

Electronic Supplementary Information for
Degradation of Novichok Nerve Agent A234 by
Phosphotriesterase: Insight into the pH-Regulated Mechanism
from QM/MM and MM MD simulations

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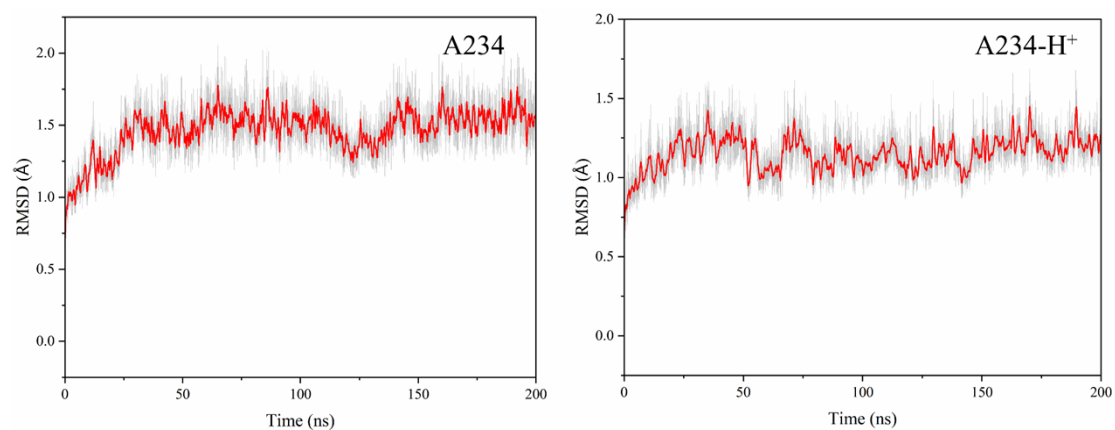


Figure S1. Evolution of RMSD values of enzyme-A234 system (left) and enzyme-A234-H⁺ system (right) during the 200 ns MM MD simulations, and the backbone of enzymes was used to calculate the RMSD value.

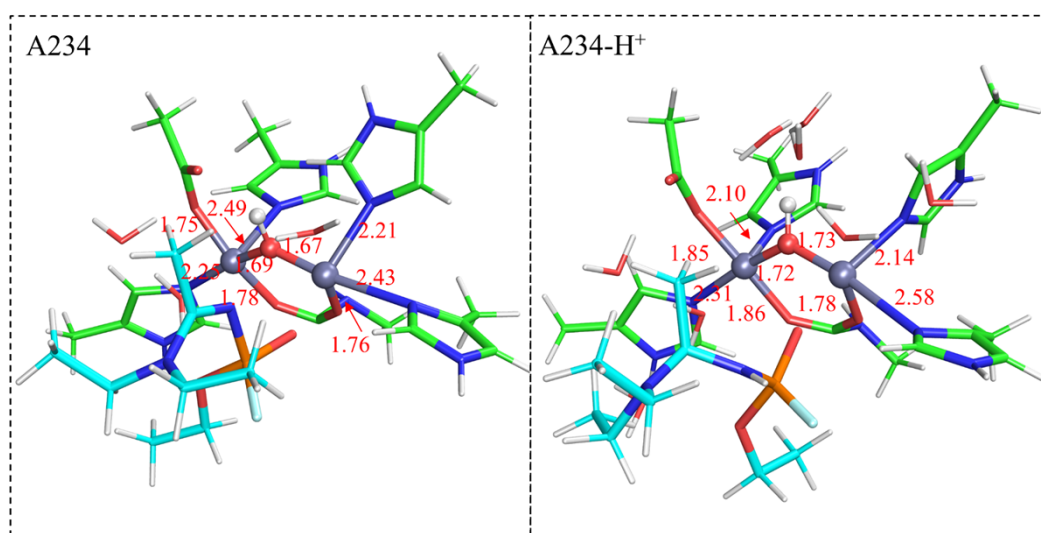


Figure S2. The selected QM region in QM/MM calculations for two models. The reference structures were obtained from the MM MD simulations, and the distances are given in Å.

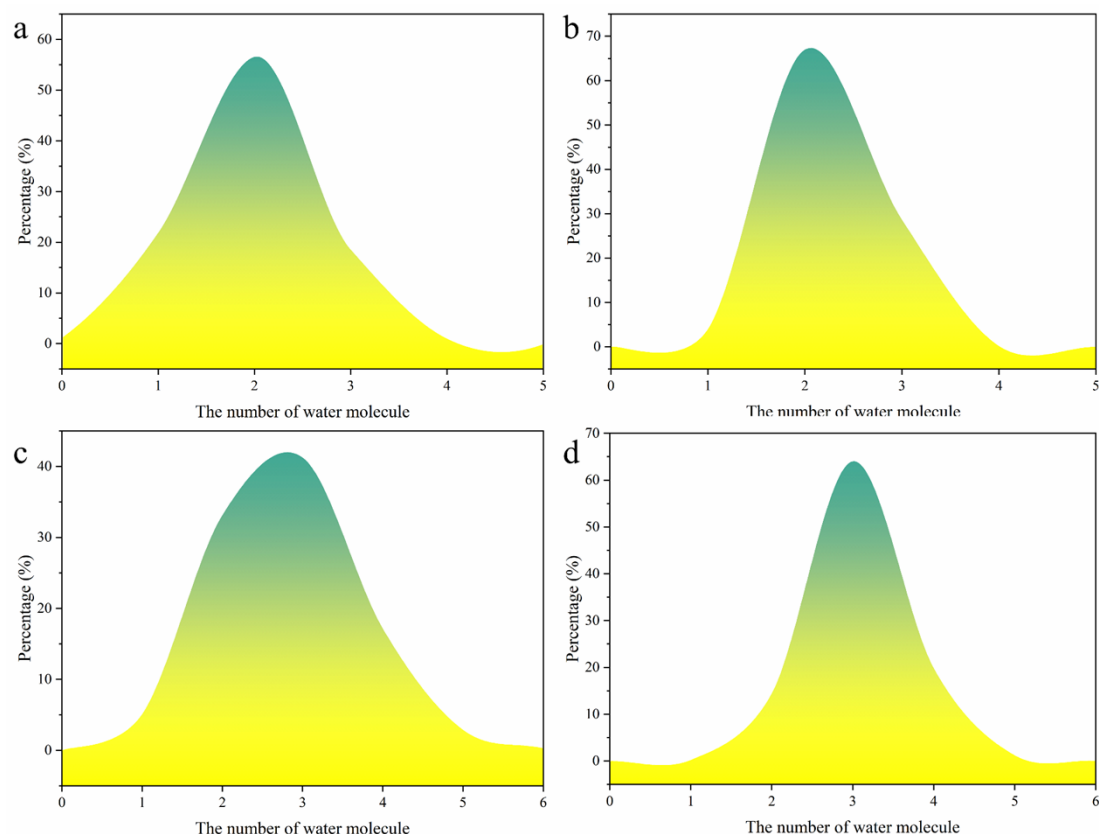


Figure S3. The evolution of the number of water molecules around the binuclear zinc ions within 4 Å during MM MD simulations is shown for each model: a and b represent the number of water molecule around the Zn_{α} and Zn_{β} in the PTE-A234 system, respectively. And c and d represent the number of water molecule around the Zn_{α} and Zn_{β} in the PTE-A234- H^+ system, respectively.

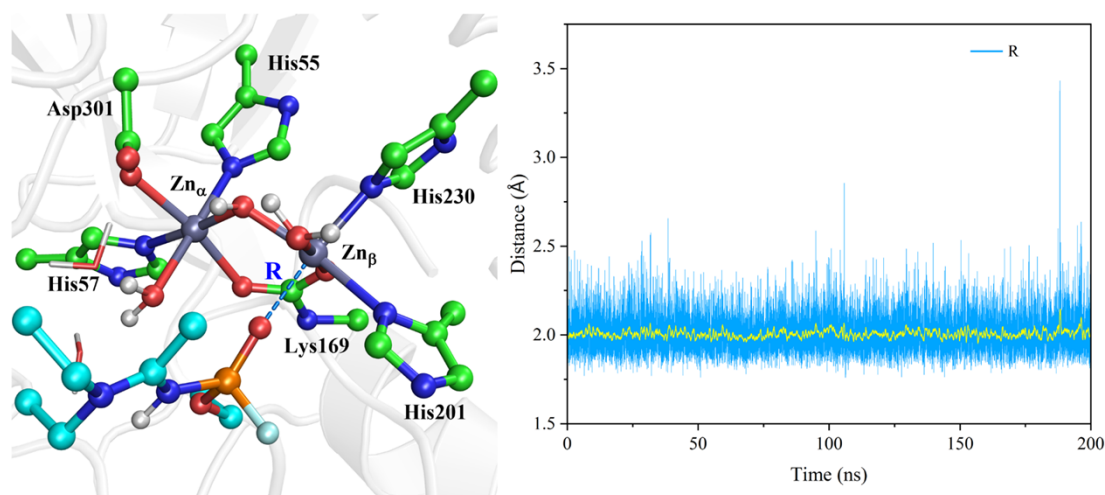


Figure S4. The most-populated structure by clustering of the last 100 ns MD-trajectories for A234- H^+ -PTE system (left) and the evolution of distance (R) between the Zn_{β} and the O atom of A234- H^+ during the 200 ns MM MD simulations (right).

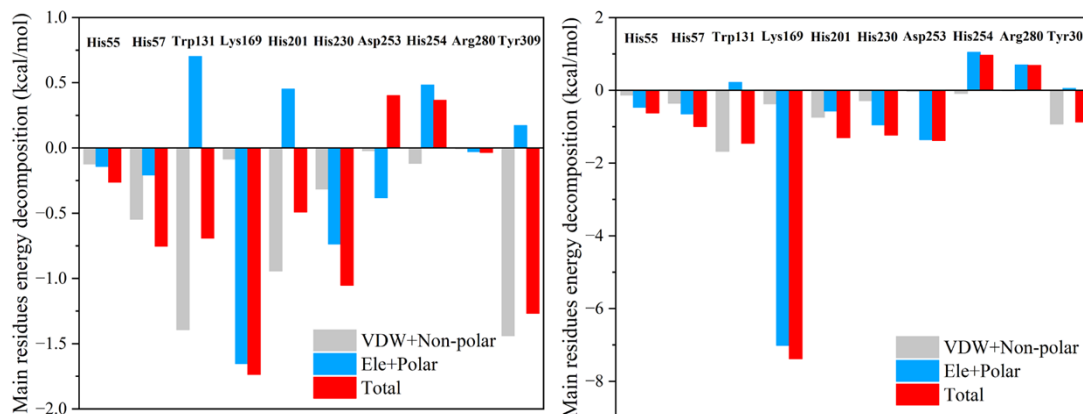


Figure S5. Detail energy decomposition for the key residues for substrates binding in enzyme-A234 system (left) and enzyme-A234-H⁺ system (right).

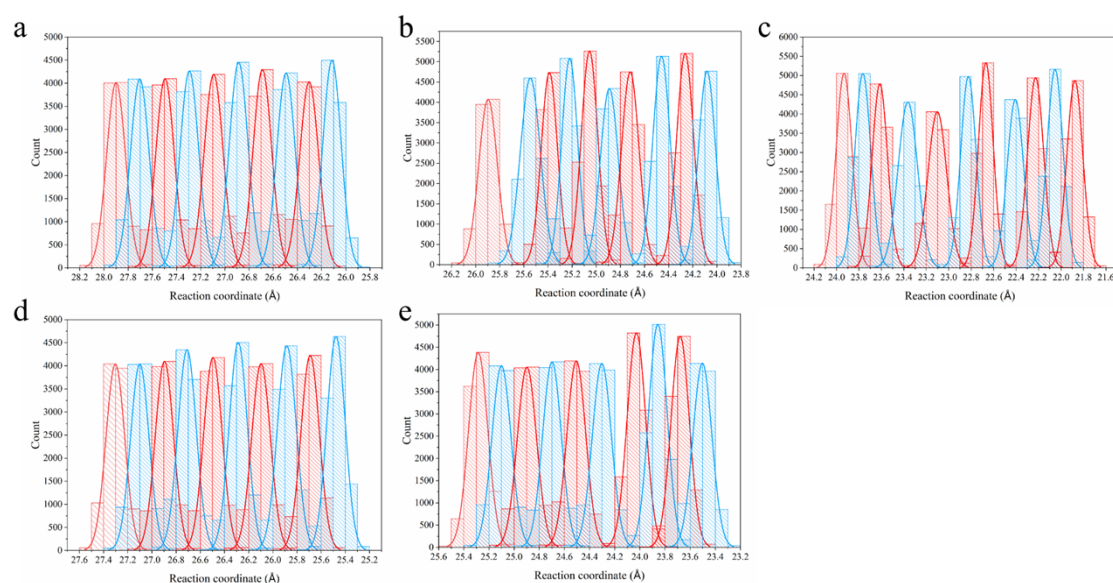


Figure S6. The selected histogram overlap between adjacent windows during the A234 (a, b, c) and A234-H⁺ (d, e) delivery using the umbrella sampling combining with WHAM methods.

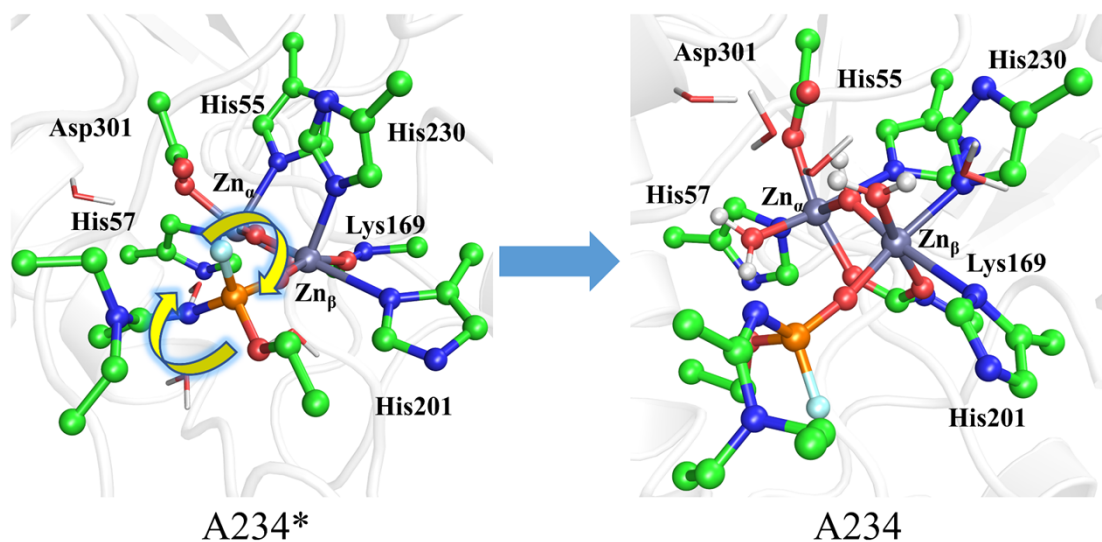


Figure S7. The conformational change during the A234 delivery into the active center in PTE.

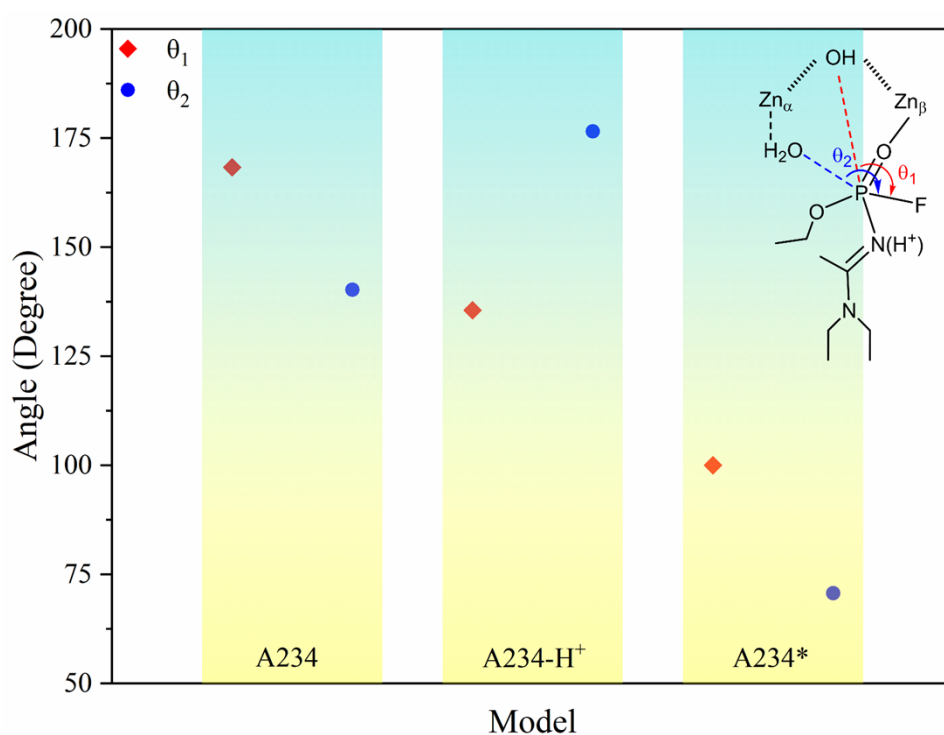


Figure S8. The angles of nucleophilic attack by hydroxide and water molecule across both three models.

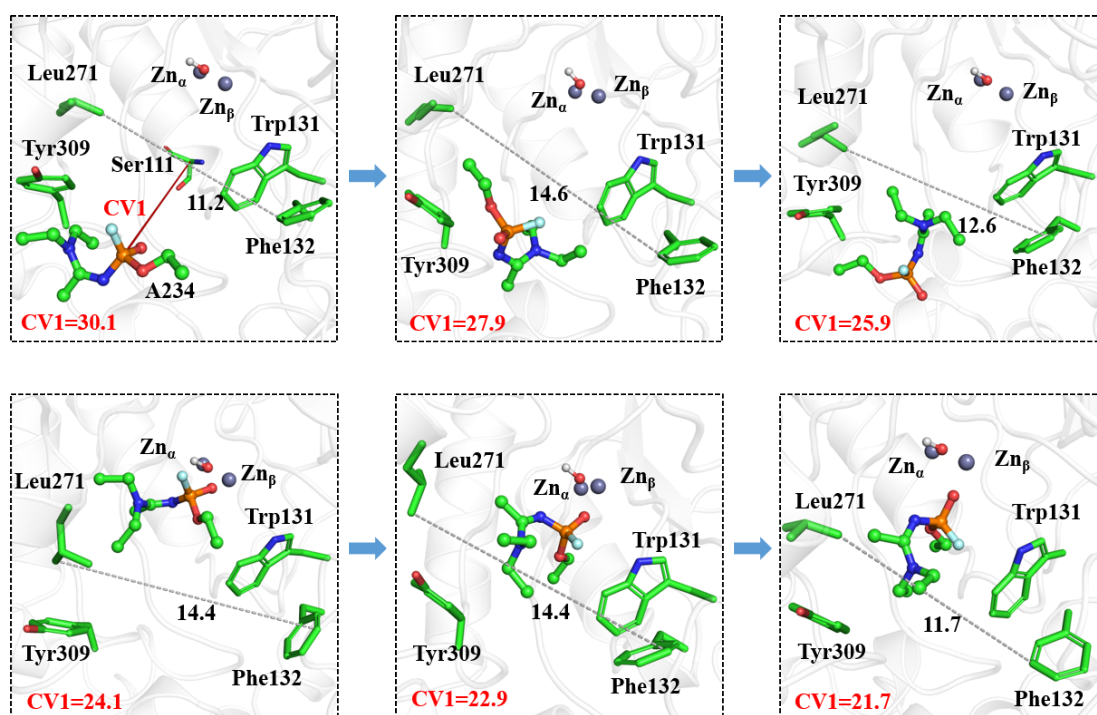


Figure S9. Representative structures and conformational changes during the A234 delivery to the active-site of PTE.

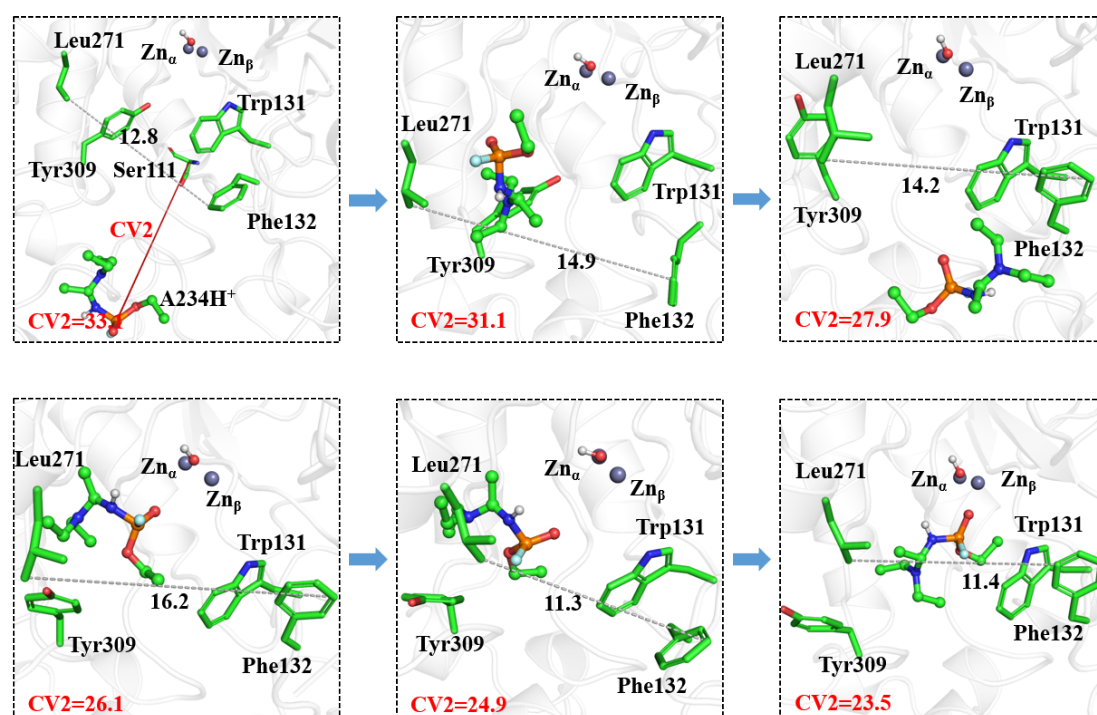


Figure S10. Representative structures and conformational changes during the A234-H⁺ delivery to the active-site of PTE.

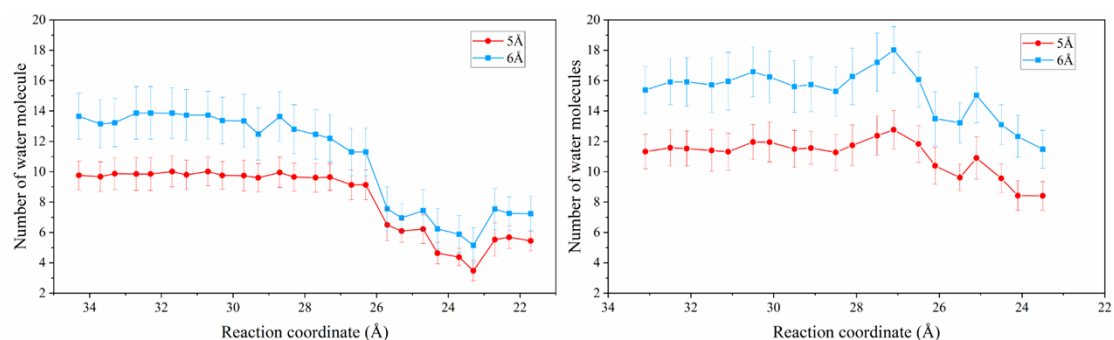


Figure S11. Statistics on the number of water molecules around the binuclear zinc ions within 5 Å and 6 Å during the A234 (left) and A234-H⁺ (right) transportation, respectively.

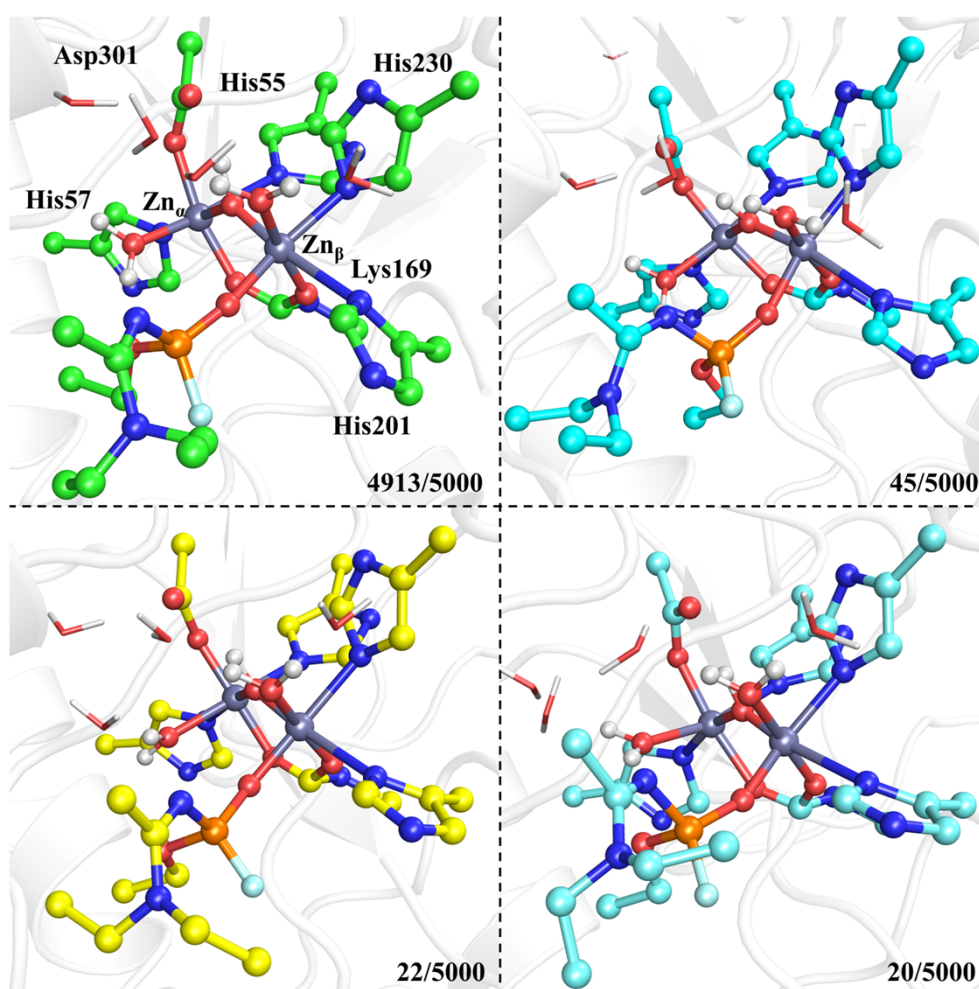


Figure S12. Four most-populated structures by clustering of the last 50 ns MD-trajectories for A234-PTE system, and the most-populated structure (carbon color in green) is applied for subsequent QM/MM calculations. The number frames of four structures are displayed in the bottom right corner.

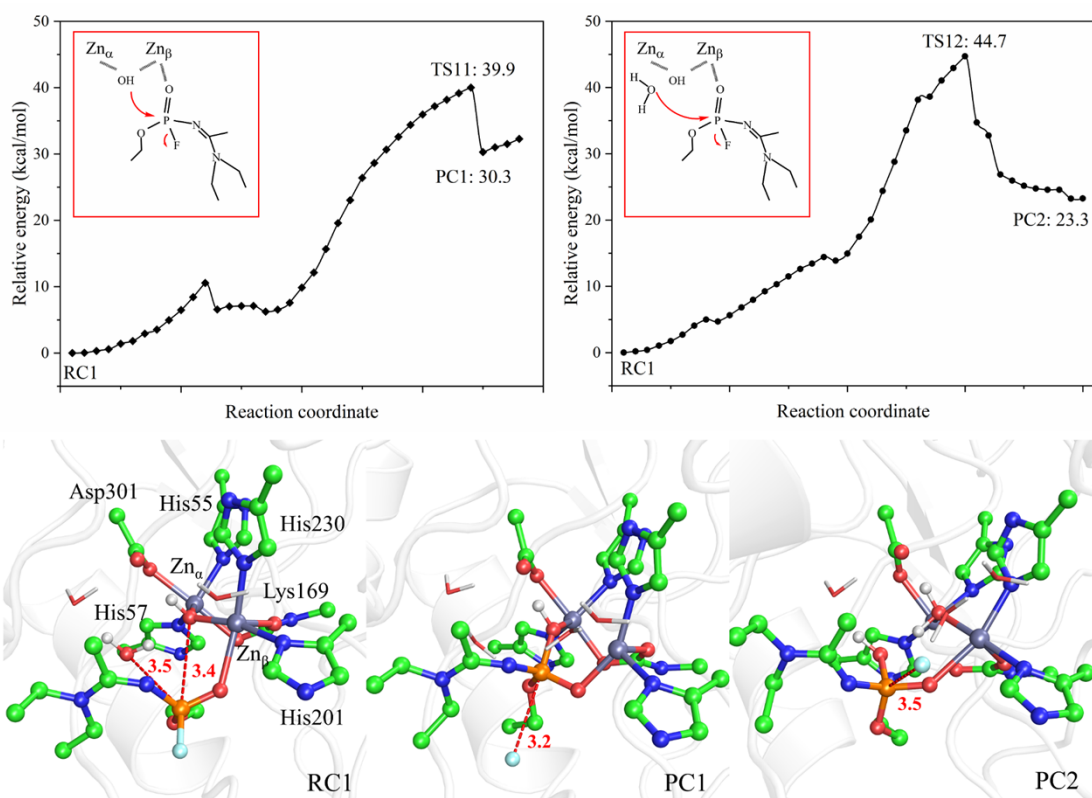


Figure S13. QM(B3LYP/B1)/MM-predicted relative energies (kcal/mol) for the enzymatic P-F cleavage of A234 initiated by the nucleophilic attack of hydroxide and water molecule. And the selected QM(B3LYP/B1)/MM-optimized active-site structures of corresponding species involved in the reactions, where selected key distances are given in Å.

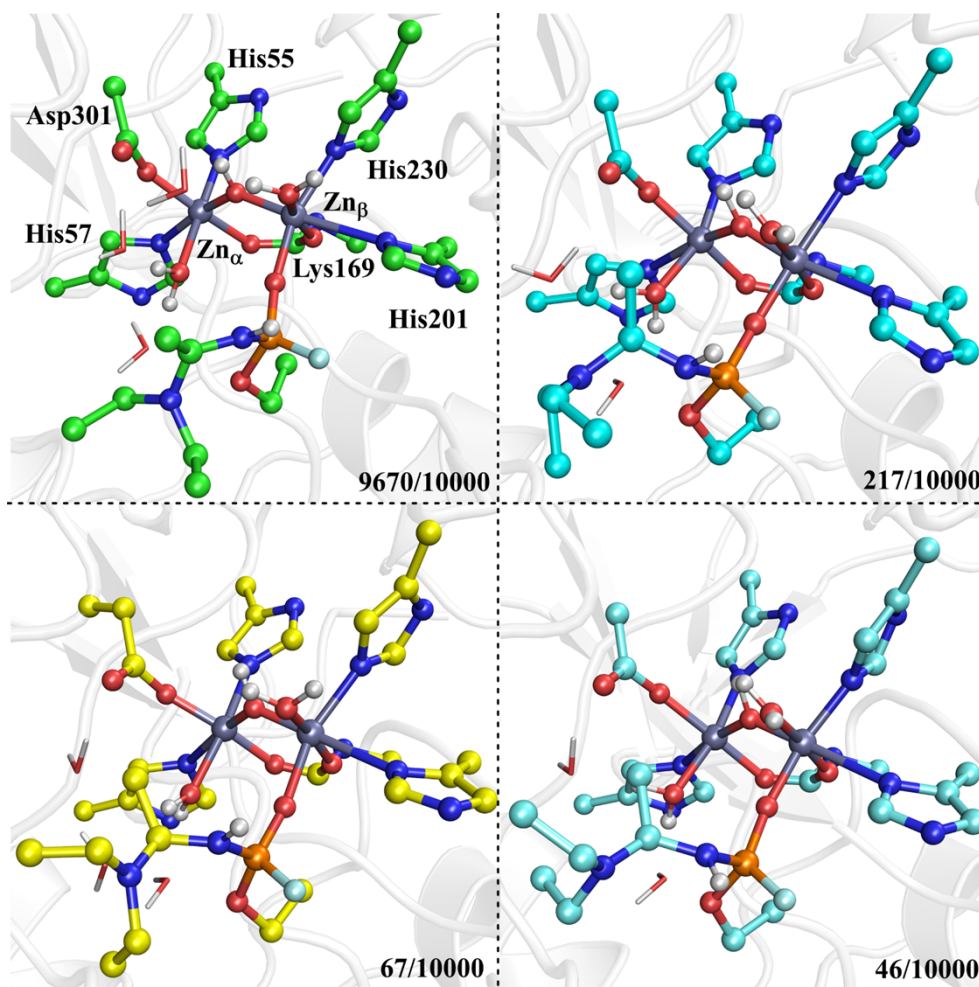


Figure S14. Four most-populated structures by clustering of the last 100 ns MD-trajectories for A234-H⁺-PTE system, and the most-populated structure (carbon color in green) is applied for subsequent QM/MM calculations. The number frames of four structures are displayed in the bottom right corner.

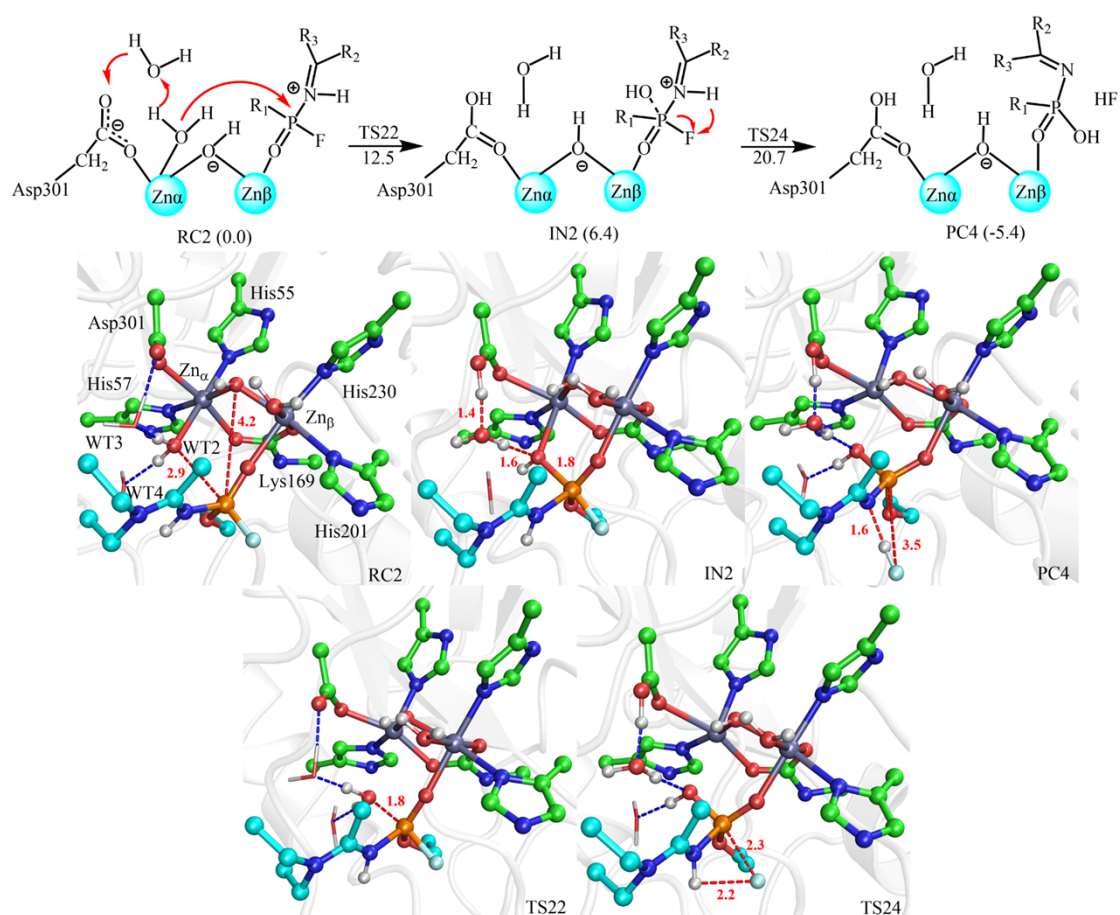


Figure S15. QM(B3LYP/B2)/MM-predicted relative energies (kcal/mol) for the enzymatic P-F cleavage of A234-H⁺ initiated by the nucleophilic attack of water molecule. And the selected QM(B3LYP/B1)/MM-optimized active-site structures of corresponding species involved in the reactions, where selected key distances are given in Å.

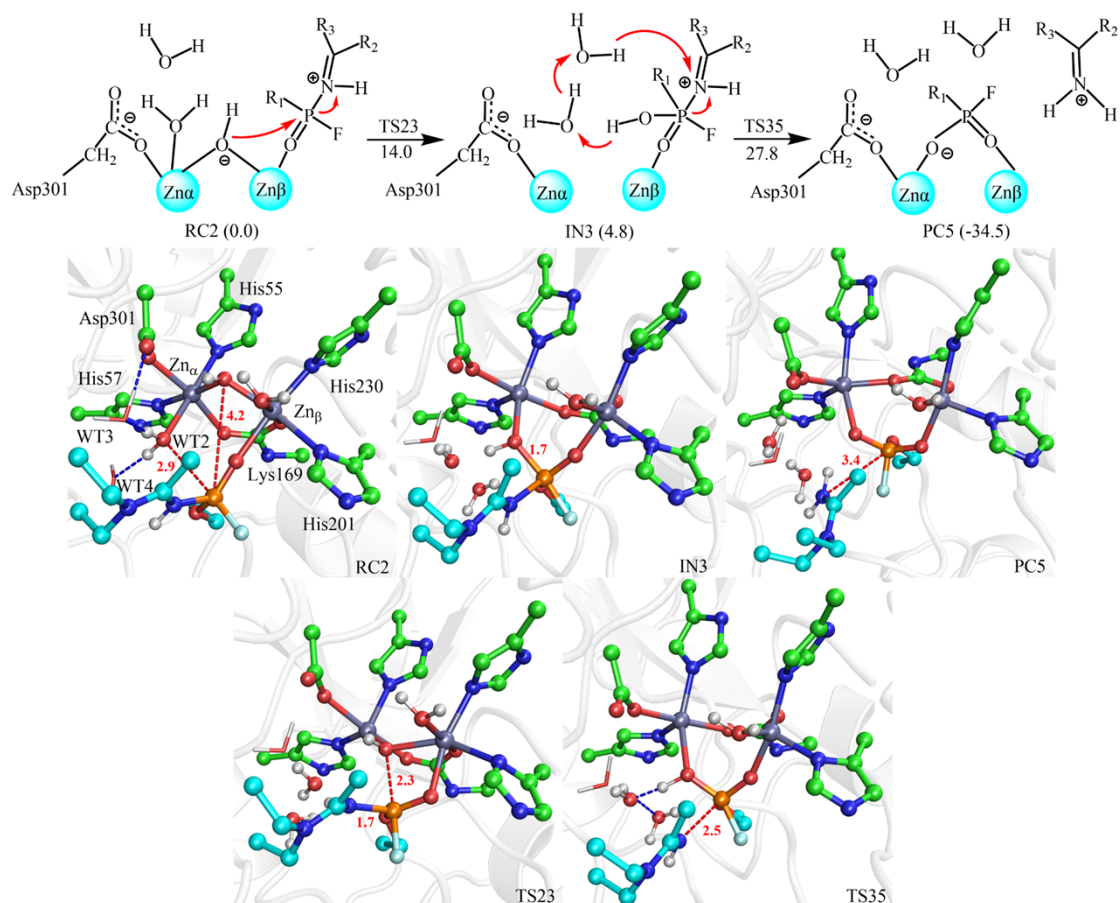


Figure S16. QM(B3LYP/B2)/MM-predicted relative energies (kcal/mol) for the enzymatic P–N bond hydrolysis of A234-H⁺ initiated by the nucleophilic attack of hydroxide ion, and the selected QM(B3LYP/B1)/MM-optimized active-site structures of corresponding species involved in the reactions, where selected key distances are given in Å.

Table S1. DFT calculated gas phase Gibbs energy using CBS-QB3 method and solvent phase Gibbs energy at M05-2X/6-31G* level (unit in Hartree).

	G_{gas}°	$G_{\text{gas}}^{\text{atm}}$	$G_{\text{solv}}^{\text{M}}$	ΔG_{solv}
A234 (A ⁻)	-1015.491387	-1016.71489	-1016.735821	-0.02093046
A234-H ⁺ (H _a A)	-1015.871165	-1016.978116	-1017.068809	-0.09069219
A234-H _b ⁺ (H _b A)	-1015.832741	-1017.000388	-1017.110372	-0.1099838
$\Delta G_{\text{solv}} = G_{\text{solv}}^{\text{M}} - G_{\text{gas}}^{\text{atm}}$				
The pK _a of the A234 when N _a atom was protonated				
$\text{pK}_{\text{a}} = \{[G_{\text{gas}}^{\circ}(\text{A}^{-}) - G_{\text{gas}}^{\circ}(\text{H}_{\text{a}}\text{A}) + \Delta G_{\text{solv}}(\text{A}^{-}) - \Delta G_{\text{solv}}(\text{H}_{\text{a}}\text{A})]627.51 - 270.29\} / 1.3644 = 8.65$				
The pK _a of the A234 when N _b atom was protonated				
$\text{pK}_{\text{a}} = \{[G_{\text{gas}}^{\circ}(\text{A}^{-}) - G_{\text{gas}}^{\circ}(\text{H}_{\text{b}}\text{A}) + \Delta G_{\text{solv}}(\text{A}^{-}) - \Delta G_{\text{solv}}(\text{H}_{\text{b}}\text{A})]627.51 - 270.29\} / 1.3644 = -0.15$				

Table S2. The calculated pK_a^c of several selected compounds and their experimental pK_a^c .

	Pyridine	3-Acetylpyridine	4-Vinylpyridine	4-Methylaminopyridine
$G_{\text{gas}}^0(\text{A}^-)$	-247.858371	-400.284054	-325.112327	-342.361404
$G_{\text{gas}}^0(\text{HA})$	-248.209341	-400.628907	-325.469286	-342.737651
$\Delta G_{\text{solv}}(\text{A}^-)$	-0.0082839	-0.0132655	-0.010315	-0.0137221
$\Delta G_{\text{solv}}(\text{HA})$	-0.100248	-0.1048118	-0.0957492	-0.0886952
pK_a^c	5.61	2.60	5.36	9.42
pK_a^c	5.32 ¹	2.87 ²	5.60 ²	9.66 ³

Table S3. The calculated reaction rate constants k (s⁻¹) during the reactions.

	Reaction process	Ea (kcal/mol)	k (s ⁻¹)
A234	RC1→TS11	39.9	3.9×10^{-17}
	RC1→TS12	44.7	2.1×10^{-20}
A234-H ⁺ (Cleavage of P-F bond)	RC2→TS21	14.0	3.5×10^2
	RC2→TS13	12.3	5.4×10^3
	PC3→TS3*	17.8	8.5
	RC2→TS22	12.5	4.1×10^3
	RC2→TS24	20.7	1.1×10^{-1}
A234-H ⁺ (Cleavage of P-N bond)	RC2→TS23	14.0	3.5×10^2
	RC2→TS35	27.8	1.6×10^{-6}
	RC2→TS24'	12.8	2.1×10^3
	RC2→TS46	21.5	3.1×10^{-2}

Reference

1. C. J. Hawkins and D. D. Perrin, *J. Chem. Soc.*, 1962, 1351-1357.
2. A. Hajduk and N. Ulrich, *ELECTROPHORESIS*, 2023, **44**, 1353-1360.
3. J. M. Essery and K. Schofield, *J. Chem. Soc.*, 1961, 3939-3953.

Cartesian coordinates of QM region from QM/MM calculations.

RC1

c	26.643982	72.065340	56.356734	c	28.203360	67.995299	51.276873
h	25.603930	71.755471	56.548275	o	27.670322	68.512595	50.245343
h	26.662941	73.166105	56.324830	o	29.417361	68.127403	51.625739
c	27.119136	71.469195	55.062972	h	25.350350	67.691132	51.888234
n	26.311594	71.446022	53.932111	h	25.954454	66.308744	50.936299
h	25.483394	72.036940	53.759271	h	27.909384	66.875418	52.910513
c	26.977112	70.804800	52.944148	c	25.322891	67.987929	48.275664
h	26.568279	70.618746	51.955586	h	25.859814	68.041805	49.233544
n	28.173944	70.426544	53.360452	h	25.050003	66.936677	48.102646
c	28.278371	70.830123	54.675043	c	26.262527	68.399146	47.181108
h	29.181642	70.622893	55.243180	n	27.327800	69.283854	47.337543
c	34.325010	68.704405	55.501447	c	27.965968	69.317410	46.174559
h	34.925099	69.578278	55.213891	h	28.867776	69.880018	45.963959
h	34.923165	67.800843	55.285592	n	27.386596	68.493983	45.283435
c	33.068796	68.695941	54.708673	h	27.775551	68.278511	44.357733
n	32.300390	67.560574	54.531906	c	26.312577	67.894814	45.897883
h	32.515335	66.631377	54.896536	h	25.687949	67.167893	45.390056
c	31.228605	67.887235	53.781738	c	24.326083	73.904127	48.472713
h	30.476578	67.195865	53.417459	h	23.585442	73.269513	47.971929
n	31.267671	69.173807	53.471403	h	24.765497	74.568018	47.706743
c	32.406184	69.697436	54.037732	c	25.394797	73.053500	49.087819
h	32.675892	70.741641	53.902973	n	26.162836	73.424286	50.178326
c	27.562360	62.865939	48.818109	h	25.963000	74.210326	50.818592
h	26.852913	63.206482	49.592417	c	27.112654	72.481687	50.371132
h	28.267274	62.191420	49.334355	h	27.885615	72.552771	51.130258
c	28.357292	64.020731	48.273448	n	26.997889	71.517699	49.473965
c	28.076699	65.375273	48.271565	c	25.935371	71.857203	48.664602
h	27.199617	65.907143	48.632795	h	25.666396	71.248653	47.804343
n	29.140870	66.084245	47.747012	c	30.215009	74.348564	53.289471
h	29.268554	67.099071	47.781206	h	29.160421	74.440863	53.599030
c	30.151287	65.205909	47.424023	h	30.480690	75.249020	52.721929
c	31.434691	65.431984	46.902473	c	30.331244	73.110948	52.403254
h	31.775065	66.425926	46.620019	o	30.522024	71.997489	52.945004
c	32.271478	64.330247	46.744406	o	30.182440	73.285858	51.148993
h	33.274194	64.480477	46.337850	zn	29.917782	70.075659	52.224607
c	31.849901	63.028513	47.092869	zn	28.467263	70.009282	49.057284
h	32.530392	62.189379	46.943154	o	29.912653	70.619430	50.338414
c	30.568934	62.801447	47.587993	h	29.999834	71.593639	50.337659
h	30.244581	61.794889	47.865247	h	31.077269	68.054856	50.260527
c	29.695786	63.893696	47.749101	h	36.175215	72.294056	46.223772
c	26.060288	66.844869	51.893412	c	35.060892	72.701067	48.062779
n	27.422525	67.264208	52.115258	h	36.481797	69.031076	48.470405

c	33.037997 67.462259 50.972057	RC2	
h	35.873132 72.445627 48.751721	c	37.579223 69.372152 34.548948
c	34.705947 70.178165 48.186821	h	38.476817 69.940306 34.845150
h	34.523820 73.525714 48.543801	h	36.859053 70.079152 34.110747
h	36.347850 73.956910 46.845130	c	36.989059 68.693511 35.750923
h	34.846390 73.456871 46.028821	n	36.893134 69.345393 36.972090
h	33.942166 66.960101 50.592598	h	37.016201 70.348644 37.176686
h	31.250394 73.077598 47.407395	c	36.356905 68.487382 37.868364
c	36.204523 70.095433 48.424881	h	36.154296 68.744214 38.899993
h	32.644718 66.887981 51.820883	n	36.102308 67.318631 37.308926
h	32.551027 73.714361 48.441654	c	36.479628 67.430628 35.991514
h	32.802063 73.576743 46.684237	h	36.368347 66.590945 35.309054
h	33.287531 68.472470 51.323093	c	35.384699 61.471212 34.601332
h	34.177886 69.756531 49.048805	h	34.304618 61.503566 34.400482
c	32.332871 73.100230 47.556870	h	35.642560 60.463901 34.977404
h	36.807692 70.559857 47.630858	c	35.699659 62.506633 35.622842
c	35.640463 73.123000 46.712305	n	36.907393 62.604935 36.296668
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h	34.444331 69.574149 47.303989	n	35.647291 64.239397 37.053980
p	31.666298 69.145241 47.784390	c	34.927911 63.537077 36.115611
f	32.254805 68.587032 46.399892	h	33.915212 63.829687 35.849471
o	30.197847 68.824563 47.878697	c	39.299091 66.151535 41.464132
o	32.550961 68.282051 48.783326	n	38.213259 65.436436 40.832843
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c	32.847333 71.690001 47.765742	o	36.695556 67.120867 40.973175
n	34.163864 71.538824 47.985574	o	36.314596 65.303087 39.679800
o	32.757479 70.681194 50.777267	h	38.957637 67.146198 41.769964
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h	32.896861 71.648748 50.791461	h	38.480441 64.652405 40.248311
o	32.902230 73.512858 50.719391	c	37.444812 68.546192 43.937390
h	33.067651 73.726101 51.671630	h	37.535102 68.230271 42.889167
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h	27.205531 71.763175 57.240717	h	33.008402 67.244412 43.968269
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h	26.976027 62.245030 48.140796	h	33.720813 67.333026 46.429336
h	25.813192 66.168798 52.711910	c	35.642889 67.988614 45.717836
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h	23.796254 74.524888 49.195212	c	34.675936 73.295970 41.736925
h	30.793990 74.342909 54.212951	h	35.325751 73.818715 42.455962

h	33.677827	73.220789	42.191861	h	30.558231	65.885083	43.032292
c	35.156543	71.913438	41.452479	h	36.183990	61.486651	40.232589
n	36.466867	71.540091	41.182944	h	31.012772	61.487582	42.416433
h	37.311829	72.105968	41.255704	h	31.607048	61.964724	39.920598
c	36.486231	70.206993	40.945600	h	30.829685	60.389111	40.188935
h	37.385921	69.630486	40.744712	h	36.226097	62.115245	42.741248
n	35.268070	69.711851	41.053890	h	29.335950	61.362113	41.950749
c	34.428090	70.754397	41.355095	h	32.416812	62.580358	41.844543
h	33.371773	70.608848	41.553426	o	32.672200	68.201009	41.720362
c	32.289000	67.835439	35.704154	h	32.170818	68.416826	40.896040
h	33.013839	68.630167	35.950593	h	32.378385	68.883051	42.378525
h	31.285038	68.278810	35.691314	o	33.637985	64.295984	39.317032
c	32.380601	66.800000	36.808573	h	32.663477	64.381359	39.172801
o	33.341967	66.004101	36.827740	h	33.848816	63.361061	39.103032
o	31.461636	66.836147	37.703889	o	31.929194	70.174813	43.307117
zn	34.871650	65.834422	38.315776	h	32.468240	70.805182	43.850424
zn	34.725143	67.699432	41.293672	h	31.109936	70.664280	43.053087
o	34.063756	67.367529	39.396094	o	33.559037	69.728024	38.151651
h	33.112932	67.194279	39.411271	h	34.184127	70.463144	38.244698
p	33.880135	64.263340	42.186735	h	33.946458	68.920816	38.586579
c	28.695620	63.796073	41.886548	o	33.900339	61.704000	38.621020
n	32.343878	63.590693	41.939332	h	34.515756	61.642017	37.876360
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c	30.279670	61.851153	41.676859	o	29.613031	68.802679	41.508934
c	30.679988	61.475497	40.250202	h	29.602533	69.656798	41.977395
c	30.929085	65.611024	42.034316	h	30.160292	68.988581	40.720457
c	28.095432	63.986399	40.496312	o	31.398567	68.932453	39.407868
c	36.141424	62.836177	41.914736	h	31.274630	68.201682	38.754866
c	31.107388	64.134605	41.935599	h	32.105970	69.480425	38.977943
f	34.020393	64.148373	43.766849	h	37.889046	68.718727	33.733404
h	36.601017	63.785501	42.225568	h	35.867195	61.624614	33.636069
h	27.987004	63.027300	39.967130	h	40.125522	66.250345	40.760346
h	29.886496	61.766140	39.549883	h	37.759911	69.588282	43.990564
h	28.683123	64.730097	42.455243	h	34.617491	73.895240	40.828340
h	28.113745	63.070146	42.474108	h	32.527648	67.476400	34.703053
h	28.738105	64.631582	39.883414	TS21			
h	27.096896	64.442118	40.584261	c	37.476105	69.395146	34.605430
h	37.796143	62.017367	40.822793	h	38.362480	69.973055	34.914041
h	31.866732	66.147908	41.866303	h	36.760993	70.092225	34.144320
h	36.740922	63.146768	39.888091	c	36.858591	68.743137	35.813758
h	30.206692	65.965986	41.292627	n	36.845884	69.392287	37.040645

h	37.039681	70.384469	37.238622	n	35.270259	69.669363	41.024581
c	36.266561	68.575455	37.948503	c	34.426562	70.720420	41.310201
h	36.152946	68.817865	38.997205	h	33.361997	70.586802	41.459592
n	35.897692	67.439793	37.389788	c	32.344340	67.763523	35.818693
c	36.248783	67.525811	36.059504	h	33.079080	68.551913	36.060678
h	36.058362	66.699442	35.379348	h	31.345376	68.216814	35.790483
c	35.340242	61.550367	34.587847	c	32.392731	66.732447	36.941320
h	34.264526	61.626571	34.379840	o	33.408568	66.017227	37.083490
h	35.538045	60.546226	35.002242	o	31.384279	66.697034	37.725394
c	35.702560	62.581732	35.596668	zn	35.060236	65.757488	38.396836
n	36.878883	62.556509	36.328357	zn	34.819644	67.652574	41.637823
h	37.657594	61.921981	36.167968	o	34.141950	66.052987	40.216501
c	36.848551	63.579617	37.221148	h	33.201115	66.196341	40.027030
h	37.643154	63.820586	37.921932	p	34.109470	64.680489	41.925118
n	35.712807	64.246199	37.104369	c	29.166570	63.463362	42.112263
c	34.990377	63.646186	36.095601	n	32.653606	64.167489	41.257710
h	34.003066	64.005011	35.818767	o	34.364149	65.918786	42.738977
c	39.376719	66.187738	41.719646	c	36.972478	62.333751	40.691389
n	38.291848	65.457808	41.090622	n	30.605836	63.304891	41.837045
c	37.217418	66.093552	40.498933	o	35.237010	63.885362	41.149280
o	36.754696	67.145268	41.053660	c	31.121459	61.928733	41.670808
o	36.800810	65.545770	39.445184	c	30.967277	61.363111	40.265954
h	39.022606	67.156173	42.086465	c	30.975129	65.730922	42.098926
h	39.784751	65.622544	42.574563	c	28.373087	63.945111	40.900845
h	38.628614	64.714331	40.486128	c	36.234841	63.055474	41.794580
c	37.513255	68.576831	44.062921	c	31.402984	64.348323	41.748740
h	37.578951	68.216544	43.027006	f	33.965264	63.606547	43.211985
h	38.255178	68.033642	44.658683	h	36.910883	63.709924	42.362236
c	36.136866	68.299001	44.583089	h	28.402374	63.216951	40.079334
n	35.010245	68.340980	43.777622	h	29.910379	61.332151	39.958962
c	33.979528	68.037413	44.556204	h	29.051345	64.143965	42.965498
h	32.943473	67.963279	44.237313	h	28.807398	62.480913	42.447064
n	34.382928	67.793905	45.820000	h	28.769192	64.892817	40.510612
h	33.781383	67.451375	46.581366	h	27.323566	64.105225	41.194530
c	35.753530	67.953002	45.863212	h	37.793455	61.739897	41.123239
h	36.331398	67.815083	46.772775	h	31.836509	66.306326	42.454645
c	34.666139	73.261456	41.716339	h	37.380804	63.061716	39.979397
h	35.307428	73.780809	42.445390	h	30.648193	66.239019	41.178113
h	33.663875	73.183423	42.161850	h	30.165254	65.783988	42.828740
c	35.153808	71.876088	41.439632	h	36.282144	61.672094	40.146597
n	36.473967	71.495096	41.224074	h	32.175103	61.937956	41.976355
h	37.321307	72.054148	41.333373	h	31.527982	61.964651	39.543512
c	36.497527	70.164835	40.981748	h	31.363867	60.338381	40.255254
h	37.402209	69.581747	40.826173	h	35.744578	62.355669	42.484141

h	30.580103 61.306537 42.396325	c	35.447910 61.436698 34.540760
h	32.854439 63.563528 40.407277	h	34.366212 61.500184 34.356455
o	32.793050 68.198856 41.624350	h	35.679622 60.418958 34.899980
h	32.324441 68.368485 40.764005	c	35.815237 62.429748 35.583005
h	32.440359 68.883824 42.249778	n	36.920808 62.322897 36.400322
o	33.452532 63.298514 38.940465	h	37.536925 61.511829 36.452966
h	32.603978 63.558620 38.516878	c	36.910093 63.354832 37.271496
h	33.829607 62.486043 38.534231	h	37.637944 63.504493 38.064544
o	31.968002 70.157335 43.217131	n	35.869565 64.138810 37.032873
h	32.499487 70.766870 43.791672	c	35.172302 63.578352 35.981275
h	31.134763 70.643869 43.000404	h	34.271056 64.040521 35.586148
o	33.560826 70.233189 38.366958	c	39.353791 66.290895 41.684694
h	33.848384 71.134658 38.048309	n	38.221982 65.623279 41.076337
h	34.289557 69.932414 38.926803	c	37.227664 66.297551 40.417335
o	34.745236 61.043449 38.083791	o	36.863674 67.441926 40.852644
h	35.681073 61.268743 38.161444	o	36.750254 65.705317 39.418178
h	34.563493 60.397205 38.833079	h	39.070079 67.295770 42.013619
o	31.022892 64.285196 38.814576	h	39.712006 65.727388 42.561872
h	30.253061 63.859697 38.367732	h	38.476156 64.783915 40.567424
h	31.121388 65.194082 38.429329	c	37.540599 68.558354 44.086374
o	29.678026 68.765467 41.423625	h	37.615117 68.208273 43.047575
h	29.669167 69.620673 41.887942	h	38.302450 68.031741 44.671343
h	30.253492 68.929475 40.651778	c	36.175395 68.214075 44.601082
o	31.547859 68.816933 39.365469	n	35.098773 68.025394 43.750784
h	31.396386 68.070039 38.735270	c	34.065283 67.652720 44.495055
h	32.166412 69.445923 38.918972	h	33.072384 67.408616 44.125473
h	37.810564 68.740721 33.800488	n	34.424016 67.590217 45.792725
h	35.842325 61.663312 33.627002	h	33.807406 67.277625 46.557231
h	40.157993 66.328983 40.972834	c	35.755789 67.943919 45.887947
h	37.828624 69.620195 44.063659	h	36.290894 67.966094 46.833035
h	34.613958 73.872269 40.815089	c	34.701989 73.334097 41.776472
h	32.583632 67.415600 34.813827	h	35.338664 73.889678 42.481571
IN1		h	33.705965 73.244126 42.232595
c	37.520211 69.413104 34.570758	c	35.215507 71.958505 41.521004
h	38.416806 69.967100 34.894163	n	36.530603 71.607021 41.238818
h	36.832102 70.129604 34.099304	h	37.371215 72.178932 41.327571
c	36.866485 68.772920 35.763418	c	36.572207 70.282014 40.982584
n	36.798544 69.426389 36.987170	h	37.474897 69.715172 40.769674
h	36.992727 70.415827 37.198358	n	35.357930 69.762163 41.090937
c	36.202821 68.606502 37.879613	c	34.505398 70.790901 41.424386
h	36.068404 68.845170 38.928185	h	33.452781 70.631123 41.628096
n	35.872145 67.463225 37.308310	c	32.466277 67.727808 35.790749
c	36.266104 67.550232 35.990905	h	33.226988 68.492673 36.026896
h	36.115381 66.715145 35.311716	h	31.479326 68.206855 35.795894

c	32.509359 66.662231 36.879941	h	32.372172 63.271328 38.307627
o	33.504691 65.898680 36.959447	h	33.649794 62.602639 37.563949
o	31.526795 66.632350 37.685235	o	32.072421 70.050809 43.235477
zn	35.180769 65.694572 38.177990	h	32.589673 70.669450 43.812774
zn	35.004369 67.755381 41.688537	h	31.253116 70.549876 42.990786
o	34.134588 64.739858 39.721611	o	33.574583 70.352883 38.443501
h	33.787336 63.926134 39.240813	h	33.854902 71.243208 38.087261
p	34.538914 64.356648 41.344727	h	34.278884 70.110528 39.060196
c	29.410800 63.685317 42.231228	o	35.555573 61.134064 38.654471
n	32.995284 63.491964 41.513241	h	35.374011 61.947005 39.151738
o	34.712170 65.804362 41.782497	h	34.935753 60.485386 39.089396
c	37.796695 62.151327 40.776785	o	31.149108 64.240854 38.821570
n	30.748308 63.169299 41.900174	h	30.312528 63.900283 38.421212
o	35.687127 63.316418 40.810159	h	31.293900 65.154273 38.458278
c	30.892860 61.708133 41.759223	o	29.830293 68.642102 41.459009
c	31.024184 61.272452 40.304119	h	29.803316 69.507143 41.900692
c	31.576095 65.470126 41.633229	h	30.373478 68.807856 40.664722
c	28.488334 63.813285 41.023346	o	31.643424 68.761633 39.339704
c	36.707202 62.732732 41.655854	h	31.534113 68.009766 38.707809
c	31.763367 63.990937 41.660220	h	32.210904 69.439650 38.901002
f	34.820868 63.791733 42.935978	h	37.848891 68.748979 33.771400
h	37.099367 63.505534 42.327999	h	35.922663 61.607387 33.574560
h	28.286926 62.836521 40.557153	h	40.151491 66.357931 40.944933
h	30.144269 61.602239 39.732047	h	37.838963 69.606699 44.082110
h	29.526616 64.643608 42.747840	h	34.625858 73.907040 40.852346
h	28.987543 62.995397 42.976340	h	32.670797 67.389051 34.775131
h	28.931952 64.457068 40.251273	TS13	
h	27.525900 64.245146 41.340531	c	37.558137 69.439621 34.524998
h	38.519994 61.622594 41.418745	h	38.460032 69.989141 34.841121
h	32.339980 65.931542 41.007411	h	36.874609 70.157539 34.049798
h	38.337623 62.933619 40.218848	c	36.905615 68.810464 35.721661
h	30.591599 65.775581 41.271818	n	36.845164 69.461907 36.946794
h	31.705639 65.854461 42.656246	h	37.040114 70.450694 37.160030
h	37.356510 61.458629 40.044858	c	36.253897 68.643249 37.842035
h	31.748424 61.358771 42.361897	h	36.126730 68.877645 38.892554
h	31.915272 61.690326 39.822502	n	35.919594 67.501281 37.268308
h	31.095140 60.180093 40.244441	c	36.304649 67.589647 35.949207
h	36.249809 61.949722 42.277074	h	36.148721 66.754819 35.271019
h	30.009338 61.253701 42.226563	c	35.457691 61.423017 34.518317
h	33.128331 62.526726 41.809991	h	34.375020 61.477544 34.337327
o	32.977995 68.178243 41.544683	h	35.700042 60.407611 34.876244
h	32.481620 68.315598 40.691955	c	35.824195 62.420959 35.554766
h	32.575059 68.811415 42.192855	n	36.918808 62.308977 36.384586
o	33.201424 62.725825 38.412527	h	37.515886 61.485077 36.462477

c	36.919778	63.356274	37.235616	h	33.719653	63.875898	39.023126
h	37.638094	63.504346	38.037691	p	34.474744	64.396943	41.059493
n	35.898468	64.156698	36.968894	c	29.456077	63.702787	42.303867
c	35.199441	63.589817	35.921751	n	33.018334	63.566613	41.495419
h	34.313904	64.062593	35.503582	o	34.757422	65.762147	41.632854
c	39.341720	66.345227	41.642011	c	37.760978	62.217966	40.782746
n	38.225490	65.659317	41.029446	n	30.798236	63.220322	41.940947
c	37.221162	66.294506	40.360947	o	35.603152	63.292952	40.727022
o	36.854042	67.455890	40.743995	c	30.992542	61.756072	41.850207
o	36.723265	65.649777	39.399384	c	31.158352	61.297531	40.405190
h	39.052071	67.359995	41.932954	c	31.522945	65.514711	41.428525
h	39.679904	65.808312	42.543073	c	28.482786	63.731162	41.129877
h	38.476372	64.789106	40.574826	c	36.629887	62.778677	41.623517
c	37.553715	68.555755	44.079842	c	31.767673	64.056283	41.607121
h	37.631894	68.213873	43.039031	f	34.779482	63.613867	43.118657
h	38.323117	68.030983	44.656975	h	36.946378	63.586849	42.289530
c	36.194060	68.184910	44.590661	h	28.292543	62.723131	40.729776
n	35.143694	67.910380	43.730818	h	30.288076	61.605978	39.805125
c	34.116047	67.511889	44.470629	h	29.556250	64.689795	42.767489
h	33.145625	67.197933	44.094591	h	29.093215	63.037623	43.100665
n	34.454251	67.517986	45.774854	h	28.873998	64.342580	40.304734
h	33.836009	67.212801	46.541594	h	27.521202	64.153975	41.461632
c	35.763787	67.942333	45.878899	h	38.491543	61.738589	41.455257
h	36.280364	68.022971	46.830979	h	32.182739	65.900683	40.648291
c	34.698559	73.328133	41.772641	h	38.283293	62.998235	40.204397
h	35.333497	73.882453	42.480401	h	30.491394	65.758927	41.168257
h	33.701800	73.237203	42.227001	h	31.781419	66.033903	42.361934
c	35.214519	71.952825	41.517982	h	37.370980	61.480657	40.065968
n	36.530305	71.605600	41.234777	h	31.850419	61.451842	42.468718
h	37.368295	72.182018	41.318039	h	32.056337	61.717753	39.939608
c	36.578083	70.279421	40.986546	h	31.244346	60.205392	40.368464
h	37.483334	69.717531	40.771938	h	36.174155	62.008466	42.254642
n	35.366714	69.753522	41.102381	h	30.111558	61.291574	42.312328
c	34.509875	70.780573	41.430915	h	33.273200	62.838024	42.172812
h	33.459146	70.616863	41.642102	o	33.003813	68.143205	41.584626
c	32.472093	67.746377	35.781723	h	32.513295	68.292233	40.731954
h	33.234150	68.510588	36.015303	h	32.612835	68.787404	42.230797
h	31.484912	68.224766	35.789720	o	33.164805	62.790557	38.283864
c	32.520052	66.675045	36.863370	h	32.292931	63.278286	38.188651
o	33.521521	65.917052	36.932773	h	33.624208	62.685829	37.437778
o	31.536936	66.627415	37.666403	o	32.094731	70.042328	43.237729
zn	35.234634	65.734811	38.075091	h	32.605363	70.661547	43.820826
zn	35.035412	67.733838	41.676671	h	31.273341	70.537590	42.993233
o	34.077143	64.713741	39.543801	o	33.602768	70.352248	38.431060

h	33.872087 71.247695 38.077603	n	38.254560 65.681151 40.931768
h	34.307079 70.120431 39.051888	c	37.193744 66.244655 40.277225
o	35.559233 61.170283 38.646188	o	36.750552 67.372857 40.674251
h	35.423445 61.954000 39.202180	o	36.739867 65.573249 39.311552
h	34.947752 60.507720 39.073616	h	38.977117 67.461097 41.776186
o	31.088285 64.209345 38.720263	h	39.649597 65.972142 42.488627
h	30.227825 63.873378 38.367515	h	38.580081 64.847899 40.454090
h	31.225544 65.128050 38.366488	c	37.556406 68.559566 44.083542
o	29.853624 68.631758 41.460870	h	37.624634 68.213246 43.043429
h	29.822676 69.492978 41.909558	h	38.328971 68.035724 44.657197
h	30.406032 68.803685 40.674585	c	36.199672 68.201144 44.609246
o	31.693151 68.752868 39.359110	n	35.122501 67.986954 43.765712
h	31.562269 68.012692 38.719557	c	34.100905 67.597660 44.519436
h	32.252311 69.434308 38.913900	h	33.112294 67.322092 44.160768
h	37.878716 68.762795 33.733037	n	34.469418 67.550655 45.815002
h	35.930488 61.601967 33.552653	h	33.862621 67.239666 46.588256
h	40.153158 66.388947 40.915566	c	35.793495 67.930352 45.899947
h	37.844731 69.606172 44.081075	h	36.333165 67.966676 46.841503
h	34.624416 73.904177 40.850284	c	34.727981 73.321349 41.776023
h	32.674039 67.403497 34.766973	h	35.373176 73.875154 42.474989
PC3		h	33.737632 73.233639 42.244552
c	37.500805 69.390208 34.585719	c	35.237085 71.941904 41.518365
h	38.399735 69.924062 34.936061	n	36.543030 71.585338 41.202517
h	36.833469 70.127221 34.115547	h	37.384509 72.159048 41.261834
c	36.805284 68.741061 35.750825	c	36.577165 70.255374 40.964132
n	36.652970 69.403103 36.963486	h	37.471393 69.690285 40.713579
h	36.856477 70.388157 37.189152	n	35.368851 69.736058 41.120329
c	36.008012 68.589206 37.824106	c	34.526139 70.770741 41.464622
h	35.808367 68.836718 38.860571	h	33.480296 70.615156 41.706567
n	35.725644 67.435946 37.241607	c	32.472641 67.659576 35.776090
c	36.208308 67.513169 35.951775	h	33.288210 68.351201 36.048678
h	36.117469 66.667821 35.274113	h	31.523022 68.207772 35.810997
c	35.510642 61.392610 34.497964	c	32.425799 66.521252 36.785674
h	34.424346 61.415619 34.327202	o	33.341138 65.639778 36.762258
h	35.785624 60.380276 34.841029	o	31.464749 66.517858 37.605824
c	35.843334 62.390546 35.546428	zn	35.122966 65.677634 38.113632
n	36.879353 62.264523 36.452822	zn	35.001342 67.710568 41.703892
h	37.538925 61.486224 36.493622	o	33.786961 65.227988 39.519306
c	36.833723 63.315902 37.301321	h	32.975257 64.165408 37.302797
h	37.513417 63.478269 38.132740	p	34.090621 64.723459 40.946779
n	35.828726 64.117471 36.974918	c	29.376418 63.568554 42.623296
c	35.205178 63.557541 35.881329	n	32.856291 63.832441 41.582175
h	34.331806 64.010822 35.422504	o	34.658454 65.761090 41.919549
c	39.317725 66.445327 41.549718	c	37.280006 62.377878 41.012644

n	30.731127 63.258966 42.164574	h	29.992726 64.017307 38.658852
o	35.220035 63.550296 40.726093	h	31.066507 65.189563 38.635631
c	31.099986 61.834993 42.021813	o	29.731779 68.584431 41.366384
c	31.293640 61.394554 40.573338	h	29.776124 69.433871 41.834173
c	31.222109 65.657498 41.838174	h	30.325121 68.710292 40.601497
c	28.360283 63.641009 41.486335	o	31.640413 68.680773 39.290956
c	36.171162 63.129168 41.724730	h	31.542917 67.938319 38.651653
c	31.612876 64.211613 41.844489	h	32.169558 69.390931 38.855596
f	33.771505 62.767639 43.695693	h	37.831938 68.738424 33.777267
h	36.555986 64.021528 42.238173	h	35.967917 61.588448 33.528112
h	28.285018 62.680330 40.952817	h	40.147223 66.482583 40.843594
h	30.390548 61.576140 39.970192	h	37.848456 69.609684 44.078526
h	29.398910 64.505350 43.190686	h	34.641076 73.898790 40.855655
h	29.095604 62.787326 43.344673	h	32.652066 67.348135 34.747072
h	28.654963 64.406284 40.752918	TS22	
h	27.365932 63.897234 41.888551	c	37.629021 69.424307 34.489250
h	37.998402 61.971299 41.742298	h	38.532276 69.992103 34.767887
h	31.644016 66.123801 40.943391	h	36.910736 70.127185 34.042746
h	37.815956 63.042665 40.317505	c	37.045482 68.771783 35.704952
h	30.150686 65.865633 41.863179	n	36.961385 69.434138 36.921121
h	31.690092 66.144146 42.704118	h	37.088271 70.437798 37.121733
h	36.864382 61.547614 40.419828	c	36.430535 68.591434 37.830365
h	32.013912 61.651311 42.601021	h	36.232758 68.856079 38.861748
h	32.133976 61.928622 40.117481	n	36.172145 67.418642 37.278470
h	31.517497 60.319403 40.551742	c	36.534182 67.514405 35.957258
h	35.651275 62.503105 42.464357	h	36.410416 66.668588 35.285051
h	30.301642 61.248376 42.496861	c	35.366901 61.513255 34.628298
h	33.397822 63.117060 42.859527	h	34.288249 61.547153 34.420788
o	32.990223 68.173509 41.516105	h	35.617632 60.509709 35.018005
h	32.496771 68.284106 40.660985	c	35.679478 62.555466 35.645628
h	32.573298 68.797693 42.162431	n	36.880676 62.648796 36.330385
o	32.621587 63.276142 37.632941	h	37.695947 62.062255 36.171134
h	31.891691 63.579248 38.327335	c	36.802669 63.698364 37.186220
h	33.379118 62.720229 38.091389	h	37.597444 64.009058 37.858826
o	32.048333 70.035305 43.214773	n	35.617117 64.274890 37.095980
h	32.563690 70.642915 43.804903	c	34.904082 63.583587 36.139372
h	31.233670 70.546054 42.972532	h	33.898130 63.886190 35.860502
o	33.497647 70.409669 38.460531	c	39.291297 66.136499 41.478582
h	33.788861 71.288313 38.082094	n	38.205372 65.425669 40.843774
h	34.153738 70.224087 39.146914	c	37.029782 65.996825 40.436264
o	34.449695 61.947118 38.713344	o	36.716250 67.138875 40.886483
h	34.777344 62.468160 39.485666	o	36.341840 65.292138 39.632919
h	34.257850 61.027836 39.064650	h	38.950979 67.131602 41.783214
o	30.862033 64.307592 39.045123	h	39.642842 65.603085 42.379114

h	38.464217	64.601929	40.314077	c	36.175177	62.658378	41.744778
c	37.445881	68.552190	43.923636	c	31.142844	64.071715	41.986380
h	37.540963	68.242661	42.874013	f	34.370120	63.851310	43.273377
h	38.191868	67.990182	44.500930	h	36.606423	63.545149	42.227872
c	36.069883	68.174665	44.395439	h	27.959177	63.128530	40.088761
n	35.029659	67.847075	43.536014	h	29.751264	61.886378	39.637354
c	34.010866	67.469234	44.295398	h	28.746020	64.771302	42.592676
h	33.048657	67.125163	43.928571	h	28.090389	63.143313	42.592647
n	34.338011	67.531508	45.606653	h	28.794447	64.691591	40.011095
h	33.735731	67.272285	46.398551	h	27.149269	64.585490	40.710109
c	35.641032	67.978249	45.694151	h	38.011305	61.807559	40.985985
h	36.151652	68.116592	46.643692	h	31.945672	66.058414	41.779259
c	34.668302	73.276216	41.720778	h	37.203717	63.002355	39.898624
h	35.317994	73.790562	42.446310	h	30.233537	65.920267	41.328085
h	33.668831	73.201916	42.173047	h	30.728343	65.871616	43.032372
c	35.145745	71.892088	41.430992	h	36.532878	61.367366	40.059225
n	36.458393	71.516199	41.176944	h	30.927634	61.398927	42.455301
h	37.303379	72.081327	41.256705	h	31.489300	61.876101	39.985302
c	36.478245	70.180500	40.948951	h	30.544804	60.384441	40.188113
h	37.380211	69.601636	40.766791	h	36.017165	61.892589	42.518424
n	35.258885	69.684988	41.044573	h	29.232868	61.381337	42.052594
c	34.417680	70.731844	41.330668	h	32.412091	62.510475	42.214842
h	33.360059	70.588838	41.523620	o	32.669499	68.195898	41.696678
c	32.356685	67.818523	35.711283	h	32.169403	68.421348	40.877626
h	33.095042	68.601063	35.957111	h	32.381018	68.873865	42.359637
h	31.361811	68.281025	35.697872	o	33.466151	64.188194	39.897472
c	32.415796	66.783622	36.816283	h	32.487005	64.465971	39.597154
o	33.376598	65.984901	36.880873	h	33.654540	63.310370	39.421570
o	31.462052	66.818209	37.672893	o	31.944495	70.196902	43.268914
zn	35.023972	65.983830	38.246371	h	32.473572	70.818102	43.831977
zn	34.724416	67.642566	41.321231	h	31.112816	70.675611	43.039820
o	34.095919	67.360428	39.365870	o	33.609279	69.734705	38.137977
h	33.145267	67.190199	39.375245	h	34.199190	70.494579	38.261851
p	33.938958	64.182512	41.634671	h	33.994508	68.944522	38.602033
c	28.713395	63.842590	42.015090	o	33.633765	61.933908	38.602333
n	32.353508	63.504133	41.998833	h	34.253514	61.983331	37.858719
o	34.115073	65.667877	41.715381	h	33.853294	61.096185	39.101965
c	37.045799	62.175492	40.602956	o	31.150972	64.786496	39.182778
n	30.070637	63.281221	41.980861	h	30.766832	64.137889	38.528065
o	34.902930	62.983434	41.150200	h	31.281961	65.625703	38.623243
c	30.190732	61.829210	41.757311	o	29.611481	68.848350	41.476503
c	30.518680	61.476009	40.306911	h	29.605124	69.698463	41.953825
c	31.003383	65.559075	42.014317	h	30.166509	69.036786	40.695620
c	28.121721	64.076263	40.624282	o	31.416427	68.962666	39.368281

h	31.269055 68.235600 38.722587	c	34.067415 67.479206 44.266562
h	32.139456 69.489971 38.938223	h	33.111303 67.145844 43.876282
h	37.927914 68.746247 33.689898	n	34.383544 67.487310 45.580294
h	35.856410 61.650737 33.664168	h	33.757211 67.182824 46.339099
h	40.119074 66.231663 40.775876	c	35.683565 67.937952 45.697324
h	37.759896 69.594258 43.983275	h	36.188097 68.037447 46.654843
h	34.615913 73.886176 40.818963	c	34.674434 73.263257 41.690690
h	32.582110 67.457296 34.707906	h	35.306216 73.782163 42.428593
IN2		h	33.672161 73.163119 42.132009
c	37.607992 69.397179 34.523468	c	35.184908 71.892890 41.391036
h	38.503424 69.974833 34.806514	n	36.510866 71.541121 41.174593
h	36.879027 70.093963 34.084235	h	37.345036 72.116934 41.289299
c	37.038900 68.725487 35.738218	c	36.560989 70.208491 40.936306
n	36.980921 69.377576 36.961120	h	37.478003 69.645441 40.780588
h	37.096018 70.383641 37.159310	n	35.347380 69.691551 40.988571
c	36.482352 68.521756 37.877064	c	34.480070 70.723104 41.253672
h	36.316636 68.774981 38.916691	h	33.419303 70.567031 41.412747
n	36.213952 67.350859 37.325624	c	32.456628 67.851717 35.665705
c	36.541077 67.461622 35.994360	h	33.228531 68.601716 35.907783
h	36.417921 66.618316 35.318722	h	31.477579 68.343899 35.672806
c	35.393298 61.497480 34.712186	c	32.493626 66.790516 36.726458
h	34.313218 61.551049 34.513671	o	33.395819 65.978629 36.861805
h	35.628896 60.484244 35.084658	o	31.432948 66.813711 37.530156
c	35.730319 62.513207 35.749558	zn	35.189411 65.874964 38.444658
n	36.878803 62.494635 36.525725	zn	34.848079 67.654077 41.347829
h	37.637876 61.820820 36.442503	o	34.185343 67.326969 39.385992
c	36.827882 63.539909 37.388980	h	33.266781 67.060324 39.509318
h	37.587195 63.775812 38.130391	p	34.245091 64.185136 41.501784
n	35.708939 64.224488 37.212274	c	29.004525 63.813322 42.082828
c	35.015077 63.604849 36.194470	n	32.639640 63.432592 41.766010
h	34.055721 63.980998 35.850646	o	34.391605 65.663957 41.776584
c	39.384484 66.196045 41.763269	c	37.449073 62.058443 40.799410
n	38.265122 65.444955 41.237184	n	30.347621 63.227552 41.938231
c	37.209551 66.040630 40.589775	o	35.295234 63.034623 41.024585
o	36.869783 67.216584 40.911909	c	30.421003 61.779539 41.690487
o	36.647984 65.317823 39.712176	c	30.575317 61.431061 40.212235
h	39.055851 67.191665 42.075188	c	31.331438 65.475746 42.064626
h	39.806087 65.683272 42.643954	c	28.346631 64.131541 40.739987
h	38.530031 64.575495 40.789506	c	36.432029 62.594727 41.787717
c	37.491916 68.581671 43.945164	c	31.437029 63.994744 41.901411
h	37.584323 68.275797 42.894659	f	34.565591 63.745555 43.117278
h	38.244527 68.027241 44.520270	h	36.844918 63.434197 42.361848
c	36.120498 68.189269 44.410590	h	28.136730 63.220775 40.159106
n	35.089160 67.893104 43.532102	h	29.755004 61.875445 39.632691

h	29.079781 64.704853 42.711973	h	34.619596 73.882111 40.795101
h	28.402248 63.095460 42.658425	h	32.646833 67.476846 34.660042
h	28.997806 64.772514 40.129112	TS24	
h	27.390819 64.652250 40.906600	c	37.633710 69.431089 34.490040
h	38.291984 61.596987 41.339748	h	38.534105 70.005462 34.763577
h	32.236065 65.977469 41.722511	h	36.909383 70.127297 34.043144
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h	30.469709 65.910904 41.551792	n	37.007051 69.441336 36.930436
h	31.231485 65.691886 43.139581	h	37.128844 70.447095 37.125300
h	36.978125 61.313653 40.139977	c	36.504672 68.597557 37.853632
h	31.231250 61.337956 42.293103	h	36.341532 68.857705 38.892295
h	31.522065 61.798990 39.791516	n	36.232890 67.424282 37.308360
h	30.545591 60.340213 40.085365	c	36.560004 67.520727 35.977069
h	36.113180 61.820652 42.500955	h	36.432333 66.671543 35.310022
h	29.500217 61.338319 42.093707	c	35.398134 61.519601 34.711008
h	32.699766 62.420860 41.861086	h	34.317657 61.574446 34.514792
o	32.760899 68.192268 41.694599	h	35.632450 60.508070 35.088154
h	32.247503 68.396285 40.881320	c	35.741405 62.540219 35.742427
h	32.471632 68.889434 42.337789	n	36.885297 62.515121 36.525484
o	33.846923 64.362340 39.798974	h	37.637330 61.832194 36.452134
h	32.328754 64.674260 39.366906	c	36.843016 63.566607 37.380475
h	33.926627 63.477427 39.351770	h	37.598676 63.794773 38.128324
o	32.042285 70.290068 43.124921	n	35.733533 64.264969 37.190402
h	32.530486 70.875628 43.760299	c	35.037558 63.644710 36.173507
h	31.171233 70.721455 42.960436	h	34.083905 64.026753 35.821113
o	33.669753 69.645406 38.107154	c	39.376171 66.198693 41.750595
h	34.254388 70.407703 38.243093	n	38.251893 65.460983 41.218811
h	34.048747 68.859198 38.588552	c	37.209361 66.059101 40.564692
o	33.666107 62.009052 38.524815	o	36.879549 67.243446 40.866276
h	34.193928 62.029197 37.712342	o	36.640206 65.333895 39.687907
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o	31.386222 64.923356 39.124785	h	39.787761 65.680280 42.632145
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h	31.467950 66.024368 38.234057	c	37.491642 68.586681 43.935850
o	29.677742 68.872930 41.496151	h	37.579365 68.287106 42.883290
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h	30.236250 69.087129 40.726456	c	36.126678 68.182579 44.409697
o	31.472789 68.988734 39.369934	n	35.104543 67.831300 43.539097
h	31.246430 68.300759 38.719005	c	34.098065 67.396840 44.284220
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h	37.916591 68.734048 33.715327	n	34.414214 67.451748 45.596402
h	35.873401 61.641402 33.744273	h	33.803241 67.153838 46.370400
h	40.154026 66.289358 40.997002	c	35.696887 67.949545 45.701057
h	37.794691 69.627405 43.998408	h	36.199545 68.082857 46.655313

c	34.672040	73.265056	41.694364	h	37.797469	62.905391	40.210169
h	35.303505	73.784294	42.432257	h	30.479447	65.906234	41.392804
h	33.669329	73.166233	42.134974	h	31.246090	65.840618	42.991844
c	35.181526	71.893691	41.397872	h	36.975858	61.342424	40.220594
n	36.506092	71.541516	41.174064	h	31.332266	61.388507	42.438809
h	37.341055	72.117834	41.280200	h	31.595050	61.824346	39.949952
c	36.556165	70.207842	40.944530	h	30.604563	60.374030	40.235245
h	37.471982	69.643437	40.788022	h	36.037322	61.905975	42.553821
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c	34.476563	70.722360	41.274082	h	32.892863	62.658265	42.414263
h	33.417636	70.566009	41.445527	o	32.781965	68.195049	41.702335
c	32.466283	67.860232	35.656096	h	32.259684	68.395170	40.894650
h	33.244487	68.604281	35.894456	h	32.483256	68.878031	42.357009
h	31.491019	68.359509	35.663458	o	33.774467	64.322756	39.733533
c	32.495364	66.796605	36.713622	h	32.187400	64.598833	39.276914
o	33.402296	65.993346	36.865226	h	33.856505	63.422875	39.267651
o	31.414970	66.802487	37.492061	o	32.035242	70.273390	43.145084
zn	35.251841	65.948640	38.381122	h	32.523879	70.863561	43.776133
zn	34.866560	67.652947	41.374523	h	31.168601	70.709808	42.970615
o	34.191415	67.292858	39.404757	o	33.668135	69.606874	38.126796
h	33.272734	67.018304	39.508017	h	34.242214	70.374559	38.274301
p	34.195540	64.214748	41.282511	h	34.045955	68.824735	38.616495
c	29.079479	63.841973	42.250881	o	33.699645	62.056694	38.503334
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o	34.462034	65.620609	41.728949	h	33.883979	61.192561	38.970095
c	37.423609	62.110927	40.870161	o	31.262965	64.870534	39.050103
n	30.422627	63.268106	42.066097	h	30.888098	64.157657	38.454894
o	35.257261	63.051373	41.017946	h	31.418582	66.002779	38.169077
c	30.507117	61.811477	41.848592	o	29.685169	68.847327	41.515359
c	30.645321	61.463405	40.367542	h	29.639564	69.693849	41.997769
c	31.348265	65.532081	41.939103	h	30.237194	69.064665	40.742226
c	28.337724	64.056215	40.930626	o	31.461038	68.961721	39.376271
c	36.381903	62.653524	41.830728	h	31.225865	68.277605	38.725565
c	31.487869	64.047722	41.929811	h	32.219909	69.430697	38.932839
f	34.579873	63.548983	43.429702	h	37.935290	68.752502	33.692145
h	36.738239	63.513648	42.406918	h	35.876075	61.656650	33.741030
h	28.107428	63.103079	40.430375	h	40.148876	66.283784	40.986558
h	29.827227	61.918835	39.792168	h	37.794649	69.632083	43.994065
h	29.176605	64.777566	42.810157	h	34.618527	73.883065	40.798111
h	28.523509	63.156889	42.906906	h	32.651298	67.481140	34.651046
h	28.937259	64.661887	40.235800	PC4			
h	27.384009	64.572809	41.119081	c	37.633610	69.425659	34.495106
h	38.264562	61.671524	41.431214	h	38.533120	69.999592	34.772261
h	32.250486	66.021975	41.577417	h	36.909515	70.122561	34.048938

c	37.061197 68.769906 35.715567	c	36.546598 70.178539 40.943783
n	37.018133 69.423248 36.938724	h	37.465199 69.615107 40.799358
h	37.139268 70.428975 37.136176	n	35.332517 69.660529 40.993652
c	36.515478 68.575795 37.858774	c	34.465549 70.697956 41.245002
h	36.360992 68.829711 38.900333	h	33.404283 70.545917 41.404244
n	36.229280 67.409372 37.306457	c	32.483164 67.853653 35.640043
c	36.549256 67.513508 35.973398	h	33.261723 68.599350 35.871638
h	36.409906 66.670582 35.300887	h	31.507016 68.350968 35.651583
c	35.412486 61.502519 34.675664	c	32.522038 66.793672 36.699594
h	34.330937 61.552355 34.485006	o	33.437716 65.995985 36.843986
h	35.655222 60.491689 35.049651	o	31.451444 66.791288 37.486086
c	35.756357 62.526087 35.702110	zn	35.233093 65.917964 38.344750
n	36.929057 62.538663 36.441952	zn	34.845367 67.601562 41.381364
h	37.697646 61.877797 36.342707	o	34.170798 67.203241 39.438594
c	36.886986 63.593382 37.291289	h	33.246141 66.944005 39.527999
h	37.668675 63.849534 38.002126	p	33.858651 64.226628 41.424151
n	35.747886 64.254473 37.143751	c	28.757154 63.828011 42.000537
c	35.034497 63.608741 36.156218	n	32.386518 63.718383 41.871695
h	34.057261 63.958372 35.836915	o	34.419412 65.542737 41.893518
c	39.373865 66.119630 41.717031	c	36.803766 62.359296 40.819755
n	38.259200 65.393536 41.147485	n	30.147568 63.380888 41.913121
c	37.191105 66.009740 40.550734	o	34.695748 62.939493 41.872562
o	36.857579 67.175785 40.912381	c	30.406097 61.933611 41.788584
o	36.604773 65.314317 39.663724	c	30.776256 61.501414 40.372359
h	39.038966 67.099823 42.069587	c	30.909466 65.712677 42.057317
h	39.789702 65.568426 42.576526	c	28.129831 64.066783 40.626775
h	38.511097 64.530001 40.679596	c	36.116040 62.861597 42.079967
c	37.485356 68.560828 43.950870	c	31.170995 64.241655 41.917983
h	37.585911 68.250793 42.902173	f	32.490572 62.515123 44.155125
h	38.236956 68.011937 44.532538	h	36.503040 63.845053 42.384014
c	36.114033 68.163439 44.414511	h	28.054380 63.132181 40.049563
n	35.085809 67.844943 43.538550	h	29.926958 61.656658 39.688088
c	34.064548 67.434071 44.278020	h	28.718332 64.727367 42.622117
h	33.111119 67.084437 43.893890	h	28.198042 63.063522 42.558156
n	34.380211 67.463827 45.590572	h	28.734676 64.770142 40.036363
h	33.754388 67.159212 46.350989	h	27.115311 64.483748 40.734523
c	35.675632 67.925637 45.703188	h	37.838530 62.055753 41.053021
h	36.178876 68.039550 46.659575	h	31.814896 66.291822 41.861768
c	34.663616 73.242742 41.675810	h	36.812984 63.148720 40.056935
h	35.293900 73.752492 42.421451	h	30.109514 66.089584 41.409403
h	33.658832 73.144977 42.112103	h	30.607897 65.918502 43.097244
c	35.170394 71.869681 41.374131	h	36.260260 61.492125 40.415252
n	36.496478 71.513625 41.167954	h	31.197647 61.666357 42.496984
h	37.331500 72.089130 41.279701	h	31.643624 62.060035 39.998411

h	31.036045 60.433542 40.367045	c	36.271142 67.520094 36.050356
h	36.243543 62.163282 42.917808	h	36.080856 66.693140 35.370919
h	29.497582 61.413838 42.123342	c	35.335142 61.557069 34.566116
h	32.544524 62.885483 43.270888	h	34.259970 61.633026 34.355764
o	32.781672 68.181941 41.687615	h	35.531915 60.553577 34.982801
h	32.263315 68.378057 40.875361	c	35.696814 62.589270 35.574302
h	32.481802 68.871354 42.337664	n	36.869063 62.557367 36.311585
o	33.868426 64.193580 39.780418	h	37.643656 61.916350 36.157107
h	32.282181 64.540973 39.245164	c	36.840159 63.580379 37.204483
h	33.993898 63.261702 39.390206	h	37.631087 63.816645 37.910964
o	32.038195 70.247849 43.140174	n	35.708812 64.253889 37.082000
h	32.532426 70.838627 43.766231	c	34.988467 63.658828 36.068989
h	31.172251 70.686207 42.968749	h	34.005047 64.024397 35.786406
o	33.692404 69.545091 38.135525	c	39.396696 66.158705 41.695613
h	34.269382 70.307491 38.296729	n	38.318966 65.425252 41.060296
h	34.054875 68.764450 38.633958	c	37.244726 66.065771 40.472899
o	33.995547 61.926237 38.616925	o	36.801828 67.127519 41.023258
h	34.503252 61.886280 37.793971	o	36.810402 65.511773 39.429622
h	34.031071 61.017049 39.043244	h	39.030633 67.118630 42.072535
o	31.376916 64.900211 39.081433	h	39.811240 65.588148 42.543631
h	30.879761 64.207479 38.555525	h	38.658390 64.685419 40.452587
h	31.483036 65.995368 38.175543	c	37.543541 68.581123 44.062094
o	29.666003 68.892348 41.483856	h	37.612959 68.219026 43.026734
h	29.628246 69.743080 41.960840	h	38.286162 68.042503 44.660913
h	30.234106 69.092160 40.717989	c	36.166901 68.307083 44.580885
o	31.462635 68.948302 39.367875	n	35.041893 68.368381 43.776693
h	31.219660 68.260854 38.723548	c	34.009000 68.071670 44.554728
h	32.228802 69.401337 38.922762	h	32.972101 68.007248 44.235811
h	37.937540 68.750513 33.695187	n	34.411021 67.814348 45.818307
h	35.887330 61.647281 33.705286	h	33.815307 67.494482 46.592496
h	40.148396 66.246478 40.960674	c	35.783403 67.958793 45.860389
h	37.785411 69.607449 44.002034	h	36.359516 67.813877 46.770163
h	34.616025 73.872363 40.787339	c	34.668490 73.235413 41.671568
h	32.666230 67.472471 34.635427	h	35.294917 73.749555 42.417096
TS23		h	33.662983 73.134205 42.105385
c	37.493245 69.390505 34.592848	c	35.179847 71.861337 41.377467
h	38.380618 69.967901 34.899528	n	36.510340 71.491240 41.210881
h	36.777631 70.087708 34.132732	h	37.349952 72.055548 41.350496
c	36.878577 68.738706 35.802210	c	36.552898 70.160891 40.968148
n	36.865448 69.389972 37.026994	h	37.467594 69.585498 40.844215
h	37.058108 70.383164 37.222190	n	35.328367 69.656443 40.963289
c	36.287915 68.573223 37.937341	c	34.467501 70.701738 41.210066
h	36.177564 68.816536 38.986846	h	33.398896 70.566185 41.314302
n	35.920624 67.435603 37.380238	c	32.365034 67.797237 35.775470

h	33.101396 68.587859 36.005019	h	32.516568 68.922067 42.249914
h	31.367783 68.254000 35.747449	o	33.480018 63.379868 38.966336
c	32.411922 66.782130 36.911193	h	32.627952 63.668995 38.565346
o	33.418247 66.054386 37.056360	h	33.827518 62.561462 38.544912
o	31.407606 66.772881 37.702194	o	32.048850 70.279961 43.089911
zn	35.061049 65.758479 38.391851	h	32.541425 70.862908 43.724824
zn	34.864769 67.651548 41.588486	h	31.183051 70.724296 42.915545
o	34.174358 66.082266 40.206677	o	33.563297 70.249853 38.260828
h	33.227527 66.200683 40.036833	h	33.856003 71.164903 37.985867
p	34.183342 64.667689 42.003638	h	34.341802 69.871206 38.690778
c	29.196801 63.535398 42.111433	o	34.711039 61.107092 38.094158
n	32.710155 64.154930 41.324618	h	35.645557 61.335450 38.181458
o	34.464362 65.942260 42.742124	h	34.528183 60.449536 38.832697
c	36.999078 62.302179 40.711143	o	31.071734 64.410209 38.865191
n	30.633299 63.340071 41.851529	h	30.327472 63.958528 38.399263
o	35.272728 63.855322 41.194194	h	31.168040 65.308626 38.451329
c	31.113000 61.954884 41.657896	o	29.717550 68.747526 41.452117
c	30.981694 61.430373 40.235071	h	29.696614 69.595019 41.929662
c	31.062742 65.747425 42.179738	h	30.296893 68.930601 40.687639
c	28.431421 64.045854 40.892567	o	31.603446 68.847255 39.397987
c	36.292961 63.039362 41.824491	h	31.438977 68.114227 38.754608
c	31.460831 64.364117 41.801027	h	32.207236 69.482251 38.939941
f	34.054035 63.653183 43.294723	h	37.825348 68.736119 33.786900
h	36.983373 63.704790 42.361006	h	35.839985 61.667308 33.606403
h	28.440384 63.314549 40.072993	h	40.174911 66.317733 40.949182
h	29.934899 61.448894 39.894462	h	37.851323 69.626750 44.063188
h	29.090387 64.216659 42.965945	h	34.617219 73.863634 40.782312
h	28.806266 62.562416 42.439050	h	32.596514 67.438215 34.772680
h	28.869818 64.975234 40.503976	IN3	
h	27.386009 64.247142 41.174578	c	37.511976 69.421237 34.563436
h	37.825978 61.706851 41.129762	h	38.406213 69.979598 34.885683
h	31.938515 66.304261 42.526884	h	36.820041 70.133526 34.091098
h	37.394125 63.020912 39.982129	c	36.862350 68.778451 35.756907
h	30.721360 66.274619 41.275438	n	36.806720 69.425065 36.984757
h	30.268632 65.800386 42.927053	h	37.005049 70.412896 37.198436
h	36.291250 61.638901 40.190959	c	36.211177 68.603676 37.876328
h	32.158913 61.923716 41.988547	h	36.086380 68.836667 38.927723
h	31.587841 62.025931 39.544701	n	35.868814 67.466524 37.300043
h	31.339405 60.391075 40.210268	c	36.255229 67.558363 35.981116
h	35.822149 62.349919 42.538290	h	36.092905 66.728818 35.297830
h	30.535973 61.327676 42.350729	c	35.463176 61.440040 34.534603
h	32.909543 63.585424 40.449385	h	34.380466 61.499173 34.354506
o	32.843755 68.202755 41.650551	h	35.701694 60.423556 34.893115
h	32.377013 68.368870 40.788507	c	35.829893 62.436677 35.573814

n	36.947967	62.346665	36.376376	zn	35.040798	67.756666	41.698002
h	37.580826	61.548373	36.417437	o	34.154601	64.728873	39.722785
c	36.932821	63.378248	37.247932	h	33.802142	63.912497	39.243686
h	37.670213	63.538229	38.030005	p	34.584536	64.355018	41.337441
n	35.877349	64.146412	37.023845	c	29.448974	63.686432	42.234958
c	35.175193	63.575208	35.981676	n	33.045834	63.488708	41.536796
h	34.261262	64.023158	35.599665	o	34.765447	65.804997	41.766251
c	39.365078	66.234316	41.685200	c	37.840859	62.141886	40.748077
n	38.227060	65.599285	41.055475	n	30.797548	63.171441	41.935328
c	37.244264	66.304894	40.413432	o	35.728891	63.311226	40.793354
o	36.907573	67.450547	40.868210	c	30.945444	61.710996	41.778725
o	36.748468	65.737994	39.408907	c	31.006992	61.292252	40.314006
h	39.089190	67.227392	42.054456	c	31.642125	65.466857	41.596029
h	39.721847	65.633468	42.537693	c	28.633396	64.047658	40.997242
h	38.468018	64.767990	40.527341	c	36.754180	62.722907	41.631373
c	37.555347	68.559143	44.095452	c	31.817044	63.992006	41.702167
h	37.631265	68.205131	43.057792	f	34.896100	63.802014	42.927732
h	38.320148	68.038849	44.682019	h	37.151374	63.492901	42.302987
c	36.192125	68.212407	44.613493	h	28.432092	63.168524	40.368729
n	35.119030	68.006588	43.763372	h	30.080789	61.586352	39.797873
c	34.086046	67.634591	44.509316	h	29.550141	64.542146	42.912634
h	33.095816	67.375023	44.142230	h	28.943945	62.901571	42.815608
n	34.442891	67.590083	45.808566	h	29.161043	64.781452	40.373225
h	33.827055	67.283522	46.576146	h	27.666584	64.475838	41.305552
c	35.771608	67.954999	45.902671	h	38.568910	61.620552	41.390339
h	36.303866	67.994975	46.848746	h	32.441903	65.981349	42.130816
c	34.699839	73.331091	41.772724	h	38.376214	62.921651	40.181253
h	35.333015	73.888040	42.479969	h	31.748671	65.728095	40.534944
h	33.702730	73.238360	42.226108	h	30.679942	65.837465	41.953307
c	35.218699	71.956974	41.519033	h	37.403193	61.442013	40.022458
n	36.535402	71.611155	41.236727	h	31.832934	61.362701	42.331919
h	37.373057	72.187528	41.322290	h	31.850900	61.755423	39.790884
c	36.584264	70.285925	40.985071	h	31.122836	60.204030	40.239015
h	37.489779	69.723090	40.773261	h	36.298544	61.937926	42.251207
n	35.372914	69.759901	41.097380	h	30.093363	61.243673	42.288010
c	34.514753	70.785172	41.427825	h	33.183733	62.519823	41.817423
h	33.463057	70.620815	41.632838	o	33.010126	68.159830	41.571095
c	32.464775	67.735013	35.778911	h	32.506169	68.266147	40.718968
h	33.228044	68.497484	36.014170	h	32.601530	68.802777	42.206010
h	31.478704	68.215866	35.784226	o	33.233645	62.726128	38.418169
c	32.503830	66.668294	36.866694	h	32.405152	63.252962	38.242092
o	33.501244	65.909535	36.955967	h	33.731527	62.550294	37.607359
o	31.511023	66.629529	37.660575	o	32.066040	70.052321	43.222942
zn	35.177111	65.697091	38.173059	h	32.583020	70.663660	43.808304

h	31.251761	70.562536	42.975932	h	34.229840	63.989658	35.617854
o	33.566274	70.334151	38.457961	c	39.387133	66.206022	41.591352
h	33.845988	71.221735	38.095391	n	38.265690	65.635655	40.883169
h	34.284072	70.085086	39.056017	c	37.264377	66.381772	40.338067
o	35.596783	61.189513	38.670527	o	36.969457	67.509006	40.854085
h	35.455496	61.988193	39.203699	o	36.695707	65.861013	39.343388
h	34.976088	60.538029	39.099510	h	39.116483	67.186051	41.997908
o	31.140723	64.198427	38.685015	h	39.703522	65.555609	42.423366
h	30.287553	63.845043	38.337340	h	38.490254	64.835449	40.302502
h	31.256454	65.115088	38.320508	c	37.580146	68.553620	44.106113
o	29.846662	68.511399	41.497282	h	37.665905	68.195377	43.070255
h	29.829836	69.356549	41.972810	h	38.347642	68.044622	44.698796
h	30.387827	68.704291	40.707756	c	36.218458	68.198450	44.622965
o	31.655446	68.722046	39.373223	n	35.147173	67.986730	43.771854
h	31.533136	67.987209	38.724353	c	34.113743	67.609242	44.516320
h	32.211862	69.410723	38.937113	h	33.125200	67.342327	44.148493
h	37.843149	68.756855	33.765321	n	34.470686	67.567323	45.815410
h	35.933258	61.611015	33.566173	h	33.853994	67.260756	46.583013
h	40.160455	66.324435	40.945389	c	35.797018	67.939240	45.911218
h	37.848566	69.608919	44.087766	h	36.327526	67.981052	46.858074
h	34.624731	73.905599	40.849488	c	34.683923	73.324255	41.766771
h	32.666187	67.395140	34.763044	h	35.315431	73.876785	42.479153
TS35				h	33.684377	73.233742	42.215029
c	37.570614	69.434245	34.519144	c	35.202068	71.949988	41.513288
h	38.477156	69.968054	34.848801	n	36.521848	71.611445	41.237097
h	36.903912	70.166933	34.042576	h	37.354410	72.195164	41.320357
c	36.893118	68.806848	35.702804	c	36.580424	70.287686	40.985020
n	36.823450	69.450786	36.931098	h	37.489140	69.730555	40.774189
h	37.031552	70.434486	37.154931	n	35.371620	69.753163	41.095427
c	36.200394	68.636486	37.809419	c	34.504984	70.773131	41.421952
h	36.067287	68.869031	38.860497	h	33.455314	70.596972	41.632489
n	35.852201	67.506336	37.221268	c	32.493727	67.695295	35.832693
c	36.265581	67.595394	35.912464	h	33.274922	68.433037	36.085718
h	36.111845	66.765206	35.227883	h	31.523427	68.206536	35.825607
c	35.449497	61.424670	34.539945	c	32.470160	66.629704	36.922194
h	34.367806	61.483597	34.354512	o	33.452399	65.848122	37.062759
h	35.687623	60.405790	34.892013	o	31.449655	66.602642	37.669577
c	35.809526	62.415905	35.585684	zn	35.187086	65.733688	38.087477
n	36.932018	62.332473	36.383018	zn	35.090162	67.748511	41.713973
h	37.568662	61.536501	36.421846	o	34.251754	64.617508	39.832574
c	36.916469	63.363187	37.253513	h	33.794039	63.772692	39.336702
h	37.654962	63.522603	38.034418	p	34.862008	64.360340	41.262169
n	35.855455	64.125766	37.033281	c	29.149600	63.658595	42.269525
c	35.149242	63.549510	35.996007	n	32.698078	63.197265	41.476930

o	35.080514 65.748186 41.822281	h	35.013352 60.593768 39.142204
c	38.087572 62.125932 40.779443	o	31.095343 64.154278 38.691523
n	30.437122 63.037984 41.981805	h	30.239390 63.812498 38.333282
o	36.074627 63.404189 40.744820	h	31.206997 65.078746 38.354017
c	30.451185 61.598658 41.710574	o	29.860101 68.591572 41.502606
c	30.483635 61.267964 40.218729	h	29.834204 69.471631 41.913112
c	31.543452 65.266041 41.779875	h	30.428172 68.724501 40.720648
c	28.363196 64.049492 41.017962	o	31.714822 68.680842 39.401952
c	37.021361 62.773056 41.633829	h	31.526403 67.964464 38.751914
c	31.567040 63.760074 41.764946	h	32.241852 69.376192 38.940800
f	34.806809 63.584622 42.710847	h	37.889441 68.758844 33.725261
h	37.436172 63.536114 42.306586	h	35.925246 61.604073 33.575816
h	28.109678 63.170132 40.406969	h	40.204151 66.314150 40.878011
h	29.616660 61.717849 39.716522	h	37.862961 69.606200 44.093548
h	29.313857 64.528312 42.917258	h	34.616312 73.902780 40.845466
h	28.573372 62.939877 42.872976	h	32.697312 67.359863 34.815783
h	28.951630 64.726985 40.382631	PC5	
h	27.422581 64.550189 41.295349	c	37.764239 69.367034 34.581325
h	38.765829 61.559625 41.433773	h	38.707021 69.821863 34.931800
h	32.443703 65.640143 42.275714	h	37.153570 70.169605 34.140719
h	38.675252 62.874406 40.220933	c	37.011070 68.744089 35.719701
h	31.574326 65.609439 40.736768	n	36.600207 69.489201 36.814683
h	30.676384 65.722772 42.262762	h	36.765860 70.482861 37.030308
h	37.609939 61.451924 40.053067	c	35.889579 68.694392 37.641873
h	31.307393 61.132345 42.226033	h	35.413081 69.053490 38.548424
h	31.391470 61.660165 39.743906	n	35.827226 67.464345 37.153083
h	30.456290 60.182325 40.061765	c	36.512612 67.478299 35.960087
h	36.496779 62.025770 42.243881	h	36.604020 66.577786 35.356598
h	29.559666 61.164576 42.182234	c	35.457341 61.532043 34.696607
h	32.745369 62.183045 41.467774	h	34.374059 61.618085 34.525719
o	33.054072 68.018078 41.583667	h	35.661423 60.515922 35.075166
h	32.561222 68.152195 40.728706	c	35.849276 62.530108 35.731918
h	32.647538 68.667677 42.213928	n	36.844553 62.324125 36.668744
o	33.218246 62.779984 38.608470	h	37.428983 61.488299 36.725962
h	32.347838 63.262387 38.419489	c	36.831263 63.350347 37.545414
h	33.717801 62.560556 37.808414	h	37.457372 63.415177 38.429648
o	32.134235 69.970243 43.216819	n	35.903109 64.232072 37.197397
h	32.640661 70.590752 43.800855	c	35.282083 63.733928 36.067065
h	31.312925 70.466091 42.975557	h	34.434703 64.236184 35.610570
o	33.569947 70.340666 38.439571	c	39.238555 67.510443 40.195386
h	33.842424 71.231894 38.078964	n	38.012187 67.011229 39.610302
h	34.275602 70.114123 39.060721	c	36.873153 67.046678 40.342835
o	35.636291 61.258033 38.733560	o	36.946272 67.341970 41.568179
h	35.589985 62.010552 39.343727	o	35.729715 66.827152 39.814090

h	39.388766	68.587548	39.983406	c	31.420280	64.785129	41.404511
h	39.160315	67.384937	41.281310	c	28.084385	63.681828	41.618115
h	37.931411	66.859553	38.611518	c	37.345130	63.600519	41.691411
c	37.543814	68.551966	44.285410	c	31.280874	63.316739	41.128644
h	37.632221	68.111388	43.286742	f	34.441597	63.152098	41.795997
h	38.300281	68.089415	44.925790	h	37.936082	64.424206	42.122703
c	36.181641	68.256568	44.843060	h	27.606309	62.836956	41.100735
n	35.074127	67.995320	44.048377	h	28.426118	61.107233	40.076220
c	34.066478	67.688720	44.856468	h	29.674662	64.057472	43.062783
h	33.064084	67.403922	44.541840	h	28.920348	62.482818	43.233126
n	34.469468	67.740434	46.139627	h	28.427874	64.384324	40.844064
h	33.885738	67.441707	46.932338	h	27.320714	64.172119	42.239660
c	35.800343	68.093869	46.159285	h	38.844620	62.053441	41.697558
h	36.371064	68.191039	47.077263	h	32.032966	65.247652	40.625625
c	34.599994	73.266407	41.714078	h	38.859841	63.100495	40.235670
h	35.226327	73.795544	42.450192	h	30.458573	65.305284	41.449073
h	33.587861	73.202452	42.138784	h	31.926516	64.926147	42.373124
c	35.093113	71.872334	41.497865	h	37.568862	61.868944	40.451115
n	36.398577	71.509418	41.206484	h	31.175117	60.694832	41.414892
h	37.220934	72.106899	41.161396	h	29.913126	61.621390	39.270024
c	36.458462	70.160681	41.113300	h	29.683492	59.899949	39.696821
h	37.377939	69.613758	40.933965	h	36.781377	63.117955	42.503763
n	35.270493	69.630604	41.346623	h	29.614527	60.689752	42.192100
c	34.406809	70.679557	41.579000	h	32.207568	61.758065	40.143611
h	33.374480	70.519210	41.881461	o	32.892656	67.882780	41.831230
c	32.396805	67.697178	35.891309	h	32.515042	68.046916	40.928482
h	33.188107	68.417394	36.162840	h	32.477234	68.568015	42.413375
h	31.436985	68.226597	35.859401	o	32.430515	63.191170	37.361692
c	32.328827	66.625312	36.975336	h	31.573065	63.345273	37.810030
o	33.324285	65.853444	37.132367	h	33.743656	62.114991	38.089970
o	31.293089	66.576033	37.688542	o	31.977642	69.935459	43.345151
zn	35.030842	65.781220	38.208395	h	32.509142	70.566128	43.893405
zn	34.909105	67.590515	42.030736	h	31.181142	70.455613	43.070021
o	34.152961	64.699048	39.813361	o	33.448625	70.573195	38.643892
h	32.792073	64.094587	37.290615	h	33.761472	71.365268	38.118337
p	34.915701	64.529792	41.118294	h	33.770033	70.769033	39.537883
c	29.253172	63.222982	42.490067	o	34.450521	61.642671	38.579388
n	32.170812	62.753211	40.336860	h	32.888287	63.326485	39.882206
o	34.794104	65.542747	42.234525	h	33.997834	60.862129	38.974359
c	38.215372	62.591385	40.973502	o	30.112448	64.145284	38.709693
n	30.324202	62.591997	41.711412	h	29.215185	64.020786	38.317524
o	36.434224	64.157781	40.729153	h	30.423309	65.033086	38.439075
c	30.182463	61.167709	41.382987	o	29.706556	68.646610	41.403235
c	29.511534	60.933921	40.026357	h	29.719944	69.508987	41.850034

h	30.381213 68.745087 40.705106	c	36.068795 68.173968 44.394933
o	31.789314 68.591739 39.497352	n	35.029483 67.843903 43.535364
h	31.534437 67.891054 38.855539	c	34.010981 67.464519 44.294564
h	32.272670 69.294898 39.006124	h	33.049455 67.118001 43.927827
h	38.027864 68.710971 33.751777	n	34.337780 67.528177 45.606017
h	35.926531 61.664295 33.721703	h	33.735554 67.268671 46.397961
h	40.129358 66.975870 39.865585	c	35.639878 67.977534 45.693655
h	37.843150 69.595615 44.189171	h	36.150053 68.117031 46.643292
h	34.572284 73.872402 40.808502	c	34.667483 73.274350 41.718979
h	32.630395 67.360767 34.881194	h	35.317199 73.787915 42.445080
TS24'		h	33.667896 73.200038 42.171018
c	37.631168 69.426204 34.486673	c	35.144657 71.890114 41.428746
h	38.534848 69.993383 34.765125	n	36.457411 71.514143 41.175132
h	36.913131 70.129273 34.040185	h	37.302330 72.079394 41.254706
c	37.047679 68.774513 35.702423	c	36.477424 70.178286 40.948040
n	36.963420 69.436887 36.918562	h	37.379392 69.599273 40.766449
h	37.089993 70.440554 37.119582	n	35.258101 69.682681 41.043796
c	36.432734 68.594156 37.827725	c	34.416712 70.729643 41.329049
h	36.234312 68.858179 38.859161	h	33.359199 70.586276 41.522514
n	36.174874 67.421375 37.275546	c	32.357709 67.815403 35.713625
c	36.536783 67.517051 35.954481	h	33.095705 68.597710 35.961130
h	36.413106 66.670956 35.282567	h	31.362730 68.277495 35.701000
c	35.366391 61.512669 34.628371	c	32.416632 66.778857 36.816347
h	34.287782 61.546519 34.420763	o	33.376304 65.980033 36.883333
h	35.617141 60.509081 35.017871	o	31.460433 66.810604 37.671670
c	35.678810 62.554670 35.645888	zn	35.030050 65.988097 38.242564
n	36.880148 62.648577 36.330126	zn	34.723774 67.640114 41.319364
h	37.695669 62.062437 36.170655	o	34.097485 67.363183 39.359959
c	36.802177 63.698213 37.185867	h	33.147815 67.188968 39.378440
h	37.596829 64.009180 37.858379	p	33.978623 64.180397 41.616743
n	35.616404 64.274442 37.095933	c	28.683384 63.839633 42.014666
c	34.903092 63.582379 36.139897	n	32.314534 63.467722 42.018340
h	33.896885 63.884206 35.861136	o	34.125203 65.670074 41.692297
c	39.291730 66.135642 41.477961	c	37.087011 62.158164 40.594197
n	38.206466 65.425554 40.841612	n	30.032241 63.262658 41.990555
c	37.032707 65.998500 40.431017	o	34.952142 62.993617 41.108723
o	36.719150 67.140727 40.880095	c	30.142087 61.812820 41.757541
o	36.346464 65.293883 39.626110	c	30.471319 61.464048 40.305571
h	38.951009 67.130307 41.783494	c	30.992604 65.532276 42.030233
h	39.642366 65.600815 42.377909	c	28.106915 64.085264 40.619427
h	38.466054 64.602334 40.311437	c	36.206630 62.650910 41.723998
c	37.444620 68.552284 43.922866	c	31.118051 64.041916 42.002307
h	37.539377 68.243194 42.873042	f	34.385482 63.853375 43.194935
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h	27.941298 63.141350 40.078407	h	40.119834 66.231380 40.775718
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h	28.721957 64.766655 42.594814	h	34.615591 73.885246 40.817769
h	28.044563 63.148167 42.584713	h	32.583039 67.455487 34.709756
h	28.791300 64.697137 40.015483	IN4	
h	27.138642 64.603794 40.695773	c	37.602192 69.405470 34.525652
h	38.045453 61.782064 40.986379	h	38.496961 69.984266 34.808361
h	31.942885 66.019855 41.801203	h	36.873907 70.100717 34.082934
h	37.258428 62.981960 39.889698	c	37.031991 68.737183 35.741764
h	30.232462 65.905004 41.338784	n	36.977625 69.390536 36.964236
h	30.713200 65.847832 43.045899	h	37.096325 70.396182 37.161712
h	36.570602 61.355441 40.046028	c	36.478380 68.536720 37.881825
h	30.876193 61.373189 42.452559	h	36.316298 68.791292 38.921777
h	31.448345 61.854793 39.990642	n	36.205926 67.366269 37.331748
h	30.485546 60.373094 40.179403	c	36.531134 67.474795 35.999928
h	36.027351 61.886293 42.494003	h	36.405086 66.631536 35.325027
h	29.181564 61.367682 42.048585	c	35.392853 61.502243 34.726173
h	32.377043 62.470089 42.202838	h	34.312425 61.554080 34.528239
o	32.667916 68.189928 41.697948	h	35.629884 60.489124 35.098226
h	32.165659 68.415050 40.880570	c	35.730772 62.518875 35.763052
h	32.381193 68.868741 42.360550	n	36.876865 62.496098 36.542899
o	33.457413 64.166062 39.921611	h	37.631508 61.816816 36.464793
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h	31.113943 70.675166 43.038060	h	34.064412 63.996142 35.855577
o	33.609624 69.733465 38.136298	c	39.392202 66.189090 41.787485
h	34.197807 70.494187 38.263089	n	38.265890 65.447881 41.261665
h	33.993930 68.942684 38.600905	c	37.227520 66.056255 40.596613
o	33.623785 61.941246 38.607358	o	36.895149 67.235775 40.914575
h	34.249746 62.002024 37.869408	o	36.673996 65.341815 39.708007
h	33.846569 61.102614 39.104691	h	39.070368 67.183041 42.110873
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h	31.320326 65.636093 38.615542	c	37.514479 68.592331 43.953205
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h	29.604464 69.699454 41.953939	h	38.269735 68.041284 44.528044
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c	34.683964 73.271945 41.700156	h	37.874748 62.870850 40.146305
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c	35.200966 71.903817 41.402293	h	37.019591 61.320949 40.110861
n	36.527805 71.555841 41.184318	h	31.256372 61.378170 42.360558
h	37.361477 72.132282 41.301396	h	31.566435 61.815681 39.860694
c	36.580677 70.223824 40.943183	h	30.565302 60.373576 40.156609
h	37.498309 69.662217 40.786043	h	36.151751 61.807496 42.471867
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h	31.473359 68.341824 35.677553	o	33.879313 64.372213 39.806363
c	32.493276 66.786243 36.727471	h	32.346394 64.644983 39.345713
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o	31.427430 66.793472 37.525615	o	32.051652 70.317332 43.120359
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o	35.347381 63.046267 41.009506	h	31.469595 65.998389 38.221260
c	30.455922 61.827512 41.750218	o	29.691581 68.822613 41.527619
c	30.611351 61.464765 40.275484	h	29.649177 69.667623 42.011982
c	31.399001 65.524027 41.975490	h	30.238106 69.040510 40.750358
c	28.359132 64.133325 40.821332	o	31.465754 68.950483 39.385281
c	36.478463 62.588526 41.769522	h	31.239021 68.267363 38.729347
c	31.496288 64.036766 41.898114	h	32.216076 69.433570 38.942707
f	34.635748 63.737422 43.112447	h	37.911807 68.740149 33.719704
h	36.897174 63.416785 42.355259	h	35.872135 61.646007 33.757831
h	28.123452 63.193398 40.298825	h	40.157554 66.286898 41.017591
h	29.803267 61.920728 39.687278	h	37.813518 69.639220 44.004825
h	29.179880 64.802440 42.729409	h	34.624630 73.886197 40.801691
h	28.490722 63.196740 42.783162	h	32.640941 67.475246 34.662391
h	28.984578 64.738773 40.150289	TS46	
h	27.411562 64.663821 41.001217	c	37.639119 69.440099 34.479289

h	38.542470	70.006335	34.759688	n	36.452974	71.490301	41.168906
h	36.925803	70.142544	34.024921	h	37.290654	72.065007	41.259708
c	37.050902	68.795531	35.697576	c	36.493537	70.152702	40.960031
n	37.009345	69.448718	36.920925	h	37.406202	69.580898	40.813726
h	37.143541	70.451979	37.121512	n	35.276703	69.641974	41.028337
c	36.487107	68.608834	37.837079	c	34.417470	70.686681	41.275622
h	36.336831	68.862439	38.879853	h	33.357744	70.536115	41.452635
n	36.185264	67.448931	37.279799	c	32.457109	67.852623	35.654532
c	36.516506	67.547798	35.950451	h	33.225725	68.607690	35.888168
h	36.367647	66.706781	35.277813	h	31.473260	68.334728	35.668335
c	35.373507	61.491816	34.718035	c	32.519699	66.788806	36.710524
h	34.295734	61.548439	34.507961	o	33.455454	66.011261	36.840740
h	35.603658	60.473890	35.080542	o	31.457548	66.758104	37.503522
c	35.698726	62.492940	35.773120	zn	35.234612	65.951242	38.323185
n	36.820801	62.443487	36.587416	zn	34.809207	67.578104	41.433422
h	37.566195	61.751434	36.525572	o	34.145942	67.137703	39.484541
c	36.768533	63.484665	37.453940	h	33.247409	66.808020	39.608775
h	37.505131	63.698701	38.223518	p	34.443366	64.033271	41.460148
n	35.672727	64.199458	37.241252	c	28.570133	63.893098	41.995208
c	34.995263	63.598484	36.200365	n	32.177516	63.295205	41.894123
h	34.056070	63.996034	35.827023	o	34.524765	65.458039	41.914574
c	39.381067	66.225365	41.715164	c	37.827327	62.086186	40.857636
n	38.284400	65.488184	41.124235	n	29.849122	63.197422	41.981600
c	37.214794	66.097908	40.518938	o	35.742454	63.217602	40.925956
o	36.824283	67.224717	40.941498	c	29.835196	61.760776	41.716703
o	36.700097	65.441000	39.566342	c	30.059253	61.385683	40.248429
h	39.043619	67.214713	42.037629	c	31.011767	65.382663	42.137926
h	39.778229	65.691995	42.595245	c	28.037858	64.237238	40.599166
h	38.583470	64.675633	40.598451	c	36.772649	62.685121	41.764791
c	37.467104	68.566295	43.950371	c	31.031908	63.886237	41.991022
h	37.548022	68.258365	42.899952	f	34.423366	63.180857	42.848244
h	38.228319	68.012300	44.515292	h	37.190676	63.487635	42.389080
c	36.104161	68.167006	44.439262	h	27.771326	63.330323	40.035046
n	35.065782	67.812024	43.587161	h	29.328671	61.896639	39.607075
c	34.063219	67.396590	44.352446	h	28.685368	64.799816	42.597796
h	33.110033	67.013405	43.997444	h	27.847574	63.259762	42.535445
n	34.403114	67.462017	45.658484	h	28.800688	64.778414	40.020156
h	33.807139	67.176440	46.448387	h	27.134634	64.863453	40.667572
c	35.690568	67.949684	45.738699	h	38.571830	61.549168	41.464284
h	36.206985	68.091137	46.684321	h	32.024640	65.773751	42.017310
c	34.642684	73.238214	41.679486	h	38.342905	62.856313	40.263475
h	35.279901	73.739914	42.425034	h	30.357275	65.882756	41.414896
h	33.636576	73.155551	42.115779	h	30.672962	65.657994	43.146568
c	35.130713	71.856981	41.382761	h	37.351958	61.389143	40.149397

h	30.579197 61.255416 42.354066	h	36.193634 68.929787 38.818909
h	31.065480 61.671626 39.904414	n	36.065015 67.504299 37.225141
h	29.947441 60.299597 40.115572	c	36.440704 67.586945 35.906635
h	36.347028 61.918993 42.428184	h	36.298775 66.742373 35.237157
h	28.862148 61.377182 42.056180	c	35.338482 61.474567 34.648476
h	32.143300 62.277207 41.865565	h	34.263754 61.521929 34.421779
o	32.742161 68.064858 41.765070	h	35.570851 60.457808 35.012314
h	32.215541 68.245625 40.955241	c	35.643549 62.475252 35.708801
h	32.453323 68.772964 42.396978	n	36.720462 62.388166 36.578819
o	33.765986 64.019263 39.997611	h	37.429062 61.653418 36.569781
h	32.176612 64.528596 39.514705	c	36.668460 63.442375 37.429795
h	33.851130 63.154881 39.469761	h	37.360262 63.625443 38.247158
o	32.021493 70.213741 43.147197	n	35.619162 64.202707 37.151376
h	32.516979 70.809476 43.766321	c	34.968509 63.616745 36.085961
h	31.160652 70.659190 42.966785	h	34.065114 64.047209 35.662507
o	33.644351 69.481371 38.194392	c	39.370775 66.265274 41.515741
h	34.226565 70.235566 38.370080	n	38.318659 65.541003 40.840691
h	33.996385 68.694689 38.691933	c	37.176426 66.124220 40.367766
o	33.666207 61.907199 38.557046	o	36.798689 67.231561 40.846524
h	34.199313 61.945366 37.748397	o	36.581607 65.454739 39.469148
h	33.838969 61.017062 38.985816	h	39.002960 67.240015 41.850286
o	31.346881 64.893618 39.123092	h	39.732463 65.708232 42.396759
h	30.962185 64.178142 38.539433	h	38.638200 64.788515 40.241022
h	31.511553 65.972384 38.206084	c	37.426617 68.550149 43.902273
o	29.626409 68.831465 41.537467	h	37.519145 68.251482 42.849892
h	29.603128 69.690521 41.998216	h	38.184845 67.989804 44.466212
h	30.204064 69.007020 40.772724	c	36.062475 68.133913 44.377937
o	31.428699 68.859994 39.440649	n	35.050536 67.717107 43.520587
h	31.192325 68.186506 38.779964	c	34.057232 67.267587 44.279258
h	32.188062 69.329265 39.003307	h	33.133030 66.822613 43.915974
h	37.940902 68.757546 33.684861	n	34.375538 67.378468 45.587595
h	35.862750 61.644532 33.756065	h	33.774923 67.093827 46.374897
h	40.165588 66.324613 40.965002	c	35.637422 67.927477 45.675289
h	37.774185 69.610934 44.000329	h	36.133187 68.111781 46.624636
h	34.605185 73.869575 40.791768	c	34.619484 73.226739 41.674308
h	32.646772 67.476856 34.649100	h	35.260362 73.716434 42.424852
PC6		h	33.610821 73.154668 42.106572
c	37.631091 69.451244 34.454743	c	35.091017 71.840111 41.373499
h	38.539262 70.001320 34.751799	n	36.407628 71.465734 41.139196
h	36.940910 70.166650 33.985212	h	37.248231 72.038689 41.207489
c	37.003655 68.823516 35.661725	c	36.439583 70.129374 40.929648
n	36.933046 69.486706 36.878462	h	37.345441 69.553104 40.761918
h	37.093746 70.484685 37.084818	n	35.220825 69.623780 41.018486
c	36.367032 68.663147 37.783567	c	34.369674 70.672493 41.282205

h	33.312099	70.526294	41.481003	o	32.681660	67.967808	41.788350
c	32.476608	67.901765	35.565731	h	32.136405	68.149115	40.988771
h	33.252312	68.655678	35.777213	h	32.415481	68.692760	42.410021
h	31.499941	68.397344	35.574174	o	33.861134	64.071092	39.821431
c	32.526122	66.876758	36.655932	h	31.533127	65.072111	40.186027
o	33.439727	66.066374	36.785369	h	33.809187	63.191611	39.292666
o	31.491584	66.922859	37.465181	o	31.964862	70.166139	43.136936
zn	35.117907	65.971993	38.214027	h	32.463850	70.760152	43.753281
zn	34.785875	67.557601	41.384661	h	31.101211	70.609212	42.970264
o	34.052694	67.078090	39.501076	o	33.460832	69.405182	38.255695
h	33.210175	66.632630	39.666288	h	34.066139	70.136762	38.442535
p	34.648504	64.012510	41.179686	h	33.803345	68.600036	38.734773
c	28.092496	63.577674	41.882960	o	33.644464	61.937239	38.485724
n	31.638123	64.295651	41.676736	h	34.160525	61.954714	37.664897
o	34.858881	65.292152	41.901139	h	33.817714	61.056717	38.935675
c	38.036565	62.078263	41.033309	o	31.156805	65.396642	39.306072
n	29.521393	63.342271	42.049505	h	30.831435	64.599593	38.807783
o	35.908121	63.103160	40.810557	h	31.528129	66.241224	38.276776
c	30.029963	61.984496	41.853240	o	29.340866	68.948219	41.541967
c	30.351920	61.579237	40.408121	h	29.392994	69.798042	42.019320
c	29.908961	65.790214	42.341580	h	30.009024	69.051116	40.839741
c	27.697295	63.987104	40.455084	o	31.265714	68.848679	39.566836
c	36.882459	62.697875	41.788738	h	30.990663	68.190112	38.909314
c	30.394731	64.405289	42.014136	h	32.020530	69.297553	39.100600
f	33.866551	62.967725	42.106708	h	37.935423	68.763166	33.666075
h	37.209073	63.575592	42.364879	h	35.843033	61.635181	33.695745
h	27.782646	63.143239	39.754032	h	40.187988	66.395389	40.806305
h	29.457430	61.647241	39.770005	h	37.735791	69.593345	43.967236
h	27.777377	64.346770	42.599015	h	34.593213	73.864583	40.790831
h	27.560885	62.658758	42.177477	h	32.659693	67.502163	34.568301
h	28.356090	64.784291	40.079233	TS3*			
h	26.658877	64.356692	40.418705	c	37.594282	69.458841	34.487123
h	38.734568	61.607722	41.737337	h	38.495398	70.029008	34.768217
h	30.786297	66.424718	42.506916	h	36.879351	70.157973	34.030097
h	38.577741	62.839140	40.449998	c	37.000801	68.810560	35.701479
h	29.346993	66.247372	41.515489	n	36.902106	69.455635	36.926394
h	29.287876	65.793993	43.247449	h	37.037304	70.453741	37.143970
h	37.655149	61.320602	40.331372	c	36.383952	68.588362	37.826740
h	30.930393	61.864512	42.475864	h	36.217036	68.820536	38.873374
h	31.136362	62.213251	39.968753	n	36.145845	67.420814	37.255767
h	30.715553	60.540719	40.388307	c	36.503870	67.546066	35.936557
h	36.412082	61.977737	42.477715	h	36.404861	66.704995	35.254435
h	29.287908	61.287642	42.270449	c	35.443054	61.372870	34.431078
h	31.885055	63.330645	41.474117	h	34.361562	61.415905	34.239459

h	35.696487	60.354656	34.773533	o	31.436543	66.718735	37.646817
c	35.788102	62.368461	35.472727	zn	35.139713	65.680386	37.880490
n	36.874948	62.265380	36.321468	zn	34.966426	67.666986	41.879356
h	37.520950	61.477034	36.365620	o	33.629541	65.392686	40.324738
c	36.890229	63.350398	37.124744	h	33.478160	64.766001	39.544107
h	37.607030	63.521048	37.923106	p	34.133315	64.661966	41.638314
n	35.879379	64.148299	36.816331	c	29.319988	63.366466	42.724898
c	35.175487	63.550624	35.798891	n	32.905440	63.752405	42.217224
h	34.270621	63.988762	35.385133	o	34.793131	65.695013	42.533368
c	39.253060	66.482906	41.222325	c	37.374423	62.502982	40.984625
n	38.256646	65.755736	40.474282	n	30.729134	63.110530	42.422671
c	36.989349	66.153090	40.205948	o	35.196726	63.518040	41.200362
o	36.566814	67.230508	40.739579	c	31.132446	61.716670	42.145088
o	36.332825	65.397578	39.429567	c	31.331305	61.460790	40.652577
h	38.914993	67.507664	41.414485	c	31.163417	65.516330	42.142314
h	39.478177	66.001676	42.191221	c	28.442950	63.556970	41.489528
h	38.582506	64.965526	39.930825	c	36.426097	63.230058	41.916652
c	37.588311	68.546807	44.149513	c	31.622246	64.096297	42.294214
h	37.647573	68.170745	43.117806	f	34.236440	62.105812	43.586556
h	38.367069	68.039412	44.727757	h	36.855138	64.178151	42.269340
c	36.238952	68.221324	44.714945	h	28.359874	62.628131	40.904199
n	35.117927	68.102448	43.913429	h	30.418304	61.680284	40.079275
c	34.109399	67.736977	44.696273	h	29.262121	64.244351	43.379197
h	33.094428	67.519773	44.370768	h	28.964385	62.515035	43.324270
n	34.528367	67.619174	45.970435	h	28.861166	64.328709	40.826112
h	33.937359	67.295975	46.750018	h	27.430714	63.865854	41.799443
c	35.873561	67.923789	46.011559	h	38.236371	62.130483	41.561130
h	36.452352	67.895343	46.929398	h	30.965861	65.682851	41.072346
c	34.698730	73.298367	41.756064	h	37.730001	63.164829	40.183137
h	35.337308	73.845104	42.467225	h	30.253464	65.751654	42.699811
h	33.701487	73.216711	42.211306	h	31.945822	66.214337	42.445039
c	35.203407	71.913709	41.513942	h	36.874226	61.651419	40.501989
n	36.514263	71.550484	41.228072	h	32.055714	61.497327	42.689378
h	37.352827	72.129119	41.270381	h	32.140521	62.082993	40.249227
c	36.552658	70.211237	41.039316	h	31.597215	60.405986	40.496116
h	37.457898	69.647313	40.828390	h	36.158035	62.614594	42.783979
n	35.344830	69.693067	41.199193	h	30.354349	61.059324	42.554944
c	34.496642	70.737507	41.489459	h	33.629401	62.697839	43.081794
h	33.447319	70.585498	41.718307	o	32.985319	68.052116	41.720944
c	32.237653	67.889213	35.714188	h	32.532466	68.169801	40.839446
h	32.916252	68.738006	35.904199	h	32.586507	68.738543	42.318517
h	31.202659	68.249904	35.674032	o	33.433560	63.949707	38.291522
c	32.415758	66.923113	36.872259	h	32.436916	63.895861	38.346528
o	33.567775	66.451614	37.020076	h	33.807220	63.035057	38.441639

o	32.047350 70.014078 43.269958	n	36.060106 64.125651 36.997851
h	32.567649 70.638079 43.839082	c	35.354394 63.599687 35.935292
h	31.236372 70.519660 43.008647	h	34.485967 64.105716 35.518745
o	33.602485 70.295549 38.482267	c	39.100974 66.722479 40.871657
h	33.861636 71.188088 38.119536	n	37.954965 66.483479 40.021163
h	34.339360 70.045671 39.056414	c	36.682101 66.707188 40.446605
o	34.786393 61.838060 39.004006	o	36.549567 67.174161 41.623243
h	34.941662 62.325956 39.837423	o	35.705432 66.476321 39.686035
h	34.479384 60.935031 39.304720	h	39.095648 67.751986 41.264356
o	30.923440 64.349668 38.900403	h	39.105071 66.044626 41.742096
h	30.079266 63.981914 38.538298	h	38.080835 66.172445 39.066856
h	31.025208 65.245747 38.499689	c	37.585549 68.569702 44.269664
o	29.763634 68.598585 41.503892	h	37.616756 68.131831 43.262248
h	29.762287 69.464633 41.943590	h	38.352143 68.077892 44.874256
h	30.381334 68.727209 40.759068	c	36.238706 68.351281 44.886331
o	31.730593 68.678205 39.504387	n	35.057267 68.621590 44.209629
h	31.568958 67.951589 38.857270	c	34.060023 68.318598 45.036747
h	32.274998 69.361534 39.043763	h	33.000428 68.390501 44.799328
h	37.899486 68.773789 33.696161	n	34.540097 67.865494 46.205939
h	35.927929 61.578193 33.476717	h	33.965349 67.482094 46.968664
h	40.152067 66.497386 40.606173	c	35.919714 67.876399 46.138403
h	37.874040 69.598190 44.117577	h	36.546293 67.550355 46.961945
h	34.628500 73.886596 40.841121	c	34.683811 73.324343 41.767543
h	32.517465 67.504240 34.733592	h	35.336390 73.863782 42.470577
PC*		h	33.687900 73.258694 42.228091
c	37.697886 69.425194 34.445163	c	35.159114 71.933685 41.522713
h	38.618238 69.948702 34.755490	n	36.467476 71.531138 41.280928
h	37.019669 70.169013 34.001842	h	37.323102 72.083607 41.344575
c	37.054839 68.764674 35.624219	c	36.466389 70.192988 41.080831
n	36.842659 69.420118 36.828871	h	37.366133 69.605516 40.914457
h	36.962947 70.417152 37.060077	n	35.235379 69.714374 41.184486
c	36.280835 68.548794 37.695072	c	34.413790 70.786136 41.453225
h	36.003591 68.798708 38.712808	h	33.351129 70.670741 41.639837
n	36.122898 67.367625 37.122395	c	32.365855 67.863383 35.703973
c	36.581441 67.486238 35.837294	h	33.078577 68.681884 35.907859
h	36.560975 66.633308 35.162680	h	31.348866 68.275328 35.708474
c	35.511865 61.428501 34.520720	c	32.521617 66.844972 36.820216
h	34.426537 61.501562 34.359054	o	33.570628 66.146803 36.821206
h	35.743033 60.400740 34.850127	o	31.614977 66.787913 37.701667
c	35.911256 62.398007 35.574866	zn	35.145518 65.690234 37.958733
n	36.964667 62.204717 36.450797	zn	34.782837 67.896298 42.270305
h	37.581834 61.389893 36.465115	o	33.373356 65.785176 40.863949
c	37.018634 63.260879 37.294986	h	33.537880 65.207554 40.055647
h	37.734061 63.351521 38.110355	p	33.964993 65.042477 42.135028

c	29.261098	63.269597	42.673158	o	34.864984	61.957979	39.736343
n	32.876898	63.849655	42.530290	h	34.766000	62.012227	40.711915
o	34.369115	66.041921	43.199895	h	34.555324	61.028901	39.552420
c	37.416122	63.270842	41.379012	o	31.299973	64.411171	38.996731
n	30.710407	63.066970	42.595636	h	30.553610	63.936326	38.551185
o	35.227008	64.237804	41.548189	h	31.326410	65.312312	38.591773
c	31.170838	61.697901	42.294362	o	29.598817	68.502174	41.369479
c	31.503430	61.492287	40.818676	h	29.621343	69.297577	41.922754
c	31.025598	65.500556	42.647388	h	30.305197	68.664964	40.714379
c	28.599368	63.488558	41.309118	o	31.798434	68.701611	39.636480
c	36.403033	63.901644	42.311382	h	31.718078	67.973719	38.976173
c	31.568700	64.094545	42.609302	h	32.299175	69.415178	39.175735
f	34.306833	61.855926	42.421452	h	37.984457	68.749980	33.638920
h	36.789366	64.827462	42.759321	h	35.969724	61.613980	33.549108
h	28.552005	62.552369	40.731986	h	40.022590	66.572875	40.309244
h	30.636037	61.700402	40.176178	h	37.889053	69.612703	44.179662
h	29.054524	64.115355	43.338896	h	34.617689	73.899996	40.844332
h	28.838900	62.383338	43.169265	h	32.596740	67.494172	34.704753
h	29.169506	64.214471	40.711662				
h	27.572279	63.867516	41.440749				
h	38.267629	62.891142	41.965794				
h	30.599229	65.773571	41.671413				
h	37.787664	64.006098	40.649582				
h	30.242873	65.611434	43.405612				
h	31.807941	66.225663	42.881651				
h	36.955310	62.437217	40.831390				
h	32.042177	61.469343	42.917350				
h	32.324500	62.142526	40.495815				
h	31.812007	60.449377	40.662152				
h	36.118045	63.197916	43.103607				
h	30.373918	61.010499	42.608692				
h	33.616595	62.637782	42.490577				
o	32.818900	68.222070	42.031411				
h	32.459857	68.256752	41.104358				
h	32.398343	68.973252	42.525984				
o	33.859306	64.220309	38.874203				
h	32.875036	64.113477	38.711671				
h	34.229817	63.334198	39.176111				
o	31.889729	70.284668	43.310318				
h	32.409638	70.913715	43.876844				
h	31.038879	70.743037	43.077254				
o	33.595048	70.328175	38.480325				
h	33.852989	71.222738	38.122321				
h	34.313328	70.097433	39.085484				