	29.2386604	29.3368234	25.2860163	C	29.3017709	33.0149221	24.3312080
C	25.7635918	30.1993085	23.1562457	C	31.7307726	26.9065182	26.8493902
C	27.4419005	31.3519753	24.0058252	C	25.1662914	24.3546888	26.3878102
C	27.2384343	25.8015364	26.3668196	C	24.4621645	29.9809878	20.4410665
C	29.2765966	26.6304768	26.5265230	C	23.6034185	30.2652109	19.3970413
C	24.9539586	27.8602768	23.3574275	N	22.2848954	29.9742291	19.4759873
C	25.3668066	26.2733435	24.8278435	C	22.6008315	29.1010521	21.6741760
C	29.5966620	30.6253965	24.9688394	C	21.7840308	29.3873134	20.5877011
C	30.3836522	28.7058466	25.7208353	H	25.5185955	30.2224474	20.3208742
C	25.5472616	31.5863916	22.8121375	H	23.9471129	30.7342914	18.4763434
				H	22.1347520	28.6757710	22.5612415

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C	23.8592472	24.5598639	26.8801503	H	31.0469005	37.2260134	22.8899117
C	23.0708420	23.4886489	27.2618466	H	30.9368046	37.5181471	24.6508785
N	23.5343682	22.2197682	27.1817055	H	32.3362248	36.6078617	23.9859466
C	25.6305859	23.0258794	26.3739840	C	21.4012979	30.2881423	18.3305146
C	24.8008059	21.9842595	26.7749905	H	20.3924223	30.4873074	18.7085034
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H	22.0492543	23.6125429	27.6281575	H	21.3818451	29.4318292	17.6402525
H	26.6300989	22.7745549	26.0175155	C	22.6139247	21.1045971	27.5096487
H	25.1251549	20.9415052	26.7622675	H	21.8152930	21.0719519	26.7571093
C	32.6497121	27.6691020	27.6009306	H	23.1723266	20.1628736	27.5123835
C	33.8571715	27.1203100	28.0115356	H	22.1806530	21.2758780	28.5019177
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C	33.3085749	25.0648954	27.0319835	H	36.2623173	25.6026108	27.4739108
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H	34.5929211	27.6929184	28.5797355	H	26.3300892	28.4908710	27.2067522
H	31.4434750	24.9066276	26.0277435	Fe	27.5253637	28.4166976	24.8161092
H	33.6143838	24.0349948	26.8438273	C	29.8787532	25.9845377	21.3251009
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C	30.1101984	34.8443354	22.9503348	C	31.1512215	25.4369427	19.3330363
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C	30.3017886	35.0179240	25.2798929	C	31.0487419	26.5782471	21.8982359
H	29.2191838	33.0774563	22.1521015	H	31.2242739	24.9474209	18.3606315
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H	30.6265304	35.6292542	26.1259118	H	30.9762098	26.9976103	22.9043827
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C	30.1821031	34.7523967	22.9273181	C	31.0123627	26.2108011	19.7176750
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H	31.5288826	24.8810347	26.1904090	Fe	27.6021917	28.3363113	24.7609619
H	33.6863687	24.0520965	27.0688209	C	30.1643074	26.3308485	20.1443090
C	29.4929162	33.5575146	23.0289824	C	30.8078485	25.2265136	19.4411473
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N	30.5694385	35.4649479	23.9797453	C	32.9613990	25.9432891	20.2908510
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H	30.8143383	35.5200228	26.0527542	H	30.4792976	28.0585767	21.3983960
O	28.2525832	27.7460460	23.4148633	C	30.0084854	24.2832581	18.6047085
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H	25.7550767	29.1058795	26.6606952	H	30.5661108	24.0563197	17.6787421
C	31.3020238	36.7461088	23.7974202	C	28.6784386	26.5152533	20.0654014
H	31.0068531	37.1998319	22.8434674	H	28.5047304	27.3552347	19.3573231
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H	21.3415144	29.3857892	17.6939909	H	26.8623503	25.5568746	19.3745190
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H	22.1582663	21.2002834	28.3624027	N	26.9818695	29.9085114	23.7008023
C	35.5052070	25.3421707	28.3995631	N	25.8005141	27.3295744	24.2309232
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N	29.3926995	29.1156908	25.1759485	C	31.8237062	26.7123543	26.8473613
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C	26.0579304	25.2943185	25.6375420	C	32.6277205	27.4763399	27.7176034
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H	23.7836922	24.6826307	23.9407476	H	34.4603228	27.5184183	28.8918691
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H	32.6682487	29.2174033	25.8389432	H	33.8034929	23.9066716	26.9281860
C	23.9539904	29.2825660	21.5455408	C	29.6058689	33.4222103	22.9605850
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C	21.2612457	30.2033336	18.3469015	H	27.3058812	25.1715611	18.2253321
H	20.2603316	30.3680886	18.7611309	H	28.6180316	26.2807759	17.7974439
H	21.6070198	31.1171049	17.8476011	C	27.7930610	26.6066940	19.7835401
H	21.2392640	29.3660701	17.6334144	H	27.1200344	27.4055663	19.4350466
C	22.6241384	20.9873463	27.3607643	H	27.2132592	26.0253336	20.5222933
H	21.8250032	20.9608253	26.6081054				
H	23.1548896	20.0300293	27.3869669	*IM(R)			
H	22.1950672	21.1935445	28.3475256	N	27.0324788	29.8992774	23.9656482
C	35.4283197	25.1252657	28.5390242	N	25.8670778	27.2814449	24.3990894
H	35.2721446	24.0626802	28.7603583	N	28.2410012	26.4779137	25.9609060
H	36.2557381	25.2563704	27.8261528	N	29.3708590	29.1565374	25.5885850
H	35.6537204	25.6592205	29.4688289	C	25.8884517	30.0369860	23.2248231
H	27.0541169	28.5311612	27.1891024	C	27.5991431	31.1447254	24.0937838
Fe	27.7150259	28.1188308	24.4661678	C	27.4077423	25.4373610	26.3018052
C	30.3006567	26.6007259	20.3314503	C	29.4187522	26.3148249	26.6368227
C	30.4258807	25.2881444	19.7150171	C	25.0300754	27.6787409	23.3848387
C	31.6779840	24.6838729	19.6866495	C	25.4932343	26.0223780	24.7778551

C	29.7305537	30.4321996	25.2225120	H	25.5342038	30.2039305	20.4261055
C	30.4996060	28.5218695	26.0523895	H	23.9047328	30.7563941	18.6424099
C	25.6842959	31.4388807	22.9302362	H	22.2395558	28.5046435	22.6839944
C	26.7267435	32.1243723	23.4861710	H	20.7656280	29.0159930	20.7633662
C	28.0863645	24.5829323	27.2513518	C	24.0084897	24.3223863	26.7898495
C	29.3250758	25.1168199	27.4532614	C	23.1706950	23.2847873	27.1549100
C	24.1349934	26.5862888	23.0572712	N	23.5632211	21.9967275	27.0201017
C	24.3944347	25.5815789	23.9431484	C	25.6835246	22.7160621	26.1895746
C	31.1492699	30.6057812	25.4456877	C	24.8057615	21.7082312	26.5750356
C	31.6286038	29.4257916	25.9304695	H	23.6557029	25.3438094	26.9292636
C	25.0174286	28.9822844	22.8265284	H	22.1669169	23.4503964	27.5535472
C	28.8831096	31.4063766	24.6349755	H	26.6594063	22.4264422	25.7984541
C	30.5362874	27.2040395	26.5915247	H	25.0712112	20.6505926	26.5187809
C	26.1154166	25.2179443	25.7726515	C	32.6866642	27.4444053	27.9677234
H	24.8303130	31.8643834	22.4118235	C	33.8790594	26.9000502	28.4267693
H	26.8625531	33.2019486	23.4942770	N	34.2298385	25.6281360	28.1314734
H	27.6685483	23.7103637	27.7470743	C	32.2491167	25.3766302	26.8398012
H	30.0741596	24.7492094	28.1474209	C	33.4292079	24.8710481	27.3491294
H	23.3924132	26.5597950	22.2664803	H	32.4357037	28.4546078	28.2895876
H	23.9091466	24.6099065	23.9803803	H	34.5788463	27.4630498	29.0441682
H	31.7276006	31.4992233	25.2317529	H	31.6467012	24.7287742	26.2084273
H	32.6646957	29.2129436	26.1703570	H	33.7648331	23.8527330	27.1473170
C	24.0455831	29.2899858	21.7394735	C	29.6400198	33.3590904	23.1961156
C	29.4401752	32.7921608	24.4701897	C	30.2068825	34.6197758	23.0614374
C	31.8252217	26.6907261	27.1415825	N	30.5845196	35.3371830	24.1437022
C	25.2920228	24.0650364	26.2609206	C	29.8075626	33.5889344	25.5750766
C	24.4863558	29.9348628	20.5619908	C	30.3729108	34.8436266	25.3880631
C	23.5956237	30.2399976	19.5507052	H	29.3748733	32.8134122	22.2894818
N	22.2874163	29.9077624	19.6450025	H	30.3806014	35.0805840	22.0871035
C	22.6754594	28.9671713	21.8017754	H	29.6373546	33.2462046	26.5967580
C	21.8274027	29.2694196	20.7457206	H	30.6677342	35.4819011	26.2251434

O	28.6560666	27.4474431	23.2378382	C	29.9127099	24.4602496	18.3346465
O	26.6630291	28.7160560	26.7593624	H	29.8432776	23.4230420	18.7082182
H	25.8139026	29.1821693	26.7242555	H	30.4073970	24.3634410	17.3574289
C	31.2837014	36.6377158	23.9625321	C	28.8450581	26.1947328	20.3926855
H	31.0324684	37.0504811	22.9777931	H	28.4576744	26.7814671	21.2410738
H	30.9618234	37.3385142	24.7416932	H	29.1083922	26.6196662	23.4580173
H	32.3676861	36.4699188	24.0384647	C	28.5182794	25.0692821	18.1838022
C	21.3686185	30.2286867	18.5303711	H	27.8546597	24.3809231	17.6445780
H	20.3648470	30.3944318	18.9383912	H	28.5845967	25.9892629	17.5795129
H	21.7191757	31.1371823	18.0266390	C	27.9134238	25.4257940	19.5430831
H	21.3499969	29.3883063	17.8205021	H	26.9525858	25.9620087	19.4569502
C	22.5913906	20.9227032	27.3314399	H	27.6548265	24.5094433	20.1236578
H	21.8254407	20.8972662	26.5450940				
H	23.1166120	19.9637451	27.3813614	⁶TS2(R)			
H	22.1203470	21.1315563	28.2989279	N	27.0214322	29.8339296	23.7307042
C	35.4956359	25.0602627	28.6444167	N	25.8563255	27.2180604	24.1693304
H	35.3577357	23.9880286	28.8241079	N	28.2752788	26.3826490	25.6475072
H	36.2951844	25.2292683	27.9081790	N	29.3917568	29.0587069	25.2762072
H	35.7500026	25.5542059	29.5887288	C	25.8470817	29.9890614	23.0439006
H	27.1759325	29.1669177	27.4463859	C	27.5823562	31.0800989	23.8846715
Fe	27.7543747	28.1146949	24.7502040	C	27.4394225	25.3510174	26.0095683
C	30.2222845	26.1539272	20.2255149	C	29.4575181	26.2175835	26.3184716
C	30.7997254	25.2329758	19.2706439	C	24.9795883	27.6342318	23.1971567
C	32.1782558	25.0515112	19.2985325	C	25.4772516	25.9650185	24.5620539
C	32.9812497	25.8252181	20.1462764	C	29.7402963	30.3462718	24.9419916
C	32.4354657	26.7847625	21.0289536	C	30.5211660	28.4321926	25.7478228
C	31.0689208	26.9344340	21.0905557	C	25.6223727	31.3986402	22.8062940
H	32.6412325	24.3297491	18.6229413	C	26.6809783	32.0729077	23.3457357
H	34.0635122	25.6857535	20.1220386	C	28.1248361	24.4948062	26.9521174
H	33.0988675	27.3757959	21.6629474	C	29.3689470	25.0201662	27.1361998
H	30.5881958	27.6099170	21.8034474	C	24.0519875	26.5574190	22.9072997

C	24.3332367	25.5469101	23.7788981	C	25.6700163	22.6563028	25.9742009
C	31.1557032	30.5283665	25.1743829	C	24.7966370	21.6662188	26.4127452
C	31.6422438	29.3463590	25.6490871	H	23.7289472	25.3236252	26.8002001
C	24.9571040	28.9443247	22.6558346	H	22.2410438	23.4590278	27.5125611
C	28.8771990	31.3342985	24.4019249	H	26.6203277	22.3493932	25.5359122
C	30.5641001	27.1168736	26.2901008	H	25.0402079	20.6035011	26.3514711
C	26.1268229	25.1482239	25.5267180	C	32.6195730	27.4156418	27.7842370
H	24.7439139	31.8348368	22.3401779	C	33.7903024	26.9011185	28.3269289
H	26.8079102	33.1506635	23.3901601	N	34.1914527	25.6377118	28.0627626
H	27.7053484	23.6295980	27.4587388	C	32.3198810	25.3402876	26.6256770
H	30.1239952	24.6476200	27.8208305	C	33.4704355	24.8621621	27.2220133
H	23.2745570	26.5434736	22.1508577	H	32.3197093	28.4185220	28.0883023
H	23.8329513	24.5842713	23.8386924	H	34.4300292	27.4829349	28.9892048
H	31.7261573	31.4304556	24.9767027	H	31.7847186	24.6832261	25.9456070
H	32.6766701	29.1383873	25.9004219	H	33.8432635	23.8518339	27.0443366
C	23.9531561	29.2765564	21.6067417	C	29.5774167	33.3664241	23.0435589
C	29.4206366	32.7308609	24.2905918	C	30.1429423	34.6325788	22.9565442
C	31.8385791	26.6390856	26.9028636	N	30.5584546	35.2910309	24.0616465
C	25.3051728	24.0119812	26.0566873	C	29.8237313	33.4703560	25.4235156
C	24.3607186	29.9588769	20.4381876	C	30.3842941	34.7330686	25.2845717
C	23.4460109	30.2835479	19.4554885	H	29.2792298	32.8710424	22.1187884
N	22.1447793	29.9309505	19.5649257	H	30.2866237	35.1445708	22.0031032
C	22.5865062	28.9427634	21.6906348	H	29.6889543	33.0749978	26.4312790
C	21.7149538	29.2591793	20.6578997	H	30.7079168	35.3265252	26.1437491
H	25.4019146	30.2444167	20.2872089	O	28.5716815	27.4038242	22.8644302
H	23.7304892	30.8303410	18.5575968	O	26.7135179	28.6400482	26.5013871
H	22.1710664	28.4587225	22.5713629	H	25.8485439	29.0767851	26.4811565
H	20.6578173	28.9894827	20.6883294	C	31.2564267	36.5982779	23.9290002
C	24.0556578	24.2951918	26.6489515	H	31.0065044	37.0467512	22.9596811
C	23.2202389	23.2743828	27.0642694	H	30.9323865	37.2693487	24.7332717
N	23.5836527	21.9792567	26.9189360	H	32.3404738	36.4291825	24.0002830

C	21.2029125	30.2625377	18.4726579	H	27.4529247	25.0852870	18.0986957
H	20.2031520	30.4021564	18.9000220	H	28.6430731	26.2730279	17.5471286
H	21.5297772	31.1876807	17.9826649	C	27.9401113	26.6213666	19.5581863
H	21.1872354	29.4371014	17.7452775	H	27.2247192	27.3980859	19.2411856
C	22.6090106	20.9238261	27.2823019	H	27.4150464	26.0759484	20.3739224
H	21.8246463	20.8860659	26.5147870				
H	23.1258880	19.9611301	27.3461747	^oPS(R)			
H	22.1629376	21.1639846	28.2542320	N	27.1898686	29.7150316	23.7023332
C	35.4234891	25.0940241	28.6775168	N	25.9197602	27.1560396	24.1951242
H	35.2511560	24.0467382	28.9535829	N	28.2940780	26.2719816	25.6768656
H	36.2532733	25.1736088	27.9599170	N	29.4698826	28.9214508	25.3328001
H	35.6567672	25.6732015	29.5777381	C	26.0508951	29.8826208	22.9431949
H	27.2242478	29.1130608	27.1747295	C	27.7979930	30.9508709	23.8133951
Fe	27.7649752	28.0223409	24.4464805	C	27.4542252	25.2203943	25.9908487
C	30.3827349	26.6883647	20.1753191	C	29.4935693	26.0454645	26.3171450
C	30.6005171	25.4278741	19.5025189	C	25.0459284	27.6009441	23.2278404
C	31.8837881	24.8879299	19.5274566	C	25.4809837	25.9225655	24.6113428
C	32.9261922	25.5592859	20.1797491	C	29.8464450	30.2250139	25.0691588
C	32.7318617	26.8041474	20.8183576	C	30.5459795	28.2982135	25.9350128
C	31.4732675	27.3606996	20.8236976	C	25.9230162	31.2732887	22.5880745
H	32.0836090	23.9388652	19.0245284	C	26.9815574	31.9344406	23.1480420
H	33.9185131	25.1045130	20.1973981	C	28.1618991	24.2868435	26.8313687
H	33.5725159	27.3090682	21.2957264	C	29.4235000	24.7790494	27.0099793
H	31.2767564	28.3098898	21.3271274	C	24.0517673	26.5804187	22.9844563
C	29.4490144	24.7253824	18.8370088	C	24.2982068	25.5651592	23.8634606
H	29.0353133	23.9900913	19.5528649	C	31.2105924	30.4161718	25.5014776
H	29.8141635	24.1314829	17.9858533	C	31.6429717	29.2334251	26.0298360
C	29.1091086	27.2482911	20.2126004	C	25.1021495	28.8769669	22.6203857
H	28.9743006	28.1886141	20.7485275	C	29.0513229	31.2041217	24.4236269
H	29.0748831	26.5882607	23.0003217	C	30.5727024	26.9618257	26.4047105
C	28.3263399	25.6726799	18.4155211	C	26.1221751	25.0676045	25.5434412

H	25.1040996	31.7163338	22.0284618	C	33.2492907	26.5549276	29.0816696
H	27.1611609	33.0042953	23.1195432	N	33.9425525	25.4897231	28.6283720
H	27.7506106	23.3829201	27.2719860	C	32.5628671	25.4069358	26.6876311
H	30.2113092	24.3280231	27.6042788	C	33.6246017	24.9301875	27.4388665
H	23.2561664	26.6051687	22.2465521	H	31.6557141	27.9387168	28.7738376
H	23.7474980	24.6322670	23.9455799	H	33.5550023	26.9558879	30.0460157
H	31.7934741	31.3266561	25.4017836	H	32.3439491	24.9207700	25.7393248
H	32.6288417	29.0328843	26.4416937	H	34.2327212	24.0825082	27.1182780
C	24.1114066	29.1964455	21.5490122	C	29.9055248	33.1713808	23.0599728
C	29.6035862	32.6007728	24.3114344	C	30.4247716	34.4571725	22.9750660
C	31.7925599	26.4927300	27.1466774	N	30.6710027	35.1893437	24.0845478
C	25.2827948	23.9360151	26.0619653	C	29.8348888	33.4103565	25.4421755
C	24.5668607	29.6206262	20.2828103	C	30.3697181	34.6859887	25.3050110
C	23.6652982	29.9039271	19.2741673	H	29.7512174	32.6160599	22.1336783
N	22.3329054	29.7786611	19.4724083	H	30.6610751	34.9288519	22.0196552
C	22.7206344	29.0739793	21.7186942	H	29.5795908	33.0662904	26.4451494
C	21.8586573	29.3593104	20.6668158	H	30.5636002	35.3327937	26.1648328
H	25.6314274	29.7213488	20.0685045	O	28.6938346	27.1268610	22.9287061
H	23.9855198	30.2212158	18.2827865	O	26.7480325	28.5962633	26.5188500
H	22.2834386	28.7761488	22.6709255	H	25.8944409	29.0572443	26.4898501
H	20.7765187	29.2583880	20.7593109	C	31.3256763	36.5204721	23.9557680
C	24.0741289	24.2328227	26.7258626	H	31.0372813	36.9760115	22.9999248
C	23.2227436	23.2199392	27.1321722	H	31.0037592	37.1666864	24.7802766
N	23.5338771	21.9227364	26.9083457	H	32.4159871	36.3824465	23.9964694
C	25.5942169	22.5759839	25.8929129	C	21.4012156	30.0926021	18.3638418
C	24.7086823	21.5952696	26.3276619	H	20.4003649	30.2419652	18.7821140
H	23.7885717	25.2632735	26.9378480	H	21.7320242	31.0118888	17.8641738
H	22.2716217	23.4161127	27.6332028	H	21.3885159	29.2551638	17.6505950
H	26.5081380	22.2585111	25.3904529	C	22.5466260	20.8767569	27.2674646
H	24.9120240	20.5298393	26.2026274	H	21.7586216	20.8544648	26.5029865
C	32.1846517	27.0810944	28.3606191	H	23.0525056	19.9074625	27.3215180

H	22.1090521	21.1142246	28.2433066	N	26.8300409	30.0097150	23.7625973
C	35.0330520	24.9025419	29.4440278	N	25.6628894	27.4239286	24.2994494
H	34.6903847	23.9458962	29.8629921	N	28.0673239	26.6578494	25.8244199
H	35.9113449	24.7458554	28.8046724	N	29.2519945	29.2251036	25.2218318
H	35.2853967	25.5954830	30.2547863	C	25.6813875	30.1349146	23.0378330
H	27.2558061	29.0128030	27.2317333	C	27.4141041	31.2478964	23.8483129
Fe	27.7696963	27.9713713	24.6251907	C	27.2235398	25.6541948	26.2406355
C	30.1807294	26.9055941	21.0217003	C	29.2664982	26.4890675	26.4654468
C	30.3831526	25.9855705	19.9691720	C	24.8274374	27.7839116	23.2661136
C	31.6952722	25.5614662	19.7004340	C	25.3023734	26.1662179	24.7046632
C	32.7854879	26.0748764	20.3999799	C	29.5999869	30.4934975	24.8298485
C	32.5855709	27.0344285	21.3993141	C	30.3918831	28.5925572	25.6620888
C	31.2899489	27.4364891	21.7107409	C	25.4757527	31.5350381	22.7212428
H	31.8639509	24.8154902	18.9194517	C	26.5288624	32.2247765	23.2476254
H	33.7941328	25.7406588	20.1543687	C	27.8980693	24.8517294	27.2372309
H	33.4375569	27.4643412	21.9290092	C	29.1597473	25.3545241	27.3679138
H	31.1257935	28.1743826	22.5011556	C	23.9409516	26.6770873	22.9693885
C	29.2319381	25.4850559	19.1173459	C	24.2082144	25.6973203	23.8813819
H	28.9920531	24.4396617	19.3797752	C	31.0295195	30.6523142	24.9707456
H	29.5479399	25.4525172	18.0629695	C	31.5240307	29.4755190	25.4533510
C	28.7904328	27.3189403	21.4544493	C	24.8107550	29.0681620	22.6712117
H	28.6486389	28.4057294	21.3405195	C	28.7253935	31.4891670	24.3207663
H	29.1866395	26.3182046	23.1454778	C	30.4127868	27.3225605	26.3036559
C	27.9720198	26.3374674	19.2773088	C	25.9319641	25.4019494	25.7229484
H	27.1160500	25.8440257	18.7920734	H	24.6115387	31.9524281	22.2124663
H	28.1044058	27.3138904	18.7758860	H	26.6710586	33.3012019	23.2372845
C	27.6687542	26.5444755	20.7633379	H	27.4648438	24.0188120	27.7835295
H	26.7078412	27.0604069	20.9145185	H	29.9247001	24.9965139	28.0517451
H	27.5767578	25.5561008	21.2458685	H	23.1934052	26.6290931	22.1841090
				H	23.7281118	24.7247915	23.9499970
⁶ TS1(S)				H	31.5983477	31.5362354	24.6978365

H	32.5696451	29.2531738	25.6395135	H	33.6575308	24.0005572	26.9930687
C	23.8605441	29.3439560	21.5557723	C	29.4342201	33.5040160	22.9351128
C	29.2911432	32.8746431	24.1858916	C	30.0259074	34.7577777	22.8370062
C	31.7084063	26.8246224	26.8562823	N	30.4815924	35.4043303	23.9328974
C	25.1425801	24.2365805	26.2423211	C	29.7373848	33.6007050	25.3110539
C	24.3498721	29.9362907	20.3709116	C	30.3231125	34.8502937	25.1597692
C	23.4938565	30.2350816	19.3295944	H	29.1084127	33.0144645	22.0162801
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N	22.1860544	29.9702444	19.5071806	H	30.1441578	35.3007702	21.9607682
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C	21.7071050	29.3338686	20.6016049	H	30.7348053	35.5459541	26.0791806
H	25.4072160	30.3115246	20.3631478	O	28.4015829	27.7756736	23.0191953
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H	22.0804061	28.5845869	22.5550442	H	25.6625261	29.3293325	26.6771437
H	20.6477798	29.0690920	20.5949781	C	31.2373965	36.7554356	23.8190812
C	23.9149516	24.4768826	26.8457653	H	30.9775186	37.1847172	22.8438905
C	23.1177094	23.4137920	27.2315717	H	30.9573594	37.4602057	24.6112954
N	23.5454834	22.1374180	27.0902070	H	32.3163010	36.5493060	23.8663737
C	25.6244474	22.9174630	26.2139278	C	21.2930140	30.2737579	18.3670041
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H	23.5323020	25.4874749	26.9889681	H	21.6646739	31.1643650	17.8461152
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H	26.6018814	22.6578784	25.8050287	C	22.6120178	21.0331942	27.4159000
H	25.0822149	20.8349963	26.5593083	H	21.8201215	21.0021772	26.6559108
C	32.6344403	27.6569134	27.6995874	H	23.1622255	20.0867354	27.4304224
C	33.8489105	27.1278230	28.1134397	H	22.1700372	21.2134795	28.4024521
N	34.1876519	25.8489985	27.8280815	C	35.4912516	25.3095111	28.2767221
C	32.1326757	25.5550419	26.6602626	H	35.4307218	24.2163738	28.3200825
C	33.3433963	25.0682797	27.1176329	H	36.2778615	25.6232052	27.5745403
H	32.3947564	28.6743815	28.0045134	H	35.7110126	25.7000941	29.2772437
H	34.5740513	27.7102820	28.6845002	H	27.0509282	29.4442641	27.3406672
H	31.4960501	24.8884527	26.0810124	Fe	27.6077460	28.2724027	24.6610306
H	33.6711237	24.0458691	26.9259092	C	30.2622405	25.8925445	20.4335131
C	29.4137335	33.5706583	23.0646904	C	30.9109513	25.0897992	19.4201841
C	30.0184018	34.8141200	22.9303312	C	32.3005772	25.0770046	19.3937480
N	30.4995281	35.4778762	24.0052832	C	33.0387779	25.8970364	20.2569736
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C	30.3561864	34.9491547	25.2453776	C	31.0429723	26.7092362	21.3260969
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H	34.1285560	25.8942745	20.1858756	C	27.9983489	24.7473449	27.0237658
H	33.0258773	27.3558698	21.8673651	C	29.2468509	25.2744094	27.1774041
H	30.5074339	27.2822305	22.0883249	C	23.9363169	26.6834074	22.9046572
C	30.0905797	24.2525649	18.4802335	C	24.2192229	25.6812029	23.7869575
H	30.1357842	23.2087669	18.8406229	C	31.0423471	30.6695949	24.9493238
H	30.5751225	24.2175188	17.4939484	C	31.5430313	29.4847408	25.4062127
C	28.8877703	25.8071252	20.6086306	C	24.8242728	29.0736389	22.6399195
H	28.4390344	28.5389568	22.4231218	C	28.7325041	31.5072189	24.3215982
H	28.4559453	26.3475915	21.4671830	C	30.4637628	27.2956176	26.1896832
C	28.6396504	24.7238639	18.3575328	C	26.0094136	25.3161273	25.5522386
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H	27.8070070	24.0610678	20.2807093	H	23.1569862	26.6641774	22.1502096
⁶TS2(S)				H	23.7226056	24.7172290	23.8558493
N	26.8625044	30.0052714	23.7251366	H	31.6094459	31.5561431	24.6808083
N	25.7290048	27.3648169	24.1710866	H	32.5915841	29.2584345	25.5709109
N	28.1577364	26.5577935	25.6133997	C	23.8525313	29.3762471	21.5506324
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C	25.6924825	30.1361311	23.0284023	C	31.7576634	26.8194784	26.7610589
C	27.4197961	31.2546296	23.8499123	C	25.2100125	24.1680532	26.0914844
C	27.3175322	25.5507009	26.0334349	C	24.3175586	29.9968866	20.3702324
C	29.3424369	26.4197069	26.2893563	C	23.4463022	30.2954904	19.3415942
C	24.8547168	27.7682506	23.1903021	N	22.1331000	29.9832386	19.4240022
C	25.3550254	26.1126099	24.5735797	C	22.4780837	29.0702358	21.6022263
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C	33.8528271	27.0720230	28.0335439	H	22.1631030	21.1374518	28.2834969
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H	32.3436810	28.5553439	27.8428843	H	35.7500947	25.7881067	29.2585315
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H	31.7110505	24.7348913	25.8835450	Fe	27.5979945	28.1382615	24.5514229
H	33.8714970	23.9859836	26.8426821	C	30.0072292	26.4732718	21.2286913
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C	29.7994748	33.5189179	25.2742905	C	32.3357923	27.1705679	21.0083769
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H	29.1368870	32.9714906	21.9794362	H	31.2384829	25.6589289	18.1575359
H	30.1594656	35.2356682	21.8630136	H	33.2772728	26.6953607	19.1149398
H	29.7021081	33.1093475	26.2809878	H	33.2308678	27.6340138	21.4291724
H	30.7390091	35.3506171	25.9867621	H	31.1623537	27.4270248	22.7958923
O	28.3316115	27.5737171	22.6504016	C	28.7649478	25.4379304	19.2452878
O	26.6333678	28.7721485	26.4680842	H	28.8501196	24.3372504	19.1874825
H	25.7711260	29.2181737	26.4665230	H	28.7121139	25.7792198	18.1989135
C	31.2288719	36.6436640	23.7673193	C	28.8149902	26.2555724	22.1300629
H	30.9351472	37.1185305	22.8230995	H	28.5710236	28.2734436	22.0212908
H	30.9670624	37.3022646	24.6040615	H	29.1373477	25.7598846	23.0538758
H	32.3109408	36.4475615	23.7706618	C	27.4905912	25.8069373	20.0051544
C	21.0913197	30.0717347	18.4142769	H	26.6254230	25.2657064	19.5918872
H	20.0842804	30.1505567	18.8371329	H	27.2764458	26.8859486	19.8837269
H	21.3729411	31.0231281	17.9471875	C	27.6636446	25.4792065	21.4890459
H	21.1270624	29.2613134	17.6713416	H	26.7420226	25.6606546	22.0621768

H 27.8860433 24.4037407 21.5943961

For Modified Cage: 'mod1'

²RS_{mod1}

N 21.8779140 25.6408914 24.2087202

N 20.8394425 23.0462256 24.6788871

N 23.2007557 22.3931033 26.1304390

N 24.2962067 24.9233937 25.5215023

C 20.7188080 25.7485000 23.4923576

C 22.4058615 26.9075831 24.3016786

C 22.4459530 21.3014351 26.5003039

C 24.4487839 22.1922714 26.6660498

C 19.9731317 23.3881592 23.6675842

C 20.5131282 21.7605358 25.0406063

C 24.6106903 26.2153709 25.1959269

C 25.4713313 24.3112215 25.8910865

C 20.4466294 27.1422026 23.2156357

C 21.4780839 27.8621035 23.7420295

C 23.2094500 20.4442858 27.3747136

C 24.4509330 20.9899464 27.4727900

C 19.1211397 22.2639514 23.3454999

C 19.4243507 21.2720901 24.2251210

C 26.0369178 26.4123172 25.3021391

C 26.5744700 25.2263153 25.7023303

C 19.8894513 24.6707193 23.0946821

C 23.7083141 27.2031268 24.7439932

C 25.5646200 23.0318188 26.4747896

C 21.1790176 20.9723728 25.9933297

H 19.5583224 27.5335805 22.7283253

H 21.5806117 28.9439092 23.7547655

H 22.8441930 19.5347630 27.8396822

H 25.2838599 20.6101425 28.0569676

H 18.3938553 22.2070127 22.5427565

H 18.9927937 20.2748291 24.2708571

H 26.5734734 27.3245698 25.0589686

H 27.6273639 25.0098853 25.8510430

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C 19.3283209 25.6335055 20.8567153

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C 17.5505488 24.5674900 22.0689021

C 16.6795045 24.9347626 21.0563627

H 20.3740774 25.9076798 20.7188105

H 18.7073921 26.5379612 18.9878298

H 17.1360411 24.0346560 22.9216840

H 15.6173423 24.6835277 21.0876124

C 19.3162128 19.5992029 27.0202497

C 18.6891798 18.3812610 27.1964472

N 19.2433399 17.2358726 26.7347846

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H 18.8247247 20.5009841 27.3867719

H 17.7204475 18.2849721 27.6871001

H 22.0720935 18.4080525 25.4011172

H 20.8497482 16.2974863 25.7896598

C 27.6422982 23.3919841 27.8498238

C 28.8639926 22.9617149 28.3314186

N 29.3409540 21.7387074 28.0101710

C 27.4248177 21.3092565 26.6605195

C	28.6446840	20.9154911	27.1938900	H	31.4241618	21.4271321	27.7990281
H	27.2744197	24.3628128	28.1756386	H	30.8627538	21.9183873	29.4360243
H	29.4827606	23.5729621	28.9881460	H	22.0723234	24.1923953	27.6169057
H	26.9186372	20.6043099	25.9964645	Fe	22.6199208	23.9494686	25.0000864
H	29.0830824	19.9394661	26.9770837	C	25.9089734	21.6560195	21.2371415
C	24.3053817	29.2507875	23.3636572	C	25.6016099	20.5873874	20.2788033
C	24.9115289	30.4933389	23.2511013	C	26.1578562	19.3162151	20.4728864
N	25.4519608	31.1115613	24.3273899	C	26.9840618	19.0638568	21.5546671
C	24.7758503	29.2883513	25.7137380	C	27.3073760	20.1207489	22.4860542
C	25.3665059	30.5303086	25.5510313	C	26.7762991	21.3873961	22.3085207
H	23.9169400	28.7794183	22.4599561	H	25.9099847	18.5084375	19.7841629
H	24.9980263	31.0163891	22.2971477	H	27.3967958	18.0671080	21.7272680
H	24.7206263	28.8642330	26.7171365	H	27.9599470	19.8801745	23.3293751
H	25.7875696	31.0919927	26.3883712	H	27.0088427	22.1875061	23.0150329
O	23.2514730	23.4171809	23.6184652	C	24.6698207	20.8347494	19.1341412
O	21.8019366	24.7410123	26.8643623	H	23.7322657	20.2952561	19.3828874
H	20.8317615	24.7276092	26.8737225	H	25.0550413	20.3027345	18.2472577
C	26.1864356	32.3896767	24.1629916	C	25.3270720	23.0236236	21.0576729
H	25.9127154	32.8443050	23.2034390	H	26.1460451	23.6619249	20.6621090
H	25.9164830	33.0751900	24.9759497	H	25.0821109	23.4371429	22.0509306
H	27.2674320	32.1910444	24.1872083	C	24.3530181	22.3057458	18.8378897
C	16.1654056	26.0939919	18.9525183	H	23.4756230	22.3590351	18.1761245
H	15.1703660	26.1922329	19.4008202	H	25.1804163	22.7690709	18.2758718
H	16.4892442	27.0649520	18.5594233	C	24.1126949	23.0921963	20.1259634
H	16.1433017	25.3534692	18.1402418	H	23.8933745	24.1475653	19.8981379
C	18.4563692	15.9841214	26.7888481	H	23.2343794	22.7001495	20.6638567
H	17.4887854	16.1733804	26.3078537				
H	18.9835085	15.2206813	26.2090053	²TS1-R_{mod1}			
H	18.3328937	15.6792821	27.8352506	N	21.9760964	25.5500237	24.0200606
C	30.6388433	21.3042402	28.5589726	N	20.8772582	23.0022862	24.5952440
H	30.5637793	20.2555833	28.8594292	N	23.2802665	22.3268801	25.9725007

N	24.4128260	24.7911195	25.2274809	C	26.9819271	22.4772929	26.7992841
C	20.7842716	25.6755421	23.3585293	C	20.5998189	19.6270295	26.2994125
C	22.5192316	26.8140615	24.1002860	C	19.3078109	25.5841947	20.7870388
C	22.5148152	21.2524474	26.3786273	C	18.3810014	25.9630558	19.8400978
C	24.5409609	22.1089774	26.4794112	N	17.0685148	25.6678412	19.9906251
C	19.9787325	23.3475140	23.6108780	C	17.5394921	24.5618505	22.0490159
C	20.5362559	21.7286381	24.9904706	C	16.6504918	24.9488184	21.0585028
C	24.7361272	26.0885850	24.9122541	H	20.3555630	25.8315706	20.6181948
C	25.5843026	24.1784614	25.6204451	H	18.6552637	26.5181165	18.9433139
C	20.5187170	27.0719281	23.1004487	H	17.1335249	24.0392591	22.9121082
C	21.5785090	27.7785550	23.5881696	H	15.5858006	24.7144282	21.1141205
C	23.2875129	20.3962310	27.2428087	C	19.3805589	19.5822981	27.0075590
C	24.5406370	20.9215574	27.3029343	C	18.7390528	18.3723393	27.1877533
C	19.0826596	22.2432161	23.3505820	N	19.2629990	17.2235139	26.6991986
C	19.3983859	21.2583994	24.2332729	C	21.1503278	18.4147342	25.8784877
C	26.1599562	26.2747927	25.0243839	C	20.4630299	17.2215180	26.0958461
C	26.6900331	25.0869511	25.4338646	H	18.9139255	20.4876641	27.3972539
C	19.9115316	24.6160159	23.0085761	H	17.7812529	18.2855258	27.7015259
C	23.8364301	27.0940287	24.5004686	H	22.0792369	18.3580679	25.3129824
C	25.6660329	22.9209799	26.2489089	H	20.8381231	16.2682354	25.7168985
C	21.2259078	20.9357143	25.9206296	C	27.6869956	23.3173418	27.6840721
H	19.6148956	27.4758408	22.6537261	C	28.8981682	22.9151699	28.2134985
H	21.6913112	28.8589548	23.6034179	N	29.4092830	21.7015627	27.9119085
H	22.9193160	19.4983072	27.7270136	C	27.5507155	21.2250939	26.4936596
H	25.3841391	20.5358262	27.8671331	C	28.7605175	20.8627982	27.0743369
H	18.3208187	22.1931548	22.5804135	H	27.2876071	24.2815839	27.9909520
H	18.9444950	20.2731002	24.3118749	H	29.4793329	23.5406316	28.8908780
H	26.6993512	27.1869212	24.7879062	H	27.0877244	20.5031340	25.8144894
H	27.7399460	24.8655115	25.5966177	H	29.2297353	19.8976959	26.8781443
C	18.9045378	24.9015760	21.9587370	C	24.3918058	29.2001831	23.1860054
C	24.3636921	28.4865933	24.4008844	C	24.9690076	30.4606835	23.1162390

N	25.5176717	31.0433861	24.2070751	C	26.8655227	19.5781554	21.4367762
C	24.9048677	29.1498392	25.5261147	C	27.2332670	20.4889394	22.4677129
C	25.4695783	30.4086674	25.4054469	C	26.6914024	21.7514216	22.4692966
H	23.9934915	28.7617980	22.2701280	H	25.7728523	19.2725920	19.5980438
H	25.0228298	31.0278588	22.1855187	H	27.2592999	18.5604515	21.4735889
H	24.8731015	28.6860771	26.5125432	H	27.9175325	20.1423968	23.2458850
H	25.8966762	30.9421970	26.2579282	H	26.9453454	22.4679765	23.2551536
O	23.1843923	23.1832498	23.3859791	C	24.4656032	21.6540301	19.3064913
O	21.9663574	24.6931499	26.6616041	H	23.4639469	21.2414350	19.5243729
H	20.9952833	24.6927719	26.6758452	H	24.7762825	21.1736280	18.3660965
C	26.2206708	32.3448671	24.0858088	C	25.0606840	23.4212865	21.5946952
H	25.9240230	32.8311680	23.1489045	H	25.6897603	24.2037354	22.0516892
H	25.9464741	32.9892761	24.9305419	H	24.2716891	23.2721704	22.5900129
H	27.3058541	32.1696690	24.0881138	C	24.3771514	23.1743521	19.1397742
C	16.1077749	26.1336470	18.9738277	H	23.5772005	23.4246610	18.4246846
H	15.1151360	26.1988993	19.4330485	H	25.3115387	23.5556557	18.6987596
H	16.4158729	27.1243264	18.6180393	C	24.1141457	23.8732659	20.4797639
H	16.0923027	25.4258234	18.1329572	H	24.1764416	24.9678540	20.3667194
C	18.4524824	15.9863509	26.7459918	H	23.0783261	23.6546283	20.7977524
H	17.4893301	16.1969289	26.2646523				
H	18.9657147	15.2164298	26.1621517	² TS1-S _{mod1}			
H	18.3211036	15.6790184	27.7906091	N	22.0393443	25.6222572	24.2992363
C	30.6966777	21.2919373	28.5033743	N	20.9695631	23.0643131	24.8906180
H	30.6264237	20.2459966	28.8148744	N	23.4498871	22.3586453	26.1322911
H	31.4995554	21.4145296	27.7621207	N	24.5196750	24.8808034	25.4450937
H	30.8886562	21.9208467	29.3775831	C	20.8566675	25.7277264	23.6148093
H	22.2340266	24.1229802	27.3999402	C	22.5902488	26.8859535	24.3327906
Fe	22.7082860	23.8540591	24.8080995	C	22.7259004	21.2411012	26.4982574
C	25.7312367	22.1483410	21.4782213	C	24.7401663	22.1328900	26.5608684
C	25.4064103	21.2304542	20.4068158	C	20.0315811	23.4164493	23.9447137
C	26.0018306	19.9756333	20.4023001	C	20.6446132	21.7841668	25.2879109

C	24.8252282	26.1792379	25.1155530	H	20.4874788	25.6849573	20.8382135
C	25.7110205	24.2682007	25.7768156	H	18.8466679	26.1888581	19.0401164
C	20.6071709	27.1111042	23.2898753	H	17.1819722	24.1572086	23.2024148
C	21.6608988	27.8326872	23.7694930	H	15.6898567	24.6767679	21.3088140
C	23.5615512	20.3359750	27.2461659	C	19.6537989	19.4900705	27.2246329
C	24.8071359	20.8820483	27.2821604	C	18.9999300	18.2762499	27.3125641
C	19.1047149	22.3273550	23.7365226	N	19.4539497	17.1878877	26.6481829
C	19.4569025	21.3350856	24.5943110	C	21.3053215	18.4361886	25.8360175
C	26.2511509	26.3740272	25.1789327	C	20.6058352	17.2381286	25.9568871
C	26.8021104	25.1877964	25.5616683	H	19.2416753	20.3486621	27.7551511
C	19.9738947	24.6664167	23.3049308	H	18.0863579	18.1403395	27.8922508
C	23.9118117	27.1740184	24.7106441	H	22.1936866	18.4238510	25.2071403
C	25.8383995	22.9845360	26.3418637	H	20.9295540	16.3303732	25.4431930
C	21.4063566	20.9460909	26.1188800	C	27.9527934	23.3081336	27.6813232
H	19.7147684	27.4977275	22.8059864	C	29.2195342	22.9030977	28.0577049
H	21.7799836	28.9120713	23.7398601	N	29.7413996	21.7449954	27.5872308
H	23.2395906	19.3920580	27.6730820	C	27.7531971	21.3142368	26.3438171
H	25.6879007	20.4642665	27.7605886	C	29.0267134	20.9470773	26.7650822
H	18.3017871	22.2819818	23.0089675	H	27.5590523	24.2329443	28.1010635
H	18.9941095	20.3553845	24.6809928	H	29.8474701	23.4873224	28.7333898
H	26.7779472	27.2882204	24.9213345	H	27.2415841	20.6289369	25.6647848
H	27.8589509	24.9705992	25.6803764	H	29.4920427	20.0162655	26.4356451
C	18.9891555	24.9003154	22.2187025	C	24.4909767	29.2177393	23.3121294
C	24.4377713	28.5651671	24.5596990	C	25.0656553	30.4757305	23.1938540
C	27.1923210	22.5259741	26.7849812	N	25.5893433	31.1113370	24.2673419
C	20.8126694	19.6021314	26.4303106	C	24.9532497	29.2811057	25.6632289
C	19.4322124	25.4640313	20.9994460	C	25.5186255	30.5349608	25.4934370
C	18.5380470	25.7449542	19.9871868	H	24.1129212	28.7331293	22.4109253
N	17.2177604	25.4817594	20.1310296	H	25.1372554	30.9980349	22.2381764
C	17.6168145	24.5924081	22.3061478	H	24.9030691	28.8638220	26.6697668
C	16.7598563	24.8887221	21.2582191	H	25.9284797	31.1094472	26.3277086

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 O 22.1211951 24.7003259 26.9714873
 H 21.1508388 24.7292004 27.0025670
 C 26.2910187 32.4079974 24.0960837
 H 25.9877215 32.8609544 23.1446446
 H 26.0210639 33.0816651 24.9188448
 H 27.3763085 32.2326032 24.0976034
 C 16.2850459 25.8445491 19.0478978
 H 15.2943052 26.0169482 19.4832105
 H 16.6403722 26.7607498 18.5618207
 H 16.2336150 25.0292706 18.3126962
 C 18.6112607 15.9733304 26.6071854
 H 17.6908716 16.2235350 26.0631907
 H 19.1404062 15.2021591 26.0404393
 H 18.4010268 15.6492042 27.6335955
 C 31.1282891 21.3910002 27.9550224
 H 31.3361392 20.3678815 27.6367839
 H 31.8198999 22.0811485 27.4529743
 H 31.2396959 21.4752503 29.0423346
 H 22.3816412 24.0869668 27.6772740
 Fe 22.8083956 23.9361050 25.0510068
 C 25.0027389 21.7517508 21.3336571
 C 25.6975164 21.3540232 20.1303560
 C 26.5645293 20.2674486 20.1989233
 C 26.7995843 19.5977050 21.4127075
 C 26.1352839 20.0003886 22.6014674
 C 25.2542164 21.0514102 22.5556959
 H 27.0423102 19.9019990 19.2861590
 H 27.4794777 18.7458522 21.4687274
 H 26.3246700 19.4493303 23.5229910
 H 24.7195333 21.3749022 23.4502517

C 25.3755225 22.0241280 18.8168571
 H 25.4821886 21.2806885 18.0157535
 H 26.1299037 22.8007113 18.6078086
 C 23.9655072 22.7553782 21.2718102
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 H 22.9994194 22.3099290 21.5733828
 C 24.0063142 22.7129165 18.7816992
 H 23.1939443 21.9688768 18.7612233
 H 23.9138454 23.3033598 17.8586565
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For modified cage: 'mod2'

²RS_{mod2}

N 22.0329668 25.8554698 23.7080609
 N 20.8188246 23.4557761 24.5334693
 N 23.1833969 22.8188304 26.0207524
 N 24.4563340 25.1393761 24.9796775
 C 20.8181167 26.0105459 23.0987693
 C 22.6835249 27.0589041 23.5658999
 C 22.3568867 21.8475497 26.5388625
 C 24.4132618 22.6430676 26.6059954
 C 19.9355944 23.7489502 23.5163613
 C 20.4139301 22.2589939 25.0562341
 C 24.8846124 26.2820713 24.3438189
 C 25.5795489 24.5207000 25.4645096
 C 20.6351213 27.3867264 22.6975428
 C 21.7885371 28.0391866 23.0046316
 C 23.0560688 21.1008991 27.5528515
 C 24.3282532 21.5868010 27.5947970

C	18.9965474	22.6670392	23.3497756	N	18.6277944	18.3062287	27.4605178
C	19.2685896	21.7599531	24.3278196	C	20.7205053	19.0799274	26.6129184
C	26.3256197	26.3483725	24.3703963	C	19.8746006	18.0506740	27.0012143
C	26.7588818	25.2525078	25.0511136	H	18.6344032	21.6576866	27.3801826
C	19.8960244	24.9737194	22.8389712	H	17.2091938	19.7241994	28.0347300
C	24.0588948	27.2601251	23.7610818	H	21.6976884	18.8242315	26.2009947
C	25.5811192	23.3755602	26.2912692	H	20.1591425	16.9997559	26.9250264
C	21.0535497	21.5586054	26.0994946	C	27.7871777	23.7779321	27.4977647
H	19.7376117	27.8074558	22.2547190	C	28.9604989	23.2886586	28.0460105
H	22.0185732	29.0881795	22.8663367	N	29.2538512	21.9668917	27.9967600
H	22.6247758	20.3097095	28.1571025	C	27.2326671	21.5490950	26.8100568
H	25.1216622	21.2635231	28.2621149	C	28.4085707	21.1066743	27.3825279
H	18.2200344	22.5978239	22.5953767	H	27.5814340	24.8404188	27.6027095
H	18.7637032	20.8129600	24.4961140	H	29.6812756	23.9357292	28.5503022
H	26.9248739	27.1211817	23.8994880	H	26.5888633	20.8287771	26.3099878
H	27.7922888	24.9712126	25.2256846	H	28.7077855	20.0576934	27.3631837
C	18.9084449	25.2252711	21.7573136	C	24.5918720	28.8159862	21.8419101
C	24.6981176	28.4948092	23.2033662	C	25.3243652	29.8728272	21.3095278
C	26.8689839	22.9118388	26.8655071	N	26.1222764	30.6164127	22.0969880
C	20.2874698	20.4184153	26.6768145	C	25.4921773	29.3387438	24.0042008
C	19.3792906	25.7364325	20.5329429	C	26.1819290	30.3876154	23.4279476
C	18.4929869	26.0790560	19.5289346	H	23.9931564	28.2257834	21.1477299
N	17.1627792	25.8954293	19.6964693	H	25.3319970	30.0880837	20.2382443
C	17.5223666	25.0146357	21.8826272	H	25.5798395	29.1793919	25.0779095
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H	20.4407894	25.8885187	20.3421958	O	23.2095282	23.4260885	23.3914251
H	18.8479027	26.5188560	18.5956986	O	21.9801116	25.3428677	26.4445098
H	17.0785166	24.6334517	22.8002502	H	21.0361917	25.5507397	26.3625054
H	15.5980256	25.2083337	20.8947358	C	27.0415475	31.6043988	21.4955819
C	19.0124081	20.6445560	27.2419273	H	26.7011721	31.8182544	20.4824681
C	18.2095311	19.5853324	27.6184394	H	27.0398214	32.5177951	22.1023027

H	28.0391694	31.1454281	21.4409692
C	16.2351217	26.3085722	18.6273084
H	15.2249561	26.3589405	19.0447001
H	16.5281273	27.3004804	18.2653146
H	16.2699026	25.5815305	17.8031131
C	17.6779452	17.2065752	27.7316938
H	16.9265736	17.1774216	26.9308607
H	18.2242449	16.2584019	27.7707930
H	17.1840791	17.3793134	28.6947964
C	30.5111359	21.4700997	28.5880805
H	30.4186248	20.3951358	28.7802602
H	31.3443428	21.6643534	27.8969678
H	30.6876009	21.9933522	29.5356723
H	22.0550413	24.8058194	27.2478247
Fe	22.6858410	24.2392186	24.6777135
C	25.7309237	24.4950412	20.3124874
C	25.7216441	23.0525626	20.0298710
C	26.9188546	22.3403605	20.1381857
C	28.0797465	22.9772766	20.5705025
C	28.0712480	24.3657867	20.9206619
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H	26.9404576	21.2775507	19.8866137
H	29.0126842	22.4131764	20.6474974
H	28.9828993	24.8417326	21.2809979
H	26.9389310	26.1831559	20.9817833
C	24.4331316	22.3656720	19.6965394
H	24.0848856	21.9219288	20.6551508
H	24.6318245	21.5076795	19.0321428
C	24.5249830	25.3007022	20.0545007
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C	23.3250885	23.2872959	19.1686940
H	22.3777776	22.7270173	19.1501997
H	23.5256720	23.6054831	18.1335682
C	23.2042244	24.5247927	20.0533851
H	22.4195574	25.1859598	19.6684806
H	22.9600904	24.2311828	21.0905935

²TS1-R_{mod2}

N	22.1917220	26.5363187	23.6503859
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N	23.5978992	23.2117648	25.3125883
N	24.6406711	25.8138427	24.8586806
C	20.9662045	26.6792352	23.0445844
C	22.6906218	27.8044953	23.8427152
C	22.7883436	22.1849013	25.7491317
C	24.7724971	23.1023043	26.0082010
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C	20.9694028	22.5969786	24.1312744
C	24.9724200	27.0874906	24.4686578
C	25.8188166	25.1827659	25.1766394
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C	26.4128622	27.2327778	24.4345998
C	26.9307620	26.0460621	24.8621598
C	20.1886128	25.6293763	22.5035978
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C	25.9034424	23.9321973	25.8255079

C	21.5539688	21.8320385	25.1685745	C	28.0427238	24.3067829	27.1618857
H	19.6878281	28.4670452	22.5952156	C	29.1410962	23.7815977	27.8238148
H	21.7841524	29.8411356	23.5963982	N	29.4127955	22.4558232	27.7791897
H	22.9990857	20.6872394	27.4337749	C	27.5481330	22.1090077	26.3415421
H	25.4113436	21.7649484	27.7267289	C	28.6390612	21.6301800	27.0367099
H	18.9408331	23.1440034	21.5665415	H	27.8407082	25.3680822	27.2805632
H	19.5562409	21.1064245	23.1894269	H	29.8097635	24.4028344	28.4231577
H	26.9564035	28.0972183	24.0587345	H	26.9657601	21.4126138	25.7422442
H	27.9797490	25.7738380	24.9164530	H	28.9228870	20.5766735	27.0197195
C	19.0350291	25.9543878	21.6103675	C	24.3297126	30.2389829	22.8299330
C	24.5779556	29.4752846	23.9775398	C	24.9563704	31.4648911	22.6521376
C	27.1785854	23.4710951	26.4236491	N	25.8191653	31.9359936	23.5721959
C	20.8198361	20.6367698	25.6471192	C	25.4576994	30.0213044	24.9323507
C	19.1770973	26.7064019	20.4317559	C	26.0715325	31.2344303	24.6987999
C	18.0548396	27.0121586	19.6671355	H	23.7333165	29.8552056	22.0041327
N	16.8280602	26.5572725	20.0094282	H	24.8311291	32.0510814	21.7407406
C	17.7438606	25.4830548	21.9198833	H	25.6696996	29.4991846	25.8646312
C	16.6702001	25.7778265	21.1044547	H	26.7739779	31.6805133	25.4035167
H	20.1466937	27.0353296	20.0537679	O	23.7190064	24.4812447	22.7684689
H	18.1334740	27.5996478	18.7521838	O	22.1233211	25.4178019	26.1797040
H	17.5577009	24.8824561	22.8044456	H	21.1828368	25.6237694	26.0656991
H	15.6707713	25.3964274	21.3035680	C	26.5447034	33.1915041	23.3070166
C	19.4315299	20.7101508	25.9125947	H	27.1826898	33.0497083	22.4242964
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N	19.3477792	18.4202579	26.5571761	H	27.1613427	33.4332620	24.1787578
C	21.4239208	19.3816023	25.8766557	C	15.6531650	26.8512805	19.1592421
C	20.6766559	18.3081438	26.3343276	H	14.7510563	26.8442551	19.7831361
H	18.8883882	21.6439363	25.7857366	H	15.7806560	27.8345265	18.6916092
H	17.6606141	19.6448442	26.5734295	H	15.5669525	26.0814229	18.3788151
H	22.4812929	19.2201166	25.6708215	C	18.5404298	17.2593987	26.9818464
H	21.1184768	17.3300798	26.5275385	H	17.7817540	17.0559688	26.2160222

H	19.1949653	16.3916301	27.1128178	² TS1-S _{mod2}		
H	18.0487293	17.4882962	27.9339516	N	22.0691008	25.9208673 23.6343638
C	30.5670175	21.9046568	28.5150545	N	20.9050675	23.4842328 24.3473291
H	30.3578630	20.8624374	28.7839236	N	23.2358814	22.8667255 25.8794466
H	31.4639408	21.9611751	27.8814348	N	24.4810567	25.2248254 24.9038167
H	30.7183430	22.4921662	29.4281592	C	20.8452749	26.0798743 23.0386391
H	22.1562127	24.7094289	26.8399168	C	22.6663097	27.1633831 23.6151136
Fe	23.0132221	24.8537963	24.2418038	C	22.4090274	21.8893657 26.3876740
C	25.6757402	27.0862586	19.0976062	C	24.4562035	22.7162545 26.4921973
C	25.6020158	26.3700011	20.3740314	C	20.0494271	23.7733956 23.3007068
C	26.8104185	25.9606482	21.0140865	C	20.5246053	22.2591687 24.8263140
C	28.0269878	26.3521037	20.5198044	C	24.8941741	26.3924757 24.2989955
C	28.0856516	27.1932147	19.3687973	C	25.6161942	24.5953518 25.3528795
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H	24.4978911	26.9422578	22.0106099	C	26.3343951	26.4564149 24.2902914
H	24.0948520	25.3445821	21.8371513	C	26.7826682	25.3395325 24.9301406
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H	24.0632452	26.6456057	17.7662613	C	24.0423196	27.3918433 23.7952159
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C	23.0912190	26.7133307	20.3197268	C	21.1306213	21.5657935 25.8963077
H	22.2847607	26.9540707	21.0211005	H	19.6842295	27.8930555 22.3721866
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C	23.3268119	27.8863331	19.3545506	H	22.6610571	20.3898194 28.0468599
H	22.4091560	28.1184342	18.8005828	H	25.1384005	21.3807973 28.1929094
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				H	18.9652662	20.7657546 24.1589867

H	26.9236500	27.2403143	23.8221677	H	26.6023454	20.8877238	26.2617063
H	27.8197369	25.0525156	25.0720732	H	28.7176022	20.1206038	27.3139270
C	18.9605085	25.3170976	21.6302046	C	24.3960618	29.1196100	21.9938641
C	24.6317835	28.6768767	23.3041154	C	25.0268166	30.2613355	21.5115037
C	26.9121160	22.9841318	26.7564721	N	25.8516297	30.9725589	22.2980282
C	20.3573926	20.4230806	26.4578714	C	25.4887220	29.4596004	24.1009741
C	19.3663890	25.9684269	20.4484968	C	26.0772528	30.5943093	23.5743491
C	18.4332441	26.3190185	19.4868253	H	23.7640003	28.5618656	21.3040024
N	17.1253382	26.0159952	19.6533080	H	24.9260776	30.5860552	20.4739324
C	17.5942283	24.9958863	21.7542960	H	25.6994070	29.1926697	25.1357247
C	16.7051928	25.3471026	20.7533575	H	26.7533898	31.2257788	24.1510929
H	20.4070347	26.2216007	20.2430291	O	23.3473188	23.4233121	23.2874129
H	18.7357285	26.8495417	18.5814467	O	21.9959531	25.3391073	26.3159613
H	17.1955021	24.5123401	22.6434623	H	21.0323188	25.4369613	26.2636508
H	15.6396616	25.1221399	20.8177423	C	26.5851944	32.1321890	21.7473577
C	19.0262552	20.6289279	26.8868504	H	26.4824871	32.1205631	20.6593454
C	18.2385924	19.5726327	27.2979478	H	26.1621856	33.0536093	22.1705841
N	18.7205254	18.3064159	27.2988087	H	27.6458450	32.0124682	21.9950582
C	20.8401138	19.1018209	26.5359788	C	16.1463854	26.4146026	18.6236046
C	20.0067862	18.0716737	26.9518309	H	15.1498595	26.4269798	19.0770194
H	18.5945683	21.6279177	26.8933036	H	16.3962540	27.4182919	18.2621854
H	17.2041149	19.7023421	27.6250930	H	16.1745958	25.6972156	17.7902935
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H	20.3390413	17.0328796	26.9926735	H	17.0427052	17.1129174	26.8384153
C	27.8412667	23.8537180	27.3669804	H	18.3700519	16.2660036	27.7070032
C	29.0111015	23.3632707	27.9230586	H	17.3088735	17.4038818	28.5877278
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C	28.4324132	21.1737662	27.3101084	H	31.3829915	21.7468662	27.8062103
H	27.6480423	24.9202878	27.4523106	H	30.7149246	22.0562143	29.4455394
H	29.7380686	24.0132493	28.4155282	H	22.1610680	24.8391575	27.1301833

Fe	22.7501868	24.2900494	24.5384110
C	25.7744475	25.2041967	20.3543807
C	25.4130157	23.8284277	20.6709096
C	26.4385693	22.8952638	21.0158133
C	27.7427118	23.3070838	21.1407957
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H	26.1574699	21.8538877	21.1713080
H	28.5328060	22.5946935	21.3894824
H	29.0880853	25.0204602	21.0939960
H	27.3949412	26.6348631	20.3317601
C	24.0203224	23.4307706	20.7168040
H	23.7683782	23.5368412	21.9145670
H	23.8752916	22.3427866	20.6063487
C	24.7319688	26.1126724	19.7868896
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C	22.9945874	24.3191654	20.0280456
H	21.9854057	24.0552282	20.3832742
H	23.0011464	24.1261067	18.9398148
C	23.3247457	25.7866277	20.2905383
H	22.6067664	26.4487273	19.7948071
H	23.2719658	25.9708216	21.3762162