

Supporting Information

How Bulky Ligands Control the Chemoselectivity of Pd-Catalyzed N-Arylation of Ammonia

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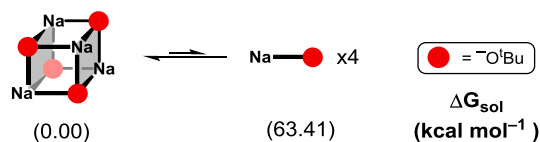
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1. Deprotonation of the Amine

1.1. Tetrameric structure of the base

The base NaO^tBu is modeled as a tetrameric cubane-type cluster, which is the most plausible form of the base in non-polar solvent environment provided by 1,4-dioxane ($\epsilon = 2.209$). The monomer-form is thought to be not the appropriate structure in a low dielectric constant media, since it cannot effectively screen the highly polarized charge of the metal alkoxide. The tetrameric geometry of alkali metal alkoxide is supported by previous experimental observations¹⁻³ and calculation results. In our own calculations we found repeatedly that the base tetramer gave the most consistent results that allows for comparing our calculations to experiments.



Scheme S1. DFT calculated equilibria between the tetramer- and monomer-form in dioxane.

1.2. Ligand exchange pathway

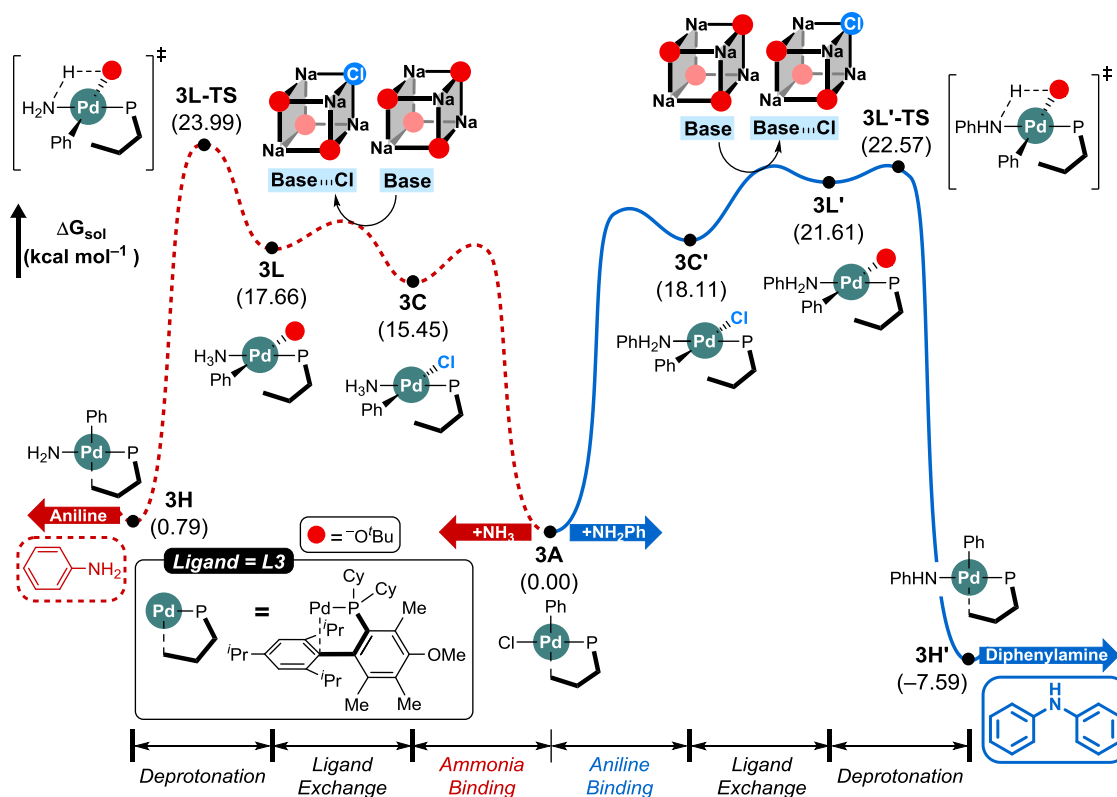


Figure S1. DFT calculated energy profile of the Pd-catalyzed *N*-arylation reaction with **L3** which follows ligand exchange pathway for deprotonation.

The ligand exchange pathway where the tetramer simply replaces the chloride with *tert*-butoxide during the deprotonation process is explored with **L3** ligand and the calculated energy profile of this pathway is summarized

in Figure S1. The calculations show that the ligand exchange step is endergonic. Both the ligand exchange product **3L** and **3L'** located 2.2 and 3.5 kcal mol⁻¹, respectively, are higher in energy compared to the reactant **3C** and **3C'** whereas binding of the tetramer to the same reactants results in a more stable intermediates, as described in the main text. Without the steric effect due to the tetramer binding, however, the step barrier for the deprotonation is reduced and therefore, the overall deprotonation barriers become reasonable for the given experimental conditions. The deprotonation transition state, **3L-TS** and **3L'-TS** are computed to be 24.0 and 22.6 kcal mol⁻¹ in energy, respectively. Although the ligand exchange pathway indicates reasonable barriers, this pathway is abandoned since it predicts di-phenylation. Note that the ligand exchange step may not be possible due to high barriers while we assume it to be possible in the aforementioned mechanism.

2. Distal Pathway with L3

The possibility of the mechanism adopting distal form intermediates for the deprotonation process is also explored since the barrier is accessible in the given condition (80 °C).

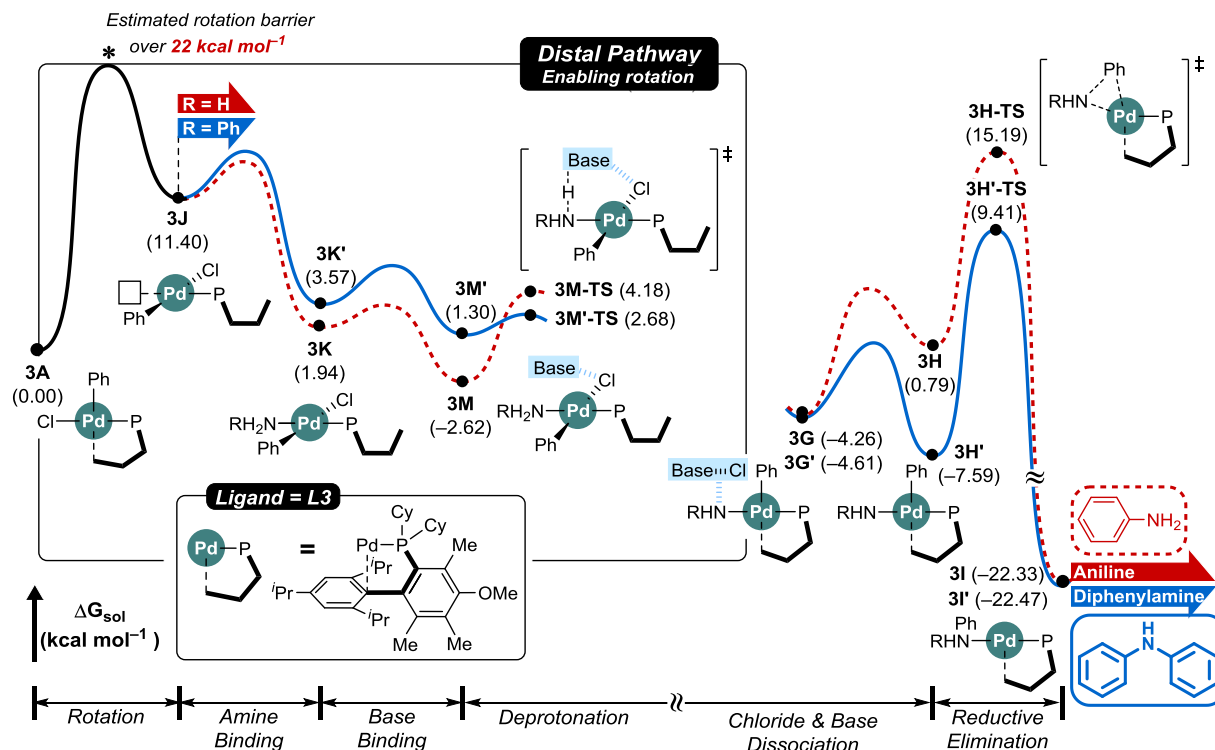


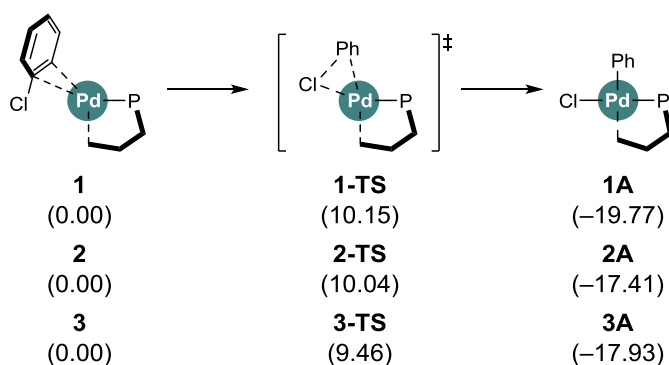
Figure S2. DFT calculated energy profile of the Pd-catalyzed *N*-arylation reaction with **L3** that involves σ -rotation of P–C₁ bond reaching for distal form during amine binding. * represents the estimated rotation barrier which is estimated over 22 kcal mol⁻¹.

Figure S2 displays the results for the distal pathway and the deprotonation process is highlighted in the square box. As expected, the access to the distal form effectively releases the steric congestion and the deprotonation process requires lower energies compared to the proximal pathway. Accordingly, the highest barrier step of this mechanism

becomes the reductive elimination step and leads to dominant generation of diphenylamine. In conclusion, this alternative path is judged to be mechanistically irrelevant because it is not only calculated to be energetically high, but it cannot properly account for the experimental observations.

3. Oxidative Addition

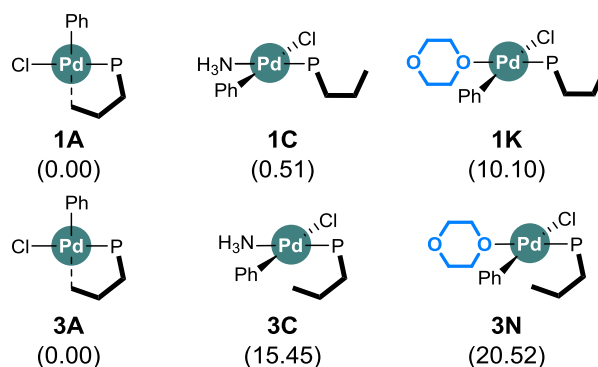
The oxidative addition step is examined and the result is illustrated in Scheme S2. The barrier for the oxidative addition is computed to be 10.1 kcal mol⁻¹ and 9.5 kcal mol⁻¹ with L1 and L3, respectively. The calculated energies are in a good agreement with the reported trend that electron-rich phosphine ligated Pd-catalyst readily performs the oxidative addition.



Scheme S2. Computed oxidative addition barrier with **L1** and **L3**.

4. Consideration of Dioxane Coordination

The effect of solvent coordination is examined and summarized in Scheme S3. The calculations show that the coordination of dioxane is less preferable than the amine binding in both ligands and therefore it would not impact to the reaction outcome.



Scheme S3. Relative free energies of dioxane binding Pd-complexes.

5. Reason of Higher Rotamer Energy for the Distal Form in L3 Compared to L2

The effect of alkyl groups on phosphine, ⁱPr in **L2** and Cy in **L3**, needs to be addressed as it has a profound influence on the rotation barrier. While it is obvious that the methylation at C₆ position impedes the rotation leading to a distal intermediate, the difference between ⁱPr and Cy is more difficult to understand. We postulated that the inherent rigidity of Cy is responsible for the higher rotamer energy in **L3** system and performed an energy decomposition analysis. We estimated the rotation barrier from the highest energy rotamer as we scan through different angles. As depicted in Figure S3, the steric clash between R¹ on phosphorus and methyl on C₆ position is expected to be a key factor that could illustrate the effect of the alkyl group on the phosphorus. Therefore, we partitioned each intermediate into “R¹-” and “catalyst-” fragments and decomposed the electronic energy of the highest energy rotamer as a sum of distortion energies of the fragments and the repulsive interaction between the fragments when the ground state intermediate is transformed to the highest energy rotamer. We found that the 4.3 kcal mol⁻¹ higher rotamer energy of the **L3** system is derived from the distortion energy of the catalyst and repulsive interactions of 2.0 and 3.1 kcal mol⁻¹, respectively, while the distortion of the R¹-fragment gives -0.8 kcal mol⁻¹. This result suggests that the flexible nature of ⁱPr in **L2** indeed reduces the rotation barrier by more easily undergoing a distortion which reduces both the repulsive interaction and the catalyst-fragment distortion.

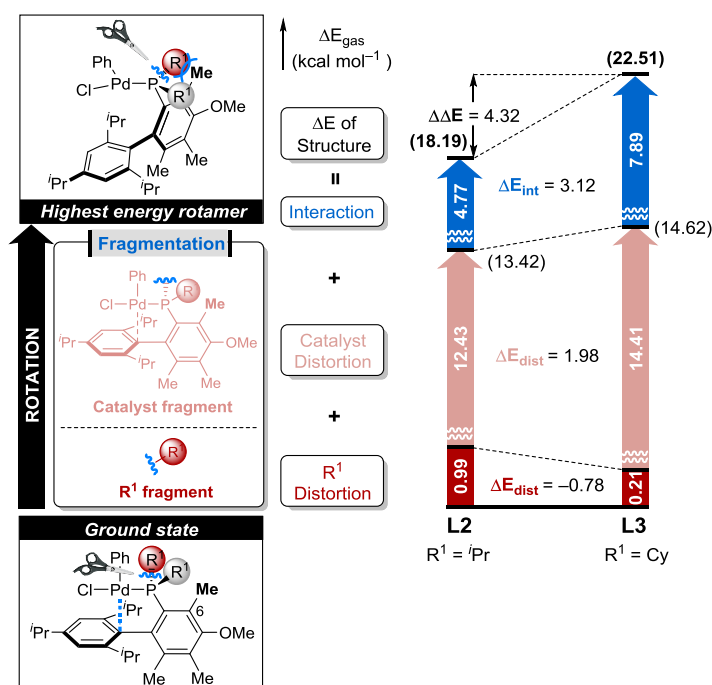


Figure S3. Schematic diagram for energy decomposition analysis that explain the highest rotamer energy difference between **L2** and **L3**. The highest rotamer electronic energy is represented as the sum of ΔE_{dist} and ΔE_{int} where ΔE_{dist} describes a fragment distortion energy and ΔE_{int} reveals the repulsive interaction between the two fragments.

6. Computed Data

6.1. Cartesian coordinates of the optimized geometries

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PhCl
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C -9.494266510 -1.132104516 -14.586632729
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HO^tBu

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1,4-dioxane							
=====							
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=====							
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=====							
L1_0							
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C	5.581313133	5.773096561	3.667891264	C	1.519561648	6.550878048	5.451066971
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H	3.435484409	-2.829691172	4.947940826	H	0.553203881	5.682558060	7.221239567
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L2_40

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C	5.823085785	5.408744812	4.462743759
C	5.164301872	6.432116985	5.148571491
C	3.801479578	6.275114536	5.400117874
C	3.092188597	5.140553474	4.999590397
C	3.141469717	2.699333429	4.411494732
C	2.124002457	2.325403690	3.479265451
C	1.344484806	1.169676065	3.780530214
C	1.696861744	0.393800437	4.903917313
C	2.719652653	0.738034606	5.789529800
C	3.413875341	1.938826919	5.567497730
H	6.877851963	5.532504082	4.230638027
H	3.263489962	7.070770264	5.903124809
P	2.262291431	3.088500977	1.775162816
C	0.608474016	2.872312069	0.912316799
C	0.626389146	3.130861759	-0.603670955
C	-0.432666421	3.756518841	1.619509220
H	0.332289070	1.829432130	1.035274982
H	1.216008306	2.380249023	-1.136223316
H	1.002742410	4.117501259	-0.864187539
H	-0.404008389	3.651745558	2.709137201
H	-0.262932867	4.807539940	1.384369254
C	3.469803333	1.897682190	0.948450267
C	4.052654743	2.450134993	-0.360339493
C	2.923141241	0.474081188	0.770401120
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H	4.512931824	3.425929308	-0.211087868
H	3.299555063	2.553452969	-1.143988371
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H	2.068466425	0.448011041	0.086346708
Pd	2.923801422	5.319954872	2.035503387
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H	1.114057779	7.184703827	5.522741318
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H	1.006796241	6.554351807	3.877936363
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H	6.922522545	2.812862158	1.439578652
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H	5.845251560	9.814859390	5.685461998
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C	2.274718285	5.958606720	0.255463779
C	3.047032595	5.797478676	-0.897399426
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C	5.247770786	4.972549438	0.276788414	H	0.394965678	3.476803303	-1.590167522
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C	5.958241463	5.073412895	-0.923880458	C	3.355412960	3.367024422	-1.279109240
C	4.041821003	6.090306282	-1.982530594	C	2.186960697	1.112816095	-1.205452919
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H	6.985332012	4.718071461	-0.967067420	H	1.770143986	0.327496767	-0.575354159
H	3.572052479	6.538261890	-2.854907751	H	1.378921270	1.528751493	-1.813155413
H	5.908769131	5.697515965	-2.989134550	Pd	3.027734280	4.993478775	1.432360768
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H	-1.002782226	4.219842911	-0.818361342
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L2_90
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C	5.356173992	1.332405448	1.622838259
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C	1.938732028	1.730311632	2.644062757
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C	1.246548772	1.149534345	4.870151043
C	2.428035736	0.444620699	5.099099636
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H 2.392403841 -0.970655322 6.971759796
H 0.749137461 -0.344688147 7.141654968
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H 4.334762096 -1.335321426 3.750956059
H -1.151586175 1.507790327 0.852291644
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L2_130
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H	6.993374348	1.079967380	5.097940445
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H	6.561801434	3.270675182	3.938883066
H	5.293118477	3.422877550	2.723759174
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C	1.553371906	-2.395815372	1.436846972
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H	0.096474491	-0.987771809	-0.458476871
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C	1.808969140	0.414895982	5.427772999
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H	0.001976565	4.949128628	0.915113509
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H	6.604147911	1.149162054	5.808714390
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C	1.597442269	-2.059577465	1.432844520
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C	2.806730032	6.815365791	0.022866698	C	3.603210926	2.769189358	0.417112947
C	5.557513237	7.269575596	0.188248932	C	5.042999268	3.171082258	0.766797245
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H	2.919943333	7.793900967	-1.891802549	H	3.214126110	4.397853374	-1.003266215
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L2_150
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C	5.420096397	-1.159381747	0.306290507	H	7.800857544	-3.426697254	-0.850119650
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L2_160
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L3_110
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L3_130
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H -2.273101091 -0.735022426 3.843798399
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L3_140
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C	-1.964864373	0.344744235	2.984754801	C	2.215908527	2.094645500	3.349510431
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H	-2.631223679	0.406446218	0.312467039	C	2.671480656	0.933224022	5.925980091
H	-2.517732143	2.074660540	0.886780262	C	2.295244694	0.117498130	4.845198631
H	-2.509055138	-0.576789081	2.747476339	H	-1.405472517	-1.695373654	1.491861820
H	-2.695094585	1.133192658	3.194422483	H	2.579200029	-2.500944614	0.198030174
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C	0.019275524	-3.528978586	-0.651081920	C	1.423330784	2.007753134	0.300437599
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C	0.100334711	-4.890030861	0.064589649	C	1.342841148	1.491838813	-2.170627356
C	0.820874274	-3.549710989	-1.966361165	C	-0.190752804	1.562770724	-2.166352987
H	0.733939826	-2.597906113	-2.499624014	C	-0.749511659	1.254716873	-0.769999504
H	1.885367513	-3.728295803	-1.776320338	C	-0.108991921	2.159765244	0.292111188
H	0.461839139	-4.347208023	-2.626626968	H	1.676724553	0.961624444	0.474260360
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C	-0.254988313	4.688474655	1.746370912	H	1.658878922	0.455317229	-1.981658816
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H	-2.208924294	3.699467182	4.341148853	C	6.507065773	2.725661278	1.739472032
H	-3.990841627	4.261093140	2.695047855	C	6.859907150	3.959388018	0.894660890
Cl	1.377563953	7.472708702	0.989257455	C	5.806064129	4.203272343	-0.195238292
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H	1.526412606	4.214508057	7.886071205	H	7.237215519	2.592201233	2.546771288
C	2.928479433	4.168980598	4.142643929	H	6.564009666	1.824334264	1.112161040
H	2.604596853	4.795265675	3.306528091	H	6.908495903	4.840641975	1.550195813
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H	4.022354126	4.101211071	4.115666866	H	5.833137035	3.377691507	-0.921702206
C	1.405356169	0.343847632	6.931000233	H	3.662383080	4.463108540	-0.397581220
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C	0.787210226	-1.260803819	4.628675938	C	3.898237467	-0.710768759	1.711735487
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H	-0.144157633	-1.189103365	5.202250957	C	4.464842319	-0.539693177	0.288638681
H	0.568210423	-1.788255215	3.704009533	C	4.679516315	-1.807983398	2.457709074

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C	1.502370834	-0.259584159	2.529330015	H	5.490221500	-0.156393185	0.329434872
C	0.109313928	-0.509809196	2.451376200	H	3.863133430	0.152591690	-0.307130486
C	-0.340993136	-1.497543693	1.566602468	C	-0.905689359	0.272443056	3.293984413
C	0.523591757	-2.226836681	0.748473704	H	-0.519645870	1.290217638	3.412321329
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C	2.396062851	-0.984124303	1.704945564	C	-2.295575857	0.386672795	2.639205694
C	2.027980089	0.685387433	3.580029488	H	-2.242770195	0.677582264	1.587733030

H	-2.847200871	-0.558383644	2.699906826	C	2.827637911	0.921335995	5.899068832
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H	-1.335731268	-1.381035686	4.656222343	H	-1.414779067	-1.660000563	1.617096782
H	-1.888698220	0.200647935	5.233981609	H	2.499150515	-2.495287418	0.141761690
H	-0.172842383	-0.209119275	5.304818153	P	2.201776028	3.005418539	1.692993164
C	-0.016601156	-3.243526936	-0.246245086	C	1.336368680	2.041387081	0.337080508
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C	0.561560810	-4.649415016	-0.007878128	C	1.144597292	1.528215408	-2.125600815
C	0.231558457	-2.780714035	-1.695799112	C	-0.384847879	1.651088953	-2.058816433
H	-0.207822502	-1.794470668	-1.877881646	C	-0.899137080	1.362129569	-0.640788972
H	1.305101871	-2.711432695	-1.906033039	C	-0.188965708	2.246953726	0.394162059
H	-0.204176664	-3.487445116	-2.410999060	H	1.559188366	0.987154365	0.502672255
H	1.645769238	-4.665163040	-0.166510001	H	2.922841311	2.291004658	-1.169245362
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H	0.368328452	-4.987980366	1.015005112	H	1.507806778	1.791209340	-3.126537323
C	-0.356549352	4.784776211	2.282717943	H	1.432563305	0.481507808	-1.948492885
C	-1.410119176	5.237154007	1.479871869	H	-0.675743520	2.671232700	-2.347098827
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C	-2.727046490	4.963299274	1.859390736	H	-0.726918101	0.307394892	-0.391095161
C	-1.943318129	3.834866047	3.839795113	H	-0.571514904	2.053803205	1.396592617
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H	-1.210238338	5.805685997	0.578917682	H	-0.851392746	0.972763121	-2.784088850
H	0.186222985	3.718374491	4.090407848	C	4.042588711	2.951054335	1.193014622
H	-3.542480469	5.313101292	1.231009841	C	5.072160244	2.766114950	2.328347206
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H	-4.026742458	4.056483746	3.326200962	C	6.874432087	3.816320181	0.875564933
Cl	1.199608803	7.547377110	1.394351959	C	5.833547592	4.063563347	-0.226234332
O	3.122320414	3.103482962	6.796628475	C	4.416738987	4.199151993	0.358397901
C	1.997820735	3.652032375	7.489085197	H	4.121480942	2.071513891	0.544774532
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H	1.359544992	2.856428862	7.895446777	H	5.060791492	3.639128685	2.990054131
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H	3.382454872	4.729239941	3.510393381	H	5.845291138	3.223615885	-0.936487377
C	2.942822933	0.348611534	7.290345192	H	3.697586060	4.372441292	-0.447812349
H	3.659023762	-0.478049219	7.231790066	H	4.383463383	5.089404106	1.006272793
H	3.346795321	1.105562568	7.962469101	H	7.868117809	3.669186354	0.435923517
H	2.026993990	-0.059763160	7.736569405	Pd	1.653574944	5.278356075	1.689527392
C	2.177040815	-1.372033834	5.104803562	C	3.904649496	-0.735959530	1.611034393
H	3.147397280	-1.786454082	5.401767731	H	4.098521709	0.199459448	2.140955210
H	1.488005519	-1.577508569	5.931541920	C	4.408319950	-0.570271969	0.163227931
H	1.827799797	-1.925165892	4.235350609	C	4.710118771	-1.842177153	2.318100929

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C	1.555011511	-0.269810081	2.543966770	H	5.436181068	-0.191452280	0.157803044
C	0.155227572	-0.505004227	2.523346186	H	3.784442425	0.122602277	-0.409279764
C	-0.345459133	-1.475808144	1.648012757	C	-0.820001364	0.276263595	3.413502216
C	0.473778009	-2.204900265	0.784613848	H	-0.423139304	1.291014552	3.524361610
C	1.845020533	-1.947330952	0.813875198	C	-0.936183214	-0.328928739	4.827742577
C	2.401186943	-0.993800581	1.671720028	C	-2.234930754	0.399623841	2.815806866
C	2.126667261	0.674635112	3.573275805	H	-2.222362995	0.692067564	1.763367891
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C	2.850780964	2.300353765	5.703372955	H	-1.208542943	-1.389032602	4.772038937

H	-1.715869784	0.190126106	5.396855831	H	3.339499235	-2.704682827	0.520581245
H	-0.003665087	-0.241321042	5.384888172	P	2.201776028	3.005418539	1.692993164
C	-0.121510677	-3.202552795	-0.197833955	C	1.237029552	2.277600288	0.248864114
H	-1.200886369	-3.250702620	-0.001463964	C	-0.261287451	2.184504986	0.571946502
C	0.451838762	-4.617314339	-0.004096664	C	-1.091647744	1.935428619	-0.698246658
C	0.066442952	-2.722225904	-1.650624752	C	-0.585137248	0.708569705	-1.473086596
H	-0.370115072	-1.729119539	-1.799498439	C	0.909056902	0.850543320	-1.799219966
H	1.130144000	-2.660914660	-1.908005953	C	1.735193253	1.038860321	-0.513316989
H	-0.408410102	-3.414562941	-2.354904413	H	1.353557348	3.126240015	-0.435906500
H	1.527584195	-4.641447067	-0.211676374	H	-0.600592256	3.099969387	1.067723751
H	-0.032387216	-5.327547550	-0.683440745	H	-0.411777139	1.364493370	1.269120932
H	0.301508963	-4.967405319	1.022114992	H	-2.148161411	1.810956597	-0.427462399
C	-0.231594399	4.946662903	2.248903275	H	-1.032065511	2.824355364	-1.339481115
C	-1.225202799	5.530704498	1.454058290	H	-0.730108917	-0.196062475	-0.864212513
C	-0.583196640	4.189750671	3.369651079	H	1.272174835	-0.033217344	-2.338669538
C	-2.570682526	5.330071449	1.778804779	H	1.057006478	1.713884473	-2.464210749
C	-1.934681296	4.007458210	3.688953638	H	2.793529749	1.142338872	-0.772222519
C	-2.932273149	4.567268848	2.892067671	H	1.638510108	0.143825889	0.095730506
H	-0.956884801	6.145503998	0.602730095	H	-1.167891264	0.571526885	-2.392269850
H	0.165649623	3.715829611	3.990906477	C	4.001518250	2.767978430	1.186965466
H	-3.338480234	5.783114910	1.156362414	C	5.006998539	3.175942659	2.283876419
H	-2.196672440	3.415029287	4.562660217	C	6.451084614	2.876341581	1.845712185
H	-3.979942083	4.419001102	3.138549566	C	6.792090416	3.557350874	0.512304008
Cl	1.550389886	7.618109703	1.480443478	C	5.773085117	3.190003633	-0.575989306
O	3.193041801	3.098773956	6.783134460	C	4.339478970	3.510047674	-0.120910123
C	2.065978765	3.599125147	7.506560802	H	4.102910519	1.694708705	1.016321778
H	1.422747135	4.219837666	6.869482040	H	4.792635441	2.659209013	3.224201918
H	1.469046116	2.776699305	7.922377110	H	4.908740520	4.253471375	2.476453543
H	2.462549686	4.208834648	8.321410179	H	7.146912575	3.199245691	2.629562140
C	2.861603975	4.408197403	4.427577496	H	6.576597691	1.789186239	1.744563222
H	1.935162902	4.986412525	4.498776436	H	6.783931732	4.647470474	0.654824913
H	3.491081238	4.684621334	5.273759842	H	5.995001316	3.728529930	-1.505324125
H	3.365353107	4.744642735	3.522443771	H	5.850818634	2.118031263	-0.806677163
C	3.168950319	0.333464324	7.245969296	H	3.628959417	3.268711567	-0.917280912
H	3.926657200	-0.452144027	7.154053211	H	4.251780510	4.588196754	0.063312113
H	3.550686359	1.101551771	7.918279648	H	7.807060719	3.289025545	0.194742218
H	2.289618254	-0.130273610	7.711063385	Pd	1.829071045	5.313591957	1.707403302
C	2.410135269	-1.392904043	5.056651115	C	4.396860123	-0.758512795	2.003971815
H	3.404277325	-1.776424170	5.313576698	H	4.482542992	0.203852803	2.517463446
H	1.757274628	-1.635193586	5.902555943	C	5.094762802	-0.645297110	0.631606579
H	2.049299717	-1.943197966	4.190495491	C	5.153189182	-1.801991701	2.851065397

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C	1.888488412	-0.378706485	2.547233582	H	6.098261833	-0.223253101	0.748749912
C	0.535695493	-0.795357823	2.414269447	H	4.539460182	-0.016348468	-0.067518629
C	0.242563069	-1.862821460	1.558765531	C	-0.610435843	-0.155623332	3.211180449
C	1.229680657	-2.557184219	0.858546615	H	-0.369758099	0.903112888	3.353920221
C	2.555363417	-2.165439129	1.043417096	C	-0.751203299	-0.781061232	4.615550995
C	2.909321070	-1.093966603	1.871016502	C	-1.982025385	-0.247908056	2.510249376
C	2.226083755	0.671464920	3.570684671	H	-1.943732738	0.029129416	1.454009891
C	2.215908527	2.094645500	3.349510431	H	-2.393184662	-1.261588693	2.573406696
C	2.372265577	2.977898121	4.448372841	H	-2.693783760	0.418277025	3.008383751
C	2.597549915	2.443323135	5.728534222	H	-0.829822123	-1.871741056	4.546141624
C	2.711248398	1.071148157	5.951939106	H	-1.657733202	-0.406886995	5.104298592
C	2.508576155	0.187334612	4.873707294	H	0.095391780	-0.534893394	5.254114628
H	-0.789352119	-2.174910545	1.433004022	C	0.860419452	-3.683741808	-0.094142653

H	-0.223102748	-3.841416836	-0.009053627	C	-0.306849450	2.257280111	0.631210983
C	1.553817153	-5.006424427	0.276682913	C	-1.174941659	2.043389082	-0.619818807
C	1.160770655	-3.287461042	-1.552543759	C	-0.716587186	0.815731525	-1.422728896
H	0.631480038	-2.369349480	-1.827755570	C	0.772834480	0.924042225	-1.783408761
H	2.233015299	-3.110811710	-1.695992827	C	1.633803606	1.075534940	-0.515424371
H	0.855389237	-4.081238270	-2.243571997	H	1.305489779	3.170337915	-0.411964357
H	2.642356396	-4.926084995	0.180333436	H	-0.611177742	3.175286531	1.145270586
H	1.222524762	-5.814332485	-0.384936452	H	-0.460092664	1.433601499	1.325588584
H	1.329491138	-5.294655323	1.308652163	H	-2.226530790	1.938694715	-0.323483139
C	1.015100241	5.491891861	-0.092931733	H	-1.110364079	2.938899517	-1.251920938
C	1.787937403	5.639029503	-1.246649265	H	-0.870095789	-0.093113951	-0.822324634
C	-0.380618066	5.523382664	-0.168161750	H	1.099693060	0.038009189	-2.341696262
C	1.155410051	5.759865761	-2.488786221	H	0.926901937	1.791138172	-2.441941023
C	-1.001764059	5.650511265	-1.414736748	H	2.688885450	1.153370619	-0.795205295
C	-0.236727506	5.755862713	-2.577941418	H	1.525740981	0.177136928	0.086998641
H	2.868795395	5.672416210	-1.191552877	H	-1.325190425	0.705416143	-2.328557730
H	-0.985748291	5.462782860	0.730260193	C	3.989972353	2.715982437	1.170691967
H	1.760077477	5.868055820	-3.385978460	C	5.003819942	3.119991541	2.262537479
H	-2.087432384	5.671847820	-1.470364571	C	6.443802834	2.804443836	1.823865175
H	-0.723016679	5.851940632	-3.544842005	C	6.791474342	3.467174768	0.483121246
Cl	1.780658841	7.652190208	1.966425657	C	5.768815517	3.095894337	-0.600139499
O	2.758424997	3.305392981	6.800597668	C	4.340428829	3.437094688	-0.145170853
C	1.540033579	3.605583668	7.486475945	H	4.066136360	1.640070558	1.010718465
H	0.817953050	4.098165035	6.821941853	H	4.787713528	2.611500740	3.207021236
H	1.082379341	2.696161270	7.897089005	H	4.915860176	4.199501514	2.448636293
H	1.799701095	4.282580376	8.303133011	H	7.143041134	3.129389048	2.603757143
C	2.330574751	4.491829872	4.343239307	H	6.560883999	1.715528846	1.734872937
H	1.323031425	4.856365681	4.107627869	H	6.792811394	4.558782578	0.612923503
H	2.633317232	4.952741146	5.283255577	H	5.992757797	3.624061346	-1.534914851
H	3.042858839	4.882800579	3.598274469	H	5.838253975	2.021945477	-0.820944905
C	3.023240805	0.557026207	7.337012291	H	3.622029066	3.202226877	-0.936944187
H	3.862610817	-0.146171927	7.318680763	H	4.271865845	4.517544270	0.028422555
H	3.282969475	1.378766060	8.004417419	H	7.804141045	3.185869455	0.169482276
H	2.169353247	0.017884117	7.766696453	Pd	2.008238554	5.335377216	1.717852354
C	2.574964285	-1.294938922	5.192031384	C	4.451153755	-0.769718587	1.878240943
H	3.575915813	-1.570969105	5.542080402	H	4.577958584	0.177266896	2.411831141
H	1.886292338	-1.556102514	6.002797127	C	5.095837116	-0.639313638	0.481427908
H	2.331635475	-1.920927644	4.336960793	C	5.221272945	-1.851113558	2.664286852

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C	1.962371707	-0.352970988	2.504658222	H	5.102486610	-2.831381321	2.188971519
C	0.602059543	-0.761774123	2.417473316	H	6.291298389	-1.614652991	2.680810690
C	0.270885259	-1.820167542	1.564654589	H	5.167605400	-1.613881826	-0.012285196
C	1.226377368	-2.512858629	0.820710063	H	6.113224983	-0.244211689	0.565435469
C	2.559786320	-2.131963015	0.963056445	H	4.526813507	0.019015649	-0.178194314
C	2.952934265	-1.072481632	1.789027572	C	-0.512248695	-0.129037246	3.264575481
C	2.325176001	0.694212735	3.525758028	H	-0.276263297	0.932020545	3.393425465
C	2.215908527	2.094645500	3.349510431	C	-0.582988739	-0.752272189	4.675245285
C	2.377336502	2.969439030	4.456571579	C	-1.913881421	-0.232908204	2.628792524
C	2.685981989	2.422668219	5.711587906	H	-1.926992416	0.045493919	1.572036386
C	2.878965378	1.051734209	5.897688389	H	-2.313732862	-1.249704838	2.710175276
C	2.670199871	0.185975775	4.808635235	H	-2.606742859	0.427494317	3.160275459
H	-0.766361177	-2.126301527	1.475420833	H	-0.664716601	-1.843006492	4.610712528
H	3.320683479	-2.672675610	0.408515692	H	-1.464181423	-0.377818435	5.208189964
P	2.201776028	3.005418539	1.692993164	H	0.294297785	-0.505228519	5.270474911
C	1.184610605	2.318823099	0.268389940	C	0.814699352	-3.626032352	-0.130388245
				H	-0.264340848	-3.784136772	-0.000866216
				C	1.521356583	-4.954668999	0.190519139
				C	1.052797914	-3.208843231	-1.594565749

H	0.510891438	-2.288129568	-1.834356070	H	-2.102344751	-3.121136427	-3.466869116
H	2.117818832	-3.027934074	-1.780297399	C	-1.077314973	-0.506294072	-3.317109346
H	0.719636321	-3.993373871	-2.283352613	H	-2.080377817	-0.565333962	-3.753362894
H	2.604680538	-4.874984264	0.046720907	H	-0.359571278	-0.452143759	-4.143475533
H	1.159081578	-5.752651215	-0.466863215	H	-1.028583527	0.421715915	-2.742371559
H	1.342772365	-5.257052422	1.227330685	C	-5.262091160	-1.448320389	-0.130997866
C	1.182570219	5.551710129	-0.073908970	H	-5.513536930	-1.358317494	-1.196084499
C	1.940363526	5.725397587	-1.234174013	C	-5.924089909	-2.736570358	0.396590173
C	-0.214268848	5.594424248	-0.131735131	H	-5.552516937	-3.621216774	-0.131618917
C	1.292626739	5.886898041	-2.463742733	H	-7.011524677	-2.691466093	0.268532127
C	-0.850683212	5.762281895	-1.365912557	H	-5.720116615	-2.874042511	1.464509130
C	-0.100354448	5.898158550	-2.535259485	C	-5.818152905	-0.207729071	0.590865672
H	3.021930933	5.751853943	-1.191994071	H	-5.623687744	-0.260307521	1.668065190
H	-0.810195565	5.505157471	0.770302057	H	-6.903440952	-0.141743109	0.450255156
H	1.886700511	6.017491341	-3.365071774	H	-5.350066662	0.705006182	0.216808960
H	-1.936901212	5.791079521	-1.406820536	C	-1.137070537	-2.062019587	2.694996595
H	-0.597998321	6.027789116	-3.492367029	H	-0.055869706	-2.161062002	2.577107430
Cl	2.247034311	7.667582035	1.929703832	C	-1.640802503	-3.391514778	3.288846731
O	2.856178284	3.269214392	6.794742107	H	-2.721091986	-3.362713337	3.467869282
C	1.668441415	3.463155746	7.567356110	H	-1.147405744	-3.597205877	4.245818615
H	0.870569408	3.917101145	6.964638233	H	-1.436509967	-4.221480846	2.605361223
H	1.303967834	2.514048100	7.981330395	C	-1.413918138	-0.882059991	3.643923283
H	1.933719158	4.137945175	8.384100914	H	-1.063926220	0.060407832	3.210802794
C	2.273813486	4.480583668	4.375090599	H	-0.915750682	-1.035478115	4.608321667
H	1.276661873	4.811815739	4.064181328	H	-2.486059904	-0.770107508	3.835188866
H	2.491156578	4.936180115	5.340550423	C	-0.045869570	2.705678940	0.001750604
H	3.030902147	4.909391403	3.694334507	C	-0.004994185	3.621353626	1.056268573
C	3.276962280	0.525200725	7.255945206	H	-0.157741591	3.293798923	2.077375889
H	4.126320362	-0.161610559	7.181480885	C	0.202444121	4.980097294	0.798874199
H	3.557903051	1.342994571	7.919738293	H	0.239239722	5.680390835	1.630301833
H	2.458462715	-0.035747007	7.725221157	C	0.342013776	5.440361500	-0.510890543
C	2.779127121	-1.299715161	5.096379280	C	0.250467986	4.533229351	-1.566860437
H	3.794912577	-1.561575174	5.410680294	H	0.329139411	4.879245758	-2.594925404
H	2.121744871	-1.583147526	5.925192356	C	0.046805903	3.173748016	-1.313944817
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Pd	-0.427212536	0.747611523	0.287520796	H	0.500337422	6.497410297	-0.707345366
P	1.830405593	-0.036048681	0.507777929	Cl	-2.665501595	1.533739448	0.229266509
C	1.689000607	-1.900144935	0.383405000	H	1.384716630	-5.786785126	0.022821222
C	2.815584421	-2.757064581	0.515483856	H	3.572318792	-4.774058819	0.433172464
C	2.702902555	-4.133236408	0.356568217	O	3.999541044	-2.165820122	0.852288246
C	1.455880165	-4.711371899	0.130473584	O	-0.941238225	-4.407943249	-0.067090221
C	0.324513912	-3.908244610	0.078596108	C	5.190642834	-2.935424566	0.834388137
C	0.420414478	-2.492475271	0.199953139	H	5.174080849	-3.727543354	1.593865633
C	-0.926439226	-1.804862142	0.140684485	H	5.365998268	-3.382592440	-0.152693182
C	-1.571671605	-1.677778959	-1.126238346	H	6.000149250	-2.239274263	1.061546683
C	-3.748502016	-1.539189458	-0.030570922	C	-1.104466915	-5.798948765	-0.288453609
C	-3.113958836	-1.669638872	1.204340577	H	-0.583648801	-6.128383160	-1.197987914
H	-3.714212894	-1.662058711	2.109094143	H	-0.751274884	-6.393017292	0.565377295
C	-1.733804464	-1.818024397	1.316916585	H	-2.177251339	-5.953886032	-0.413258076
C	-0.782027245	-1.726562142	-2.425661564	C	4.315348148	-0.175475791	-1.137524486
H	0.278126955	-1.710342288	-2.164813280	H	4.816334248	0.285964608	-1.998492360
C	-1.045176029	-3.037515163	-3.191573620	H	4.975973129	-0.078733750	-0.277746826
H	-0.788305223	-3.907808065	-2.581820726	H	4.188127041	-1.236269474	-1.361159205
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H 0.971974432 1.606506228 2.834344864
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H 1.220605373 -0.844444811 3.323062181
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H 0.245218143 -2.055989742 2.833004951
C -1.231155515 -3.220525503 3.833251715
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L4_40

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C 0.240186140 -0.072354883 -2.332567453
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L4_130
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H	-0.183826581	-3.615459681	-1.772823572	H	2.626171112	-4.009336948	5.349651337
O	-0.174756944	-0.965276241	-1.719378471	C	1.783926725	-1.349068761	5.414677143
O	2.812144279	-4.166020870	1.611334801	H	2.287218094	-1.707411766	6.319374561
C	-1.070675492	-1.521826744	-2.695093155	H	0.707147479	-1.390756607	5.608211040
H	-0.499873936	-2.081570387	-3.444414377	H	2.062917233	-0.302908957	5.271350861
H	-1.819983602	-2.155252934	-2.213900566	C	7.009059429	-1.337601304	5.172060013
H	-1.577155113	-0.667853057	-3.139910460	H	6.534194469	-1.277163744	6.160420418
C	2.701485395	-5.580278873	1.577938437	C	8.059080124	-2.461910486	5.228134155
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H	3.035332203	-5.991456032	0.615655184	H	8.808655739	-2.254359245	5.999915123
H	3.355042934	-5.946832180	2.370941162	H	8.585428238	-2.559858084	4.271959305
C	2.463736057	-0.190530345	-2.885439157	C	7.670674801	0.024351142	4.888360023
H	2.992079020	-1.013294220	-2.395975351	H	8.178262711	0.019186050	3.917042255
H	1.480857253	-0.539539874	-3.194076777	H	8.417160988	0.262376875	5.654541492
H	3.022062778	0.066945881	-3.793319941	H	6.926896095	0.827588022	4.870937347
C	3.842029333	1.556760192	-1.829711199	C	5.596138000	-2.172593117	0.381923378
H	4.278622627	1.694173694	-2.826851845	H	4.714794159	-1.922887564	-0.219126701
H	3.918113947	2.514768362	-1.316745400	C	5.984149456	-3.627622604	0.048823766
H	4.458414078	0.825189888	-1.302439332	H	6.848984718	-3.933332682	0.648912251
C	1.563160896	2.143351316	-2.738559484	H	6.255762100	-3.718755245	-1.009277701
H	0.548825145	1.789229512	-2.944972992	H	5.169750214	-4.319873333	0.261936277
H	1.480834365	3.073224306	-2.170564175	C	6.740374088	-1.233383894	-0.043392956
H	2.047660351	2.376236916	-3.695366859	H	6.576910973	-0.206052989	0.293152541
C	2.018738985	3.318902016	0.598103881	H	6.838266373	-1.227587700	-1.134288907
H	2.605459452	3.595336914	-0.280499458	H	7.702120304	-1.564919591	0.362519294
H	0.967374563	3.515708208	0.395909041	C	-0.873693883	2.233587503	0.993229449
H	2.327570438	3.986207008	1.411758780	C	-1.282298565	2.375853300	2.323187113
C	3.768829346	1.721659422	1.408743739	H	-1.393856049	1.502790928	2.959128618
H	4.432538033	2.005986929	0.595204115	C	-1.569696426	3.646185398	2.833803177
H	3.981451750	2.399342775	2.245448828	H	-1.881232381	3.746925592	3.870937824
H	4.019812107	0.719204724	1.737727642	C	-1.471974134	4.776244164	2.019874334
C	1.476912737	1.617766738	2.352262259	C	-1.100092173	4.626837730	0.682623148
H	1.753394365	2.380325794	3.091314077	H	-1.038445592	5.496966839	0.032970604
H	0.400808960	1.679273605	2.201873064	C	-0.807540357	3.360136032	0.165360168
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L4_140
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Pd	-0.508978546	0.441141695	0.229407147	H	4.351541042	-1.649807215	5.617788315
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C	1.952894211	-1.666367173	0.525554538	Cl	-2.852706671	0.175493032	-0.066579692
C	0.904696167	-2.320403814	-0.198662296	H	1.550047636	-5.586639881	0.391171545
C	0.773456812	-3.698199749	-0.252286136	H	-0.024079848	-4.154451847	-0.822591126
C	1.659160614	-4.511024952	0.446085602	O	-0.004082641	-1.516225934	-0.859484255
C	2.642197132	-3.920171261	1.223306775	O	3.539379597	-4.646501064	1.962678075
C	2.786410570	-2.505197763	1.311222315	C	-1.003096938	-2.107433081	-1.707478285
C	3.861169338	-2.099847794	2.279625893	H	-0.516862869	-2.693059206	-2.495453358
C	3.546077013	-2.007746935	3.656844616	H	-1.689917088	-2.724800110	-1.123037457
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C 1.978584290 1.136540771 2.899254322
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L4_150
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Pd -0.540170550 0.456699073 0.365998924
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C 0.792545021 -3.761043072 -0.278614253
C 1.814222813 -4.557385445 0.218850091
C 2.832383633 -3.964094639 0.949676096
C 2.908489227 -2.554187775 1.133700609
C 3.987994432 -2.173851490 2.119290829
C 3.633046865 -2.087335110 3.492090940
C 5.978788376 -1.696380377 4.074747086
C 6.315816402 -1.876079082 2.733106375
H 7.360289097 -1.819760919 2.439748764
C 5.354792118 -2.130911350 1.750474691
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L4_160
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L4_170
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 H 5.315235138 -1.808591485 -3.641829967
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 H -0.827039182 -7.835270882 -9.106229782
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 H -1.105059028 -7.157831669 -5.025612831
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 Pd 1.584404230 -3.610908985 -7.474261284
 Cl -0.406051397 -1.950817585 -7.309890270
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 C 3.092739105 -5.837376118 -8.783344269
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 C 4.249602795 -6.473202705 -9.246306419
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H 5.098528385 -0.434163481 -2.373090744
H 2.257967472 -1.399120808 -8.519067764
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O 2.049326897 0.895435929 -12.613918304
C 2.403374195 1.681084633 -8.213567734
O 1.924937129 0.918657303 -9.290594101
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H 1.405653119 0.450474203 -6.704672337
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H 1.231531978 -4.541191101 -10.499708176
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Na -0.108697236 -0.196072251 -9.295036316
Na 1.110681653 2.149137259 -10.999530792
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C 4.714010239 -1.620522618 -8.981367111
C 3.952792406 -3.226316214 -10.618583679
C 6.002961636 -1.693404317 -9.510279655
C 5.247520447 -3.308574200 -11.127870560
C 6.282023430 -2.537954569 -10.587682724
H 4.516121387 -0.989882529 -8.120444298
H 3.165215969 -3.844755411 -11.030913353
H 6.796664238 -1.100216150 -9.061473846
H 5.451382160 -3.991428375 -11.949186325
H 7.289542675 -2.608675718 -10.988253593

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3N

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C 4.952768803 -2.323413134 -10.064398766
C 4.170999050 -1.465880036 -9.285219193
C 3.810393333 -1.758491755 -7.964312077
C 4.128156662 -3.303179502 -5.932307243
C 3.155958891 -4.147412777 -5.300702095
C 3.412889481 -4.598218918 -3.976498127
C 4.527907848 -4.087141991 -3.289602518
C 5.403471470 -3.155960321 -3.841264963
C 5.239302635 -2.815911770 -5.196281433
H 5.963356018 -4.204102993 -10.093490601
H 3.846484423 -0.525243461 -9.716155052
P 1.596191525 -4.702601433 -6.221796036
C 0.156501934 -4.879312992 -4.993663788
C -1.219025254 -4.888147831 -5.708664417
C -2.326991796 -5.247869492 -4.701474667
C -2.352410555 -4.263374329 -3.522491693
C -0.974713743 -4.172733307 -2.848279476
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H -2.629816055 -3.268690109 -3.896644831
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H -0.738072455 -5.134171486 -2.366137028
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H -0.079700619 -2.849529982 -4.317333221
H -3.118610144 -4.557809353 -2.794314861
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C 0.729162157 -7.242379189 -7.239000797
C 1.117897511 -8.532670975 -7.980367184
C 2.005602598 -9.431719780 -7.108366489
C 3.233501911 -8.660754204 -6.602184772
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H 1.648563027 -8.260770798 -8.903459549
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H 3.725249529 -6.840871811 -5.520244122
H 2.242395163 -7.627667427 -4.993474960
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Pd 0.779479325 -3.311028004 -7.883533478
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H -1.116055608 -5.026009560 -9.385720253
H 3.214926720 -5.860025883 -11.662664413
H -1.051941514 -6.387095451 -11.440207481
H 1.109187245 -6.821695805 -12.599018097
C 3.042566776 -0.706951022 -7.157605648
H 2.375765800 -1.235328794 -6.472430229
C 2.163115501 0.201363459 -8.035491943
C 3.963588476 0.190096155 -6.303097725
H 4.379963875 -0.346605480 -5.451771259
H 4.788510323 0.599138260 -6.898553371
H 3.384518862 1.031266928 -5.906702042
H 2.766410589 0.919149637 -8.606483459
H 1.483304143 0.767267764 -7.394055843
H 1.543114305 -0.373919874 -8.722536087
C 5.314058781 -1.981724739 -11.502449036
H 5.979804039 -2.775249720 -11.868205070
C 6.072669983 -0.647828281 -11.612494469
C 4.060937405 -1.977529526 -12.399384499
H 3.510653019 -2.920827866 -12.316500664
H 3.384278774 -1.164632201 -12.111718178
H 4.332093716 -1.826163411 -13.450407982
H 5.449107170 0.191207230 -11.284342766
H 6.368240356 -0.454724461 -12.649908066
H 6.975604534 -0.654652119 -10.993825912
C 5.454321384 -5.262034416 -7.672929287
H 4.803466797 -5.540021420 -6.841262817
C 6.894527912 -5.198359966 -7.127028465
C 5.356600285 -6.382975578 -8.725853920
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H 6.071029663 -6.240067482 -9.543184280
H 5.595986843 -7.345879078 -8.263364792
H 7.581129074 -4.820262909 -7.893039227
H 7.236038685 -6.196545601 -6.829349041
H 6.962847710 -4.546731949 -6.255156517
C 6.339326859 -1.971442699 -5.818408966
H 6.442288876 -1.012021303 -5.302227497
H 7.308001995 -2.476806879 -5.729003429
H 6.171003342 -1.760375023 -6.870751858
C 6.524672985 -2.576187372 -3.013423204
H 6.385753155 -2.807569027 -1.956824183
H 7.503453255 -2.960225821 -3.328725815
H 6.565635204 -1.487442255 -3.120359898
C 2.649691105 -5.641688824 -3.182834625
H 1.784996867 -6.037871361 -3.693533421
H 3.306988716 -6.488509655 -2.963232517
H 2.330585718 -5.238436222 -2.218544722
O 4.732576370 -4.527782440 -1.989279747
C 5.721082687 -5.551771641 -1.866546512
H 5.470503807 -6.429714680 -2.477154493
H 6.715966225 -5.196309090 -2.163707733
H 5.742799759 -5.840456486 -0.813089907
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 C 0.353683740 -0.695276260 -11.583284378
 H 1.702973723 -2.156047583 -10.697736740
 H 0.245066583 -2.861277103 -11.441668510
 O -1.046446919 -0.460937411 -11.683222771
 H -2.712387562 -0.269910425 -10.528628349
 H -1.227284193 0.395402700 -9.790895462
 H 0.749647439 -0.728034079 -12.603541374
 H 0.843576431 0.129353121 -11.039044380

6.2. Vibrational frequencies (in cm^{-1}) of the optimized geometries

PhCl

189.80 300.67 416.25 418.68 479.57 626.00
 698.33 710.51 756.14 844.86 917.67 972.78
 998.77 1012.13 1049.15 1107.52 1108.38 1195.35
 1210.89 1330.33 1354.44 1486.03 1520.33 1640.62
 1640.82 3184.36 3193.91 3206.43 3216.06 3218.88

NH₃

1095.37 1692.51 1692.70 3460.41 3588.78 3589.29

NH₂Ph

223.84 287.30 392.79 418.01 508.38 537.29
 634.43 635.12 704.34 764.23 828.03 835.37
 881.56 955.33 980.02 1009.23 1057.05 1079.95
 1147.56 1193.40 1214.51 1313.64 1368.47 1371.72
 1513.80 1546.38 1644.59 1661.62 1679.92 3165.74
 3167.36 3182.53 3188.44 3206.15 3559.45 3662.49

NHPh₂

33.48 56.69 108.11 219.63 234.87 312.18
 334.78 350.65 417.53 425.39 503.53 513.98
 581.31 627.08 631.63 651.79 704.11 712.66
 760.71 762.98 823.25 833.76 849.26 893.82
 898.23 911.43 962.91 969.16 985.37 992.59
 1009.54 1010.43 1058.19 1058.70 1114.15 1125.90
 1194.66 1195.25 1214.82 1220.94 1260.28 1280.85
 1355.26 1356.09 1371.59 1373.42 1460.44 1506.75
 1538.31 1543.71 1566.55 1639.47 1645.83 1657.78
 1670.77 3167.46 3168.58 3179.62 3180.16 3188.65
 3189.38 3205.74 3206.74 3214.89 3220.66 3636.99

NaO'Bu

47.86 48.67 233.81 286.67 287.81 329.97
 346.94 347.21 478.87 479.24 518.60 760.27
 881.85 883.13 947.24 1038.92 1039.32 1059.35
 1236.42 1237.93 1266.65 1387.57 1387.94 1413.05
 1482.20 1492.25 1492.67 1505.21 1505.42 1526.54
 3013.73 3014.25 3024.76 3085.19 3085.87 3094.12
 3097.62 3101.17 3103.00

(NaO'Bu)₄

21.02 23.04 26.35 27.34 31.48 36.11
 39.65 40.42 53.61 63.50 66.78 67.79
 108.15 108.32 108.54 141.81 142.34 147.87
 207.72 207.94 208.16 223.52 223.75 224.06
 224.39 224.85 250.60 250.77 250.99 258.90
 270.51 271.20 276.94 293.93 320.11 320.40
 320.75 320.96 324.67 325.24 335.72 335.89
 365.34 366.13 366.47 369.20 369.69 371.76
 373.48 374.30 454.44 454.62 455.10 457.64
 494.84 494.97 495.48 498.18 498.26 501.66
 502.24 502.39 742.97 747.80 749.66 751.46
 885.04 886.23 887.63 888.05 888.38 888.90
 888.96 889.09 951.61 951.91 953.03 957.37
 1005.96 1006.29 1007.18 1016.68 1042.64 1042.76
 1042.95 1043.05 1043.11 1043.47 1043.95 1044.38
 1236.60 1237.40 1237.93 1238.36 1238.98 1241.82
 1241.94 1242.57 1243.30 1243.64 1243.91 1260.61
 1389.15 1389.28 1389.45 1389.77 1389.84 1390.06
 1390.47 1391.05 1414.43 1414.51 1415.05 1416.27
 1487.24 1487.59 1487.88 1488.92 1495.33 1495.44
 1495.80 1496.07 1496.60 1496.89 1497.87 1497.91
 1509.72 1509.79 1509.96 1510.57 1510.66 1510.79
 1511.23 1511.41 1526.26 1526.59 1527.09 1528.53
 2982.66 2984.58 2993.73 2998.50 2999.22 3002.47
 3002.87 3003.11 3003.37 3008.97 3012.89 3013.11
 3044.24 3050.57 3052.08 3062.86 3068.03 3068.41
 3069.25 3070.13 3074.01 3074.49 3074.68 3075.20
 3079.97 3080.52 3083.17 3083.48 3085.62 3086.02
 3086.16 3086.46 3092.28 3095.36 3097.33 3098.16

Na₄(O'Bu)₃Cl

13.54 15.87 18.84 30.39 31.99 38.97
 56.26 60.52 76.25 99.49 101.34 114.97
 135.14 136.24 157.33 175.34 178.21 213.92
 216.66 217.70 220.46 225.93 228.13 238.78
 246.64 248.86 251.62 251.99 253.51 255.27
 300.53 303.24 303.87 305.58 307.14 310.35
 363.73 364.57 365.35 368.72 369.70 370.29
 453.77 454.34 456.66 496.73 496.75 498.46
 502.56 503.74 504.32 751.70 752.86 753.77
 889.49 890.23 890.59 893.10 893.20 893.69
 949.17 949.61 950.04 997.65 998.21 1006.41
 1041.61 1041.88 1042.30 1042.52 1042.94 1043.13
 1232.66 1233.09 1241.12 1242.25 1243.02 1243.46
 1244.10 1244.58 1249.80 1393.60 1394.23 1395.41
 1395.80 1396.59 1397.80 1419.82 1420.82 1422.42
 1484.82 1486.07 1486.49 1487.00 1487.28 1488.25
 1489.89 1490.07 1491.12 1507.84 1508.49 1508.67
 1509.04 1510.10 1510.62 1516.69 1519.54 1521.08
 3003.47 3006.03 3009.52 3011.62 3012.09 3012.24
 3020.06 3021.28 3021.61 3070.59 3073.32 3075.56
 3078.36 3079.49 3080.28 3082.27 3083.29 3083.81
 3093.77 3095.03 3096.04 3098.64 3099.89 3100.77
 3106.41 3107.63 3109.70

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HO'Bu							1387.09	1391.63	1395.10	1396.08	1396.94	1401.27
=====							1403.60	1404.87	1413.35	1414.83	1416.36	1433.50
217.73	277.46	284.01	312.36	347.34	348.97	1435.24	1436.92	1466.19	1467.04	1478.25	1492.56	
423.22	470.42	471.65	756.12	916.90	931.22	1494.72	1497.93	1498.28	1499.10	1500.87	1501.35	
944.29	968.96	1036.82	1054.53	1170.25	1251.70	1503.44	1503.70	1504.76	1505.89	1506.42	1506.50	
1267.33	1377.04	1412.83	1419.62	1440.36	1486.71	1508.27	1510.88	1512.45	1515.92	1517.05	1517.69	
1496.70	1500.34	1512.37	1520.50	1534.99	3030.70	1518.92	1521.08	1522.84	1523.48	1527.85	1531.00	
3035.84	3051.34	3098.48	3105.62	3124.74	3124.86	1603.58	1612.85	1618.65	1624.94	1641.83	1660.18	
3132.22	3132.47	3799.71				3001.34	3010.35	3012.02	3014.08	3015.30	3015.77	
=====							3022.14	3027.44	3030.18	3032.12	3034.40	3035.16
NaCl							3036.20	3039.11	3041.38	3041.87	3057.43	3063.25
=====							3065.22	3069.79	3071.48	3073.88	3075.21	3077.60
355.69						3080.73	3082.80	3092.75	3098.00	3103.29	3103.75	
=====							3105.82	3108.58	3108.91	3111.64	3112.56	3113.72
1,4-dioxane							3118.70	3121.29	3124.87	3126.20	3134.51	3135.94
=====							3140.92	3165.49	3173.76	3174.87	3179.03	3184.00
251.21	280.95	424.74	447.34	488.80	618.95	3193.44	3195.00	3200.50	3206.43	3209.60	3221.72	
853.37	874.25	895.17	899.63	1024.57	1072.09	=====						
1117.12	1143.02	1150.64	1153.82	1245.16	1287.48	L1_10						
1326.47	1335.78	1365.38	1405.47	1420.52	1437.49	=====						
1491.63	1494.18	1507.20	1512.77	2974.84	2982.49	20.66	25.79	33.80	37.15	40.56	46.28	
2986.33	2993.17	3092.36	3094.20	3096.35	3099.60	51.98	57.74	58.76	67.16	71.84	76.84	
=====							79.95	84.41	88.46	90.83	99.36	104.14
Ligand(L1, L2, L3, L4)_ (dihedral angle)							109.28	112.31	136.27	137.45	142.49	153.93
=====							160.46	173.15	178.13	187.76	202.23	204.82
L1_0							208.28	214.54	225.40	241.58	246.34	252.23
=====							258.81	262.20	262.81	263.24	270.44	276.42
19.53	25.49	33.46	36.38	40.55	47.94	276.72	285.97	289.24	291.85	309.33	321.02	
51.79	58.28	59.65	68.31	73.06	79.30	325.55	336.13	339.45	363.83	377.69	387.52	
82.72	88.43	90.50	91.77	99.08	105.99	396.23	415.47	420.69	435.62	450.04	451.10	
109.20	112.47	135.66	138.70	144.10	155.61	453.62	466.87	479.66	484.82	489.69	495.55	
164.77	175.25	179.35	188.55	201.83	206.28	508.68	526.34	535.29	541.17	563.48	586.84	
209.21	214.65	224.58	242.64	246.60	252.18	611.32	623.23	637.27	648.86	664.10	672.79	
259.60	261.75	263.37	264.50	270.35	278.24	682.86	708.15	730.33	747.22	749.48	754.59	
279.66	286.19	290.83	293.34	310.50	320.18	767.54	778.18	783.86	807.13	816.51	828.39	
325.66	336.06	339.75	364.14	377.29	389.89	828.93	833.37	848.55	856.43	868.31	872.53	
396.49	415.92	422.08	436.80	450.32	451.44	893.39	895.05	902.27	903.40	906.18	907.65	
454.37	468.68	479.74	485.17	491.88	494.87	913.09	914.21	920.12	941.12	944.20	945.22	
509.55	527.20	537.51	541.33	564.20	584.76	948.25	949.20	957.83	962.33	971.24	973.89	
611.57	623.47	637.31	648.80	663.29	672.47	975.16	975.94	976.50	989.92	1000.66	1009.88	
683.15	708.55	731.36	748.00	750.08	754.84	1020.48	1024.53	1030.04	1042.15	1047.46	1049.36	
768.96	777.39	785.40	808.31	817.66	827.98	1062.18	1065.79	1070.27	1083.27	1090.13	1093.85	
829.70	834.06	847.97	856.37	868.81	872.89	1098.72	1100.80	1102.54	1105.81	1108.37	1112.58	
894.27	896.30	902.27	903.54	906.02	908.08	1128.29	1130.47	1133.55	1137.59	1139.20	1150.97	
912.99	914.17	920.48	941.70	944.61	945.28	1156.21	1163.83	1190.61	1191.81	1202.86	1203.26	
948.12	949.03	957.57	963.35	973.10	973.63	1209.90	1210.33	1215.62	1218.24	1234.69	1246.33	
975.24	976.31	976.84	990.05	1001.20	1009.88	1262.31	1288.80	1289.55	1295.31	1296.51	1300.91	
1020.67	1024.92	1030.54	1041.89	1047.49	1049.45	1307.87	1309.10	1314.19	1315.94	1319.14	1322.85	
1060.68	1065.23	1070.16	1082.99	1090.35	1093.53	1334.46	1341.94	1342.87	1344.00	1346.15	1349.78	
1098.95	1100.24	1101.92	1106.22	1108.24	1113.24	1361.93	1365.13	1367.95	1369.61	1379.95	1380.76	
1128.67	1130.45	1134.27	1137.86	1139.38	1151.26	1385.94	1391.35	1394.94	1395.91	1396.72	1401.29	
1155.78	1163.26	1190.19	1191.58	1201.98	1202.97	1403.47	1404.51	1413.68	1415.05	1416.64	1433.86	
1209.33	1210.06	1215.52	1218.52	1234.28	1245.96	1435.45	1436.90	1467.43	1468.10	1478.37	1492.17	
1262.38	1287.67	1291.39	1295.21	1296.72	1301.06	1493.67	1497.36	1498.10	1499.15	1500.90	1501.58	
1307.05	1309.08	1314.02	1317.45	1319.69	1322.77	1503.43	1503.75	1504.72	1505.64	1506.09	1506.43	
1334.32	1340.47	1342.38	1343.26	1345.53	1350.15	1508.57	1509.89	1512.62	1515.80	1516.94	1517.25	
						1518.03	1520.73	1522.31	1523.32	1527.47	1530.44	

1602.78 1614.03 1619.26 1625.03 1643.39 1659.56
3003.46 3009.63 3012.46 3014.28 3015.33 3015.89
3021.76 3028.37 3030.24 3030.40 3034.52 3034.90
3035.07 3039.37 3039.61 3040.54 3057.22 3061.26
3065.83 3069.35 3071.51 3073.14 3075.39 3077.71
3081.48 3084.47 3089.93 3098.16 3101.19 3103.86
3105.80 3107.99 3108.94 3111.49 3111.75 3117.15
3118.78 3119.55 3122.12 3129.05 3132.33 3140.34
3141.90 3165.52 3173.56 3176.34 3180.13 3183.90
3193.52 3194.66 3196.70 3205.56 3207.04 3219.76

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L1_20
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20.69 28.72 33.72 37.69 41.23 46.01
52.04 58.45 58.95 66.35 72.85 73.33
77.63 82.27 86.58 91.29 99.73 102.82
109.10 112.38 133.23 137.35 140.25 152.06
158.79 170.81 176.96 187.49 201.93 204.73
207.38 215.69 225.93 240.88 245.46 252.26
254.88 261.49 262.08 262.79 271.77 272.94
273.21 281.63 289.48 291.53 308.38 320.69
325.96 335.96 338.55 363.46 378.96 385.24
396.84 414.92 420.12 434.42 449.75 450.41
453.34 464.96 479.70 484.44 488.50 495.96
508.37 525.05 533.58 542.11 562.30 589.45
611.03 623.09 637.65 649.39 664.61 672.04
680.56 707.99 729.20 746.70 748.66 754.09
767.31 779.09 782.92 806.18 815.48 828.34
828.50 833.36 848.63 856.64 867.76 871.99
891.41 895.56 902.11 904.03 906.20 907.79
912.87 913.67 921.11 940.55 943.34 945.33
948.57 949.20 958.04 961.56 969.83 973.88
975.48 975.92 976.14 989.25 999.44 1009.49
1019.68 1024.07 1029.68 1041.05 1047.26 1049.23
1063.67 1065.57 1070.87 1083.06 1090.02 1094.08
1098.55 1099.49 1102.99 1105.31 1108.09 1112.43
1127.98 1130.91 1132.90 1137.65 1139.39 1150.85
1156.62 1163.96 1191.01 1191.46 1202.75 1203.40
1209.94 1210.55 1215.71 1217.87 1235.23 1247.22
1261.77 1287.26 1290.25 1295.64 1297.03 1301.11
1308.56 1309.19 1313.27 1314.61 1317.58 1323.14
1335.56 1342.73 1344.47 1345.04 1345.47 1349.72
1361.66 1364.07 1368.23 1369.94 1378.47 1380.48
1386.00 1390.80 1394.81 1395.72 1396.83 1401.26
1403.31 1404.03 1414.39 1415.30 1416.87 1434.51
1436.23 1437.03 1466.28 1468.18 1478.98 1491.82
1493.30 1496.84 1498.07 1499.04 1500.81 1501.58
1503.23 1504.15 1504.59 1504.76 1506.00 1506.46
1508.23 1509.28 1512.46 1515.27 1516.47 1516.86
1517.93 1520.63 1521.85 1523.04 1527.75 1529.60
1601.82 1615.00 1617.70 1623.00 1642.54 1659.10
3006.09 3009.14 3010.86 3014.42 3014.99 3016.32
3021.98 3029.16 3029.64 3031.52 3034.54 3034.91
3036.07 3039.08 3040.82 3043.08 3056.41 3061.24
3066.02 3069.69 3071.94 3072.99 3075.49 3078.06
3080.79 3087.33 3088.26 3097.99 3102.68 3105.10
3105.11 3108.28 3108.92 3111.84 3112.73 3116.91
3118.48 3119.33 3121.41 3129.13 3131.20 3142.13

3147.29 3165.63 3173.20 3178.64 3183.87 3186.16
3189.56 3194.17 3195.95 3205.25 3206.79 3218.91

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L1_30
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19.76 25.30 39.63 43.49 45.43 50.56
55.22 60.00 64.16 66.54 72.09 74.43
80.77 84.03 88.69 93.36 99.71 103.96
109.37 117.60 125.38 136.42 140.86 147.90
162.56 171.34 177.15 185.43 191.66 206.01
206.60 219.63 224.48 239.30 246.59 253.21
253.85 258.13 263.52 265.03 266.49 269.36
276.08 281.64 290.52 296.67 305.86 318.14
331.71 336.49 339.79 363.58 379.85 384.03
395.78 412.59 415.74 427.73 447.60 450.16
451.95 475.73 479.33 485.07 489.28 495.48
506.98 522.23 532.90 543.12 560.22 591.19
608.99 622.52 637.51 648.82 665.03 672.67
679.05 707.44 722.62 747.45 749.03 758.00
771.53 779.78 784.48 807.46 811.78 826.87
830.41 832.58 847.14 857.02 866.05 869.83
895.79 895.88 900.55 904.07 906.87 908.67
911.14 913.91 922.25 938.71 942.96 944.99
947.77 950.04 957.58 962.04 972.21 972.65
975.07 975.96 976.56 988.87 1000.59 1009.35
1019.45 1024.01 1028.25 1040.96 1044.44 1048.43
1065.43 1069.19 1070.12 1083.59 1088.67 1095.84
1097.02 1099.29 1103.52 1107.41 1108.05 1112.87
1127.07 1129.90 1132.33 1137.44 1142.22 1148.34
1156.13 1163.86 1191.23 1191.28 1203.26 1204.78
1209.91 1210.70 1212.76 1217.68 1239.74 1245.23
1263.30 1286.72 1290.24 1296.61 1299.08 1301.75
1306.99 1308.47 1310.11 1313.94 1317.47 1321.29
1330.73 1335.93 1344.72 1345.72 1346.73 1348.37
1359.20 1361.32 1368.58 1370.82 1374.10 1382.87
1388.09 1392.41 1393.39 1395.57 1397.63 1399.37
1400.95 1401.57 1414.87 1416.16 1416.81 1435.52
1436.46 1437.34 1466.41 1469.39 1477.84 1491.42
1495.60 1496.76 1498.19 1498.84 1500.75 1501.76
1503.41 1503.97 1504.56 1505.38 1505.98 1506.16
1507.73 1508.43 1510.25 1514.92 1516.40 1516.96
1517.40 1521.12 1523.00 1523.42 1524.79 1527.46
1602.07 1614.74 1617.62 1622.04 1641.39 1658.55
3008.70 3011.82 3016.64 3020.64 3026.14 3026.44
3028.66 3031.94 3034.68 3034.80 3035.21 3038.21
3039.06 3039.57 3039.87 3050.95 3056.03 3056.97
3060.81 3068.17 3070.15 3071.84 3073.78 3075.36
3077.77 3079.31 3079.61 3094.00 3098.11 3102.31
3105.26 3105.97 3108.52 3109.91 3110.08 3111.58
3113.66 3115.55 3120.40 3126.79 3130.13 3144.61
3163.10 3165.63 3173.05 3179.08 3183.58 3188.76
3192.15 3193.54 3200.84 3201.02 3210.44 3223.10

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L1_40
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13.02 20.78 39.19 39.97 44.77 50.22
55.64 59.54 65.02 66.28 71.52 74.03
76.61 83.14 88.21 92.83 98.08 103.38

110.12 118.32 123.06 136.82 140.06 147.39
162.84 170.59 176.16 184.77 190.84 204.55
205.72 219.27 224.12 237.88 246.61 252.89
253.58 258.74 263.90 266.04 267.28 269.56
276.12 285.20 290.02 300.60 304.32 317.34
332.45 337.09 339.07 362.06 380.29 385.05
398.18 410.15 415.25 427.69 447.20 449.81
451.85 475.52 477.48 483.58 488.79 494.61
508.49 522.00 532.91 545.47 558.17 592.21
609.11 622.19 637.48 646.48 664.41 673.01
681.07 706.45 725.23 747.00 747.59 759.12
770.62 777.99 785.18 807.31 812.15 826.11
830.50 832.43 845.74 857.50 866.39 870.26
894.30 895.89 900.56 902.58 907.05 907.85
910.74 913.87 923.07 938.67 943.18 945.49
947.90 949.99 957.69 960.61 969.97 970.98
974.99 976.15 977.02 988.74 998.70 1009.01
1019.89 1023.82 1028.15 1040.48 1044.33 1048.62
1064.60 1069.22 1070.04 1083.54 1088.20 1095.91
1096.78 1098.79 1102.63 1106.94 1107.42 1113.70
1127.53 1130.57 1131.96 1137.34 1141.96 1148.90
1154.93 1163.33 1191.34 1191.43 1203.54 1204.44
1209.23 1210.43 1212.36 1218.18 1238.79 1246.30
1263.97 1284.09 1290.93 1296.78 1299.30 1301.64
1306.86 1308.24 1309.58 1313.63 1317.21 1321.87
1328.17 1335.37 1344.46 1345.98 1347.22 1348.41
1359.61 1361.39 1368.64 1370.74 1373.29 1383.07
1388.81 1392.71 1393.38 1395.87 1397.28 1399.44
1400.93 1401.15 1414.65 1416.07 1416.82 1435.58
1436.53 1437.24 1466.67 1469.06 1476.88 1490.55
1495.58 1496.76 1498.24 1498.80 1500.85 1501.67
1503.32 1503.96 1504.73 1505.46 1505.95 1506.00
1507.22 1508.13 1510.36 1511.56 1516.58 1517.17
1517.59 1521.21 1522.92 1523.37 1524.78 1527.62
1603.59 1614.01 1617.31 1622.02 1639.74 1659.20
3008.65 3011.51 3016.59 3020.90 3027.38 3028.08
3029.67 3032.01 3034.35 3035.32 3035.46 3037.07
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3062.13 3067.86 3070.44 3072.07 3073.82 3075.15
3078.51 3080.75 3083.90 3092.87 3097.81 3102.72
3105.54 3105.84 3110.13 3110.29 3111.75 3113.19
3114.85 3115.36 3121.99 3125.00 3129.54 3142.53
3159.65 3166.00 3173.42 3180.47 3181.89 3191.28
3193.78 3199.45 3201.42 3202.88 3212.33 3220.77

L1_50

11.06 20.94 40.30 43.38 46.88 54.31
59.96 61.67 65.28 73.35 75.97 79.11
81.11 87.65 95.97 99.69 101.78 108.08
112.00 121.41 122.99 141.78 145.70 154.68
164.67 172.67 178.79 188.91 195.18 205.17
207.37 221.39 225.32 244.43 249.85 250.28
253.91 259.78 266.76 271.15 272.53 276.20
282.82 286.28 291.93 299.76 303.50 316.39
334.94 338.80 341.53 361.70 380.71 390.01
400.44 408.32 415.63 429.52 447.73 450.59
454.37 474.45 477.23 483.74 489.90 494.59

509.19 523.20 533.03 545.64 558.71 593.55
607.72 621.63 638.89 639.35 661.59 673.79
682.13 705.20 724.39 746.58 747.51 759.67
771.39 776.57 786.59 808.22 811.13 826.14
829.34 831.76 844.53 857.40 866.52 869.80
894.49 896.10 901.05 901.39 906.56 908.06
910.53 913.10 923.99 939.98 943.79 945.70
947.32 950.52 956.39 960.07 971.34 971.58
974.68 976.17 976.64 988.16 999.97 1009.25
1020.77 1022.98 1027.66 1040.98 1044.46 1048.32
1064.83 1069.24 1070.84 1083.23 1087.45 1095.72
1097.88 1098.73 1103.07 1106.85 1109.28 1114.88
1125.65 1129.43 1131.61 1137.34 1142.98 1147.45
1155.07 1164.65 1191.12 1192.10 1202.86 1205.01
1208.77 1210.38 1213.15 1218.92 1240.89 1243.94
1267.81 1282.35 1291.00 1297.15 1299.64 1302.46
1307.56 1308.55 1309.24 1315.92 1316.95 1322.00
1327.49 1336.70 1340.22 1343.92 1347.69 1349.60
1357.80 1360.24 1369.39 1371.56 1373.09 1385.21
1390.40 1393.48 1394.97 1395.62 1396.92 1398.13
1400.34 1401.56 1415.15 1416.82 1417.47 1436.35
1437.40 1439.99 1466.49 1469.40 1475.72 1489.87
1496.92 1498.19 1499.50 1500.28 1501.13 1502.19
1503.56 1504.50 1504.99 1505.49 1506.31 1507.68
1508.12 1508.53 1511.24 1513.36 1518.34 1518.54
1519.62 1522.20 1524.14 1524.77 1526.28 1530.26
1605.77 1614.74 1617.03 1622.27 1640.37 1658.52
3008.39 3010.63 3016.53 3021.07 3028.92 3029.35
3031.29 3034.59 3035.66 3036.39 3037.76 3040.30
3040.43 3042.06 3043.30 3051.74 3053.06 3061.72
3068.56 3071.96 3072.14 3073.73 3076.24 3078.02
3078.85 3081.97 3083.71 3091.92 3096.62 3100.83
3104.98 3105.30 3105.99 3110.56 3111.66 3112.86
3118.67 3122.03 3127.84 3132.18 3137.03 3139.87
3161.36 3167.01 3174.48 3181.12 3181.59 3193.85
3195.46 3205.63 3205.87 3214.93 3218.31 3225.53

L1_60

12.11 18.09 40.85 46.15 47.35 56.05
60.87 62.06 65.12 73.62 76.49 79.32
90.14 93.21 97.09 103.09 104.58 110.78
114.10 124.36 127.86 144.20 147.78 161.48
164.96 177.08 180.43 193.11 198.43 204.52
207.35 222.65 226.67 241.48 246.57 251.94
253.85 256.56 266.23 274.24 276.28 280.44
285.18 289.27 294.08 298.91 305.96 316.90
334.95 338.60 345.67 360.22 379.59 396.18
402.21 405.64 417.51 429.57 447.43 450.12
455.26 472.80 477.10 484.52 489.45 495.00
508.29 523.62 532.16 544.43 558.99 593.21
604.39 622.40 630.62 641.60 663.11 673.29
683.65 706.71 722.90 744.99 747.76 757.66
771.76 776.59 789.11 808.10 808.73 824.68
827.65 830.79 845.00 857.31 865.98 868.99
895.26 896.00 901.20 905.22 906.38 908.12
911.06 913.57 920.04 940.25 943.79 944.72
947.07 949.60 955.09 959.80 971.36 971.99

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1513.52 1514.76 1516.46 1518.13 1522.09 1524.29
1524.87 1526.48 1528.44 1528.96 1531.13 1535.53
1537.63 1586.17 1591.77 1606.26 1615.88 1621.19
1655.74 2957.97 3012.24 3014.14 3016.54 3018.28
3020.50 3029.11 3031.53 3033.96 3037.21 3037.88
3039.36 3041.70 3042.55 3045.54 3046.24 3048.53
3051.19 3054.23 3061.47 3066.31 3067.05 3069.29
3070.71 3073.68 3077.99 3079.20 3083.50 3085.39
3094.30 3094.71 3097.44 3099.35 3103.55 3104.38
3109.72 3110.59 3112.13 3112.81 3115.28 3118.22
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L3_100

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279.87 288.39 291.87 296.45 298.65 302.65
311.82 313.10 323.83 333.70 347.70 353.14
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456.31 464.10 471.80 476.62 479.97 489.17
497.45 510.72 522.33 529.08 535.89 555.65
582.49 601.50 607.98 621.02 632.96 644.49
662.01 672.12 676.11 699.80 719.23 721.80
739.94 744.54 745.84 785.45 798.91 805.88
813.40 817.02 823.01 827.86 830.37 836.85
856.25 863.48 867.78 895.93 901.34 902.60
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1295.35 1296.16 1302.74 1311.91 1313.94 1314.42
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1344.74 1350.56 1355.13 1367.69 1368.26 1368.92
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1500.39 1500.98 1502.14 1502.99 1505.12 1505.39
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1536.12 1585.62 1592.93 1607.66 1615.91 1620.93
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3068.74 3070.74 3078.66 3080.22 3084.99 3085.50
3090.62 3091.22 3091.34 3101.70 3104.35 3104.50
3110.30 3110.80 3111.65 3111.89 3115.82 3117.21
3118.21 3119.56 3128.09 3134.36 3141.37 3141.49
3144.47 3152.81 3161.85 3168.60 3173.06 3174.92
3176.21 3178.53 3181.06 3195.01 3196.91 3196.99

3199.57 3208.28 3213.50

L3_110

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75.77 82.67 84.03 85.96 95.19 99.36
104.03 107.81 115.10 119.46 124.04 134.49
141.75 143.09 153.13 159.75 167.20 172.74
175.34 178.08 183.03 191.66 194.16 199.55
209.16 218.49 219.74 233.36 237.26 239.98
250.23 255.33 259.54 263.95 266.98 268.46
272.24 276.11 283.15 293.06 299.55 307.47
311.99 315.27 332.42 335.35 338.43 358.84
360.60 369.79 375.30 378.34 397.09 397.58
408.53 413.68 416.39 421.73 441.80 450.47
455.38 455.91 459.38 476.61 478.97 479.70
488.58 504.75 517.84 529.71 534.39 549.90
577.18 598.28 612.97 620.82 624.51 641.47
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959.76 963.16 970.28 971.25 973.59 980.44
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1039.48 1043.30 1043.76 1045.77 1053.99 1060.27
1063.04 1071.43 1072.24 1079.37 1083.35 1091.14
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1145.70 1164.81 1183.93 1188.97 1192.03 1197.62
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1236.35 1247.13 1265.64 1280.94 1285.42 1292.71
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1437.07 1438.06 1465.09 1472.98 1481.47 1485.91
1491.85 1492.89 1495.15 1496.88 1497.19 1498.41
1499.60 1499.95 1501.33 1501.76 1502.55 1502.74
1504.02 1504.72 1506.03 1506.79 1507.85 1508.27
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3102.88 3103.22 3108.89 3109.09 3113.65 3116.70
3119.26 3123.88 3124.60 3126.08 3130.85 3133.88
3135.10 3139.79 3154.02 3159.50 3167.83 3168.73
3176.54 3177.91 3183.32 3195.28 3195.52 3195.66
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L3_120

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140.75 142.84 153.07 161.79 164.84 174.10
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456.57 459.17 465.82 477.32 479.36 481.62
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581.97 604.90 610.89 620.82 625.54 643.24
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734.07 743.51 752.08 782.99 792.00 808.99
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855.23 865.50 869.16 894.73 900.57 903.61
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1122.62 1125.07 1128.74 1130.32 1136.61 1141.05
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1201.81 1210.66 1214.35 1214.84 1219.51 1234.45
1238.23 1247.68 1269.22 1282.47 1285.84 1294.42
1296.67 1299.68 1305.15 1306.07 1311.75 1318.38
1318.90 1320.34 1334.52 1347.02 1347.69 1351.49
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1397.09 1397.90 1404.06 1408.54 1412.05 1415.95
1416.94 1417.76 1420.67 1432.66 1436.02 1436.54
1437.58 1438.49 1466.21 1473.39 1482.25 1485.04
1492.99 1493.34 1495.67 1497.32 1497.72 1498.68
1499.75 1499.85 1501.61 1501.99 1502.47 1502.74
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1509.64 1513.10 1515.76 1517.53 1518.18 1519.31
1521.53 1523.92 1524.32 1524.93 1526.78 1529.82
1533.52 1587.34 1600.18 1606.32 1615.80 1623.69
1656.28 3014.95 3015.16 3015.21 3017.09 3020.32
3022.51 3024.90 3028.01 3030.58 3034.25 3036.20
3038.12 3038.40 3039.78 3040.95 3041.75 3043.34
3046.02 3057.12 3057.17 3066.00 3067.85 3068.29
3071.34 3074.85 3076.35 3078.38 3080.01 3084.16
3085.65 3089.75 3092.39 3093.36 3094.51 3098.99
3102.93 3103.43 3105.82 3109.13 3114.51 3116.75
3118.66 3122.20 3124.12 3126.13 3130.18 3136.69
3139.66 3140.11 3148.43 3160.02 3167.52 3168.89
3177.10 3177.89 3180.78 3187.55 3194.66 3194.94
3200.60 3222.77 3267.98

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14.70	26.11	30.14	33.86	39.92	44.22
47.48	48.57	58.68	64.28	67.68	70.53
75.50	78.68	85.54	90.05	95.22	99.46
106.55	109.17	110.80	115.64	125.06	136.90
140.48	141.32	153.29	160.59	162.80	173.45
175.97	177.49	181.97	190.06	194.31	200.03
201.49	218.83	220.64	230.27	237.25	239.53
248.79	255.75	260.05	263.23	267.82	270.14
271.96	274.91	278.66	291.37	302.48	303.53
313.18	314.76	331.53	335.61	337.25	355.93
358.99	369.51	378.73	385.32	398.82	405.80
412.66	413.97	423.74	435.37	451.32	453.42
456.68	460.36	468.57	478.02	480.12	483.42
490.00	511.49	520.18	534.70	537.64	555.00
583.62	607.16	609.98	620.85	626.38	643.43
657.98	673.61	673.93	697.41	717.78	721.13
737.93	744.82	754.47	782.26	793.74	809.32
810.58	817.74	820.96	824.39	830.43	836.36
856.50	865.69	869.31	895.04	900.68	903.26
907.84	908.34	911.15	912.58	919.98	935.12
936.34	943.14	943.89	946.63	949.24	959.13
962.53	965.94	970.70	973.49	976.80	980.13
988.65	1007.98	1023.04	1026.35	1033.36	1039.34
1040.72	1043.91	1044.38	1045.12	1054.94	1061.34
1064.48	1069.96	1072.24	1080.41	1085.10	1093.36
1094.48	1103.46	1105.79	1106.40	1108.68	1111.59
1123.48	1124.70	1128.64	1130.74	1137.09	1140.43
1146.26	1168.35	1184.16	1189.15	1193.05	1201.51
1202.13	1210.38	1214.07	1215.45	1219.88	1235.14
1238.19	1246.36	1270.18	1283.32	1286.42	1295.62
1297.59	1299.82	1305.38	1306.97	1311.34	1318.03
1320.29	1323.54	1334.56	1346.20	1348.80	1352.17
1353.19	1353.78	1358.53	1365.57	1369.21	1373.63
1376.12	1382.73	1390.31	1393.04	1394.20	1394.52
1396.58	1397.80	1404.67	1407.15	1411.89	1416.00
1417.68	1417.96	1420.51	1432.10	1435.63	1436.39
1437.70	1438.62	1466.47	1474.62	1481.64	1483.47
1493.08	1493.59	1495.73	1497.43	1497.85	1498.57
1499.54	1499.76	1501.15	1501.90	1502.26	1502.69
1504.32	1505.29	1506.60	1507.16	1508.39	1509.17
1509.77	1513.32	1515.64	1517.39	1518.07	1519.38
1521.26	1523.67	1524.13	1524.83	1527.25	1529.06
1532.78	1588.27	1601.72	1608.15	1616.15	1623.93
1657.57	3014.46	3014.64	3015.35	3017.91	3020.85
3021.21	3024.33	3028.94	3031.02	3034.44	3036.41
3038.32	3039.15	3040.29	3041.14	3041.21	3043.70
3046.36	3056.37	3065.15	3067.58	3067.96	3069.13
3071.98	3074.93	3077.52	3077.77	3078.95	3080.06
3085.82	3089.90	3092.25	3092.70	3093.71	3099.84
3103.14	3103.94	3104.88	3109.37	3114.61	3116.98
3118.11	3120.28	3123.24	3125.05	3128.86	3133.78
3139.39	3140.12	3146.25	3160.61	3167.02	3168.83
3177.76	3177.85	3178.54	3184.22	3193.05	3193.19
3194.90	3220.25	3250.83			

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19.96	26.86	28.66	32.62	37.24	40.16
43.27	49.86	55.51	60.51	65.92	70.00
70.83	72.16	83.83	86.78	88.90	95.78
100.35	106.25	112.25	121.03	125.21	129.33
136.88	145.27	146.39	150.97	156.43	163.09
169.38	179.41	182.33	184.23	194.02	201.09
201.59	203.51	213.95	225.94	231.06	234.23
240.96	249.58	251.77	253.76	257.03	265.04
268.23	270.18	273.00	280.56	295.18	301.96
310.71	318.95	321.50	335.28	342.93	353.86
364.01	372.24	378.88	391.89	394.33	397.78
410.64	413.96	427.79	439.91	447.18	449.53
455.16	465.04	471.54	476.32	481.96	489.85
494.85	509.95	519.39	531.02	533.50	556.04
583.15	608.74	611.16	620.81	630.53	643.73
658.64	672.92	675.64	697.46	714.12	714.51
740.16	745.08	750.36	783.13	795.60	808.24
812.42	818.30	823.63	828.61	831.14	837.31
856.80	865.19	869.31	896.28	901.63	902.63
903.61	908.07	910.01	913.46	914.56	935.19
936.90	939.89	945.73	946.70	946.85	958.28
964.33	966.33	973.36	973.82	974.53	980.34
987.52	1007.84	1024.21	1026.11	1030.92	1038.96
1041.04	1042.24	1044.58	1047.96	1051.71	1062.28
1065.97	1071.26	1071.92	1082.07	1083.88	1094.33
1095.31	1101.20	1103.15	1105.36	1106.45	1108.46
1122.39	1125.79	1129.05	1132.51	1137.19	1138.87
1155.15	1168.00	1185.80	1190.24	1193.13	1201.20
1202.80	1211.74	1212.50	1214.67	1219.35	1232.97
1237.74	1263.83	1265.60	1281.76	1286.44	1291.90
1293.16	1298.48	1303.28	1312.66	1313.52	1316.71
1320.35	1324.64	1329.11	1339.84	1349.56	1350.83
1352.91	1358.28	1359.27	1364.18	1369.36	1371.01
1378.24	1381.82	1387.52	1392.78	1393.52	1395.01
1396.24	1398.04	1399.51	1403.73	1406.47	1411.73
1414.01	1417.88	1419.10	1425.68	1435.08	1436.46
1437.04	1438.21	1467.00	1473.53	1480.62	1488.17
1491.70	1492.68	1493.97	1495.55	1497.39	1498.33
1498.92	1499.42	1499.77	1500.74	1502.65	1503.56
1504.33	1504.60	1505.06	1506.68	1507.07	1508.12
1509.27	1510.24	1511.77	1518.30	1518.69	1519.54
1522.04	1523.26	1523.99	1525.99	1526.58	1529.27
1533.07	1583.43	1601.88	1607.58	1615.48	1623.36
1656.87	3013.18	3015.07	3015.25	3019.83	3024.84
3025.13	3027.33	3030.02	3033.23	3035.08	3036.75
3038.40	3039.97	3042.40	3042.57	3045.19	3045.70
3047.02	3050.27	3058.80	3061.18	3068.36	3069.46
3072.05	3074.78	3075.32	3076.55	3077.39	3085.22
3089.49	3090.64	3094.42	3095.71	3096.62	3098.66
3103.40	3103.91	3109.50	3112.92	3115.86	3117.10
3118.22	3119.67	3120.37	3123.95	3131.85	3133.13
3139.56	3148.66	3149.83	3161.68	3167.68	3173.32
3177.51	3179.96	3183.26	3185.13	3191.27	3194.99
3204.30	3214.11	3228.02			

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22.86 29.59 31.14 36.65 42.18 43.41
49.14 52.58 54.96 59.57 68.77 71.58
77.59 83.62 88.10 90.76 92.73 101.56
106.13 109.74 111.91 118.20 125.20 138.73
145.77 146.93 157.61 158.90 163.51 172.62
174.97 181.28 183.50 188.12 193.69 197.88
203.33 216.07 223.82 226.35 236.81 239.26
246.00 248.69 254.86 261.13 269.55 271.21
273.68 280.19 287.56 292.42 297.86 304.19
314.50 315.57 328.80 337.65 338.32 353.79
362.34 368.04 379.49 384.83 397.48 410.43
417.65 424.38 426.39 429.20 450.09 453.57
458.11 463.98 472.24 477.49 481.46 482.47
488.47 512.59 524.04 534.27 538.43 554.74
584.71 609.41 610.04 620.48 626.87 644.39
658.62 673.32 673.53 700.80 714.20 724.92
743.21 747.20 758.23 781.90 793.28 810.83
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857.94 866.63 869.43 895.38 900.46 904.65
907.03 910.49 912.75 913.47 918.75 935.51
937.56 943.71 944.29 946.48 948.37 959.93
962.83 971.64 973.30 973.58 975.79 978.85
991.94 1007.25 1023.00 1027.99 1035.36 1038.63
1039.30 1044.75 1045.32 1045.80 1054.22 1061.65
1063.96 1066.00 1073.05 1081.45 1085.08 1092.62
1094.59 1103.56 1105.07 1105.99 1111.96 1116.62
1124.44 1125.42 1128.61 1132.99 1138.62 1140.13
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1241.20 1245.51 1269.49 1281.79 1286.29 1294.74
1297.68 1299.84 1306.39 1308.08 1311.86 1316.30
1319.47 1319.97 1337.74 1343.85 1350.55 1351.08
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1346.32 1348.10 1352.57 1357.81 1364.88 1392.92
1414.87 1415.05 1416.75 1417.12 1418.70 1419.91
1421.74 1424.02 1435.99 1437.43 1438.04 1448.29
1449.45 1455.71 1468.11 1476.48 1488.57 1489.19
1492.13 1492.96 1495.48 1497.17 1498.83 1501.14
1501.54 1503.00 1504.49 1506.08 1506.73 1506.92
1508.63 1509.94 1511.46 1512.92 1515.26 1517.96
1518.24 1518.49 1519.90 1521.03 1522.70 1523.38
1525.24 1527.07 1533.04 1534.08 1543.64 1544.12
1610.66 1623.04 1623.84 1628.17 1637.22 1660.53
3007.78 3028.82 3034.80 3035.44 3039.09 3039.89
3041.34 3041.57 3041.91 3042.13 3046.24 3046.81
3047.65 3048.87 3053.28 3070.28 3073.26 3092.55
3102.89 3103.13 3104.27 3110.30 3110.99 3112.13
3113.09 3114.89 3115.59 3117.58 3117.67 3119.65
3123.40 3135.55 3136.81 3143.76 3145.54 3150.57
3156.45 3158.93 3163.63 3171.64 3174.14 3181.21
3183.61 3185.19 3189.50 3191.50 3197.54 3197.71
3202.98 3208.00 3217.70 3230.58 3255.87 3266.71

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16.64 22.35 24.44 32.53 43.11 52.96
55.71 64.19 71.77 73.67 79.59 92.66
99.94 106.31 108.46 115.26 118.15 123.89
129.49 135.86 139.80 141.62 148.05 151.81
156.36 159.27 166.08 182.58 189.29 198.22
215.74 225.13 227.79 231.83 236.00 241.68
243.46 249.82 252.95 257.48 261.60 267.52
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294.18 301.87 307.33 314.30 316.23 318.93
319.70 327.55 338.75 351.19 356.35 362.47
365.91 377.33 391.51 396.96 405.52 408.99
417.39 421.01 427.20 435.24 452.83 459.77
471.95 482.49 492.14 497.80 513.28 517.07
559.46 565.67 579.91 592.94 599.77 623.62
624.05 626.70 634.65 657.33 669.87 672.36
675.93 710.06 738.23 749.39 779.44 783.14
808.34 814.63 822.40 823.04 834.26 848.02
853.55 886.69 896.90 903.52 910.64 913.51
931.20 941.48 944.75 946.52 949.66 952.26
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1064.67 1083.73 1087.24 1093.87 1101.05 1103.60
1120.58 1128.64 1129.01 1136.09 1158.66 1176.91
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1203.24 1211.86 1212.97 1219.29 1222.08 1223.25
1227.46 1233.75 1243.04 1244.31 1263.60 1273.52
1281.60 1288.84 1295.03 1313.81 1314.96 1341.41
1345.41 1347.04 1352.75 1357.46 1363.77 1393.45
1411.89 1414.95 1415.65 1417.06 1417.09 1420.22
1421.70 1424.64 1436.16 1437.49 1438.87 1447.44
1449.08 1456.37 1466.82 1475.58 1488.15 1490.63

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1508.39 1509.56 1510.86 1513.13 1514.87 1516.11
1517.64 1518.08 1520.42 1520.84 1524.24 1524.84
1525.08 1527.57 1531.93 1535.26 1543.98 1547.63
1610.18 1621.50 1622.41 1624.21 1635.95 1660.81
3007.76 3028.81 3034.85 3034.87 3038.46 3038.61
3041.16 3041.22 3042.26 3043.03 3045.65 3046.53
3047.67 3048.70 3052.73 3070.45 3081.73 3098.79
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15.93 23.70 27.43 34.36 38.23 40.12
42.47 52.22 57.25 59.51 61.97 68.18
73.73 76.56 81.43 87.27 89.27 98.13
103.07 107.05 118.36 128.50 137.71 144.47
150.56 159.33 167.76 174.18 193.01 204.63
210.37 221.20 228.88 240.29 248.64 255.36
257.41 259.53 264.09 267.84 277.63 279.91
288.36 291.87 294.22 297.80 318.38 327.31
336.80 340.19 365.47 379.80 381.48 391.03
394.47 407.39 414.78 438.77 448.11 451.21
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508.64 528.39 532.90 537.57 562.83 586.89
610.86 612.24 640.29 646.74 665.44 673.33
678.66 680.88 731.56 732.64 749.83 753.84
768.79 781.95 789.29 808.41 812.47 817.63
819.81 828.03 833.18 855.90 868.60 870.85
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906.20 912.17 914.49 940.29 943.17 945.54
945.95 946.97 950.58 954.88 962.14 972.63
973.38 975.07 975.32 976.64 994.85 998.67
1018.79 1021.82 1022.41 1030.32 1046.26 1049.99
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1093.24 1098.73 1101.15 1103.93 1107.24 1111.44
1128.78 1129.59 1132.63 1133.21 1136.54 1147.10
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1203.45 1206.12 1211.97 1217.01 1225.30 1236.55
1261.55 1285.29 1291.17 1293.97 1296.43 1301.25
1302.36 1304.37 1307.17 1309.42 1316.39 1318.23
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1400.56 1401.69 1411.84 1414.16 1415.67 1431.52
1433.74 1435.15 1455.08 1466.47 1474.41 1491.19
1494.34 1496.07 1496.44 1497.22 1499.01 1500.39
1501.57 1502.73 1503.42 1504.02 1505.01 1506.11
1507.59 1509.01 1510.56 1513.84 1516.93 1517.44
1518.65 1520.94 1522.00 1525.28 1527.29 1531.05
1585.73 1605.03 1610.74 1613.20 1644.08 1658.63
2997.13 3009.92 3011.48 3011.66 3013.51 3014.12
3017.19 3018.99 3021.91 3030.23 3031.82 3032.03

3033.48 3033.86 3035.59 3038.19 3039.02 3045.13
3050.89 3064.01 3065.62 3065.90 3067.23 3071.12
3073.55 3084.68 3086.65 3090.16 3092.02 3097.89
3098.50 3102.33 3103.97 3105.88 3107.80 3108.71
3111.67 3111.79 3115.23 3116.09 3121.00 3133.62
3140.16 3170.20 3171.92 3177.32 3178.31 3180.06
3188.03 3191.42 3201.84 3202.65 3218.19 3252.10

1-TS

-199.69 14.28 17.35 30.86 33.53 37.53
43.62 45.64 51.40 54.85 59.93 63.96
76.15 76.92 83.74 85.82 86.27 93.56
97.80 108.83 121.36 126.54 133.93 140.14
147.80 154.79 162.77 175.64 184.43 194.99
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279.51 282.02 287.60 293.21 302.42 312.29
331.11 333.70 340.91 360.05 379.27 383.33
393.19 419.38 423.51 430.30 434.51 449.25
449.38 451.07 456.68 480.38 488.95 500.62
516.36 524.86 533.96 540.87 563.40 587.83
609.76 614.79 624.89 640.80 645.99 662.46
673.78 691.05 729.88 736.62 747.79 748.87
770.47 779.12 786.30 809.02 817.11 824.81
828.11 829.48 834.30 856.18 868.79 871.63
878.33 895.47 900.89 900.98 903.82 907.59
908.95 910.31 911.88 941.54 944.41 945.49
945.73 946.62 956.37 962.95 965.38 973.07
974.44 975.14 977.40 979.79 984.25 999.96
1001.80 1018.92 1024.79 1027.49 1043.70 1049.20
1049.90 1060.88 1064.55 1072.83 1086.81 1095.01
1098.93 1099.47 1100.59 1103.30 1105.14 1113.35
1127.31 1128.69 1133.08 1135.36 1138.83 1149.03
1155.13 1162.98 1189.34 1189.51 1202.33 1203.35
1204.07 1205.71 1215.24 1217.19 1229.02 1244.42
1259.44 1286.71 1293.82 1297.19 1298.97 1300.15
1301.53 1305.14 1307.66 1310.02 1317.25 1319.09
1320.82 1333.92 1342.34 1347.75 1348.10 1349.81
1350.15 1359.46 1367.73 1369.61 1379.20 1379.94
1385.49 1388.99 1392.45 1393.95 1394.40 1397.83
1399.94 1402.49 1412.17 1413.57 1416.66 1431.56
1432.58 1436.83 1466.29 1470.32 1475.94 1487.53
1492.98 1494.34 1496.06 1498.35 1499.46 1500.15
1501.07 1501.63 1503.58 1504.23 1505.15 1505.99
1506.97 1507.90 1511.24 1514.09 1515.93 1517.03
1517.51 1520.95 1523.68 1524.49 1524.61 1526.74
1604.27 1609.22 1611.05 1611.54 1640.21 1658.29
3010.04 3012.73 3013.21 3014.81 3017.45 3018.94
3024.36 3027.23 3028.18 3031.73 3033.17 3033.62
3034.22 3037.56 3037.79 3039.94 3040.62 3043.75
3057.39 3064.53 3066.00 3067.77 3068.04 3072.57
3073.49 3080.44 3085.23 3091.31 3095.25 3099.95
3100.87 3101.25 3101.45 3107.32 3110.72 3113.57
3114.02 3119.14 3120.60 3123.01 3123.37 3127.52
3134.72 3164.10 3170.54 3177.18 3178.23 3185.96
3186.94 3193.77 3200.98 3206.37 3207.60 3211.25

1A

23.19	29.22	36.14	40.01	43.50	47.81
53.57	58.80	61.64	66.39	76.39	79.11
85.12	90.08	93.08	96.68	98.98	102.43
109.10	112.02	131.08	136.79	140.71	153.10
162.05	171.55	182.09	187.50	195.66	206.05
211.96	221.12	231.01	237.81	250.45	250.99
253.29	257.51	263.62	265.40	271.33	275.46
277.89	280.91	288.21	303.40	309.28	317.06
333.02	333.98	342.28	364.37	379.22	387.25
398.18	414.50	423.22	438.01	450.11	451.30
453.19	458.63	481.62	485.23	489.14	500.20
520.47	526.68	539.11	544.86	563.59	587.51
611.37	623.53	638.01	652.34	664.53	672.67
679.51	709.27	733.64	745.27	747.57	755.45
769.15	779.06	786.47	808.40	820.15	827.05
829.53	833.67	849.96	856.93	867.98	872.83
895.71	899.99	903.35	904.46	907.93	909.92
911.40	912.09	919.35	940.24	946.36	946.87
949.02	949.45	957.30	965.22	972.06	974.58
975.41	975.82	977.68	989.21	1003.35	1009.07
1018.86	1026.44	1028.84	1041.45	1044.26	1048.02
1064.88	1067.12	1073.98	1084.76	1089.11	1094.28
1097.87	1099.33	1103.21	1104.99	1107.40	1113.29
1125.93	1128.77	1132.50	1137.86	1143.15	1152.81
1158.09	1164.12	1190.74	1191.67	1203.26	1204.07
1206.64	1210.58	1216.59	1217.83	1239.50	1250.20
1259.24	1287.22	1293.28	1298.14	1300.05	1301.40
1306.50	1307.22	1309.55	1313.51	1318.07	1320.00
1328.89	1336.81	1342.09	1346.69	1346.93	1349.85
1350.86	1360.10	1368.29	1370.00	1377.86	1382.18
1385.23	1390.32	1393.68	1395.05	1395.51	1398.57
1401.74	1402.84	1414.90	1415.64	1416.61	1435.06
1436.02	1438.07	1467.12	1467.78	1477.35	1490.47
1492.04	1496.70	1498.64	1500.07	1500.96	1501.91
1502.35	1503.54	1504.11	1505.10	1505.59	1506.90
1507.33	1511.73	1512.51	1514.61	1515.85	1516.85
1516.98	1520.64	1523.66	1525.01	1526.12	1529.18
1599.52	1612.78	1619.08	1622.72	1641.96	1657.21
3009.84	3014.14	3015.83	3018.56	3022.43	3025.17
3026.82	3033.10	3033.27	3034.49	3035.11	3035.85
3037.37	3038.90	3039.67	3040.00	3048.40	3058.17
3067.37	3070.81	3071.02	3073.44	3075.17	3077.27
3077.67	3086.15	3088.70	3089.36	3098.90	3103.24
3104.06	3106.06	3107.10	3109.19	3111.23	3112.11
3112.50	3119.37	3121.28	3126.72	3128.78	3140.44
3149.73	3164.91	3171.87	3180.78	3187.69	3189.05
3191.23	3192.71	3197.11	3201.63	3203.56	3214.23

1B

14.64	26.84	34.98	37.72	40.94	45.23
50.88	56.16	66.61	69.64	73.31	78.75
83.73	86.86	93.29	96.25	99.55	104.15
107.45	110.97	127.27	137.72	149.73	153.82
171.35	180.77	190.09	192.29	196.68	209.20
219.69	221.29	229.76	240.48	243.05	246.94

250.69	254.20	263.57	265.84	269.99	273.43
278.67	285.88	290.03	301.54	308.13	312.79
333.88	337.54	341.13	364.30	379.49	382.89
389.63	411.36	426.43	438.44	446.92	450.01
452.43	473.65	485.93	488.58	497.17	500.18
509.50	533.06	535.92	547.44	559.75	588.83
608.52	625.11	642.13	653.86	667.16	669.69
672.45	707.21	726.39	749.15	750.76	755.14
772.89	788.40	798.32	807.25	814.41	823.10
828.78	833.31	850.72	857.14	865.74	868.50
896.96	899.34	903.90	904.88	906.36	907.88
915.84	916.76	919.86	933.88	945.44	946.93
947.37	948.54	955.70	965.78	973.82	975.07
975.63	978.71	988.36	995.17	1006.34	1009.07
1019.78	1024.16	1030.46	1039.27	1044.55	1050.36
1051.96	1057.85	1064.34	1079.91	1086.80	1092.22
1097.26	1102.00	1104.18	1105.84	1109.63	1119.46
1126.86	1129.65	1131.60	1135.82	1141.05	1148.20
1148.83	1163.39	1190.10	1194.54	1204.67	1205.71
1206.12	1212.20	1219.16	1220.77	1231.75	1246.55
1265.35	1284.62	1289.25	1292.91	1299.00	1300.42
1302.70	1304.97	1306.79	1309.83	1309.98	1323.70
1325.64	1331.83	1342.83	1352.86	1353.81	1356.34
1359.83	1361.77	1362.75	1369.39	1376.87	1383.31
1387.80	1391.41	1394.03	1395.62	1400.48	1402.17
1402.97	1408.41	1413.63	1416.22	1417.09	1435.40
1436.68	1437.68	1458.98	1462.33	1476.12	1495.57
1496.70	1497.91	1498.49	1499.01	1500.61	1501.53
1502.10	1504.07	1504.76	1506.65	1507.73	1508.27
1509.60	1511.54	1513.20	1517.84	1518.36	1521.50
1522.20	1523.81	1524.67	1525.37	1528.68	1530.41
1611.08	1613.56	1616.01	1619.63	1641.64	1659.31
3004.23	3008.13	3017.74	3023.65	3025.48	3029.90
3032.37	3035.97	3036.57	3036.81	3038.88	3039.92
3041.63	3045.16	3048.07	3052.68	3058.90	3065.23
3069.56	3070.64	3071.16	3074.47	3078.08	3081.18
3083.84	3085.28	3101.16	3104.01	3105.21	3107.04
3108.89	3110.17	3112.80	3116.69	3117.17	3117.55
3118.07	3122.19	3123.45	3129.30	3134.47	3162.83
3166.55	3173.89	3175.49	3178.93	3182.65	3185.76
3186.25	3186.75	3196.23	3198.47	3209.41	3216.67

1C

14.73	18.82	23.36	32.66	39.99	43.65
54.70	57.32	63.23	68.01	72.20	78.20
80.47	84.73	91.57	92.98	100.86	102.91
105.89	110.16	117.94	121.35	129.41	140.92
152.98	163.54	166.60	173.97	182.52	190.05
200.86	203.93	217.27	221.37	224.82	232.98
233.85	240.64	247.30	251.99	255.83	266.53
269.35	272.21	280.99	283.81	284.96	295.66
304.61	309.44	315.16	336.66	342.33	353.01
359.09	378.57	384.35	392.90	413.90	415.33
425.79	435.93	453.01	455.00	457.78	463.50
484.58	488.14	496.00	504.35	522.18	537.10
544.27	548.57	562.71	588.68	603.55	608.50
627.92	645.02	652.19	653.97	663.93	667.28

672.06 716.98 733.07 752.97 757.37 758.00
769.39 789.98 798.30 810.21 821.87 827.11
828.60 833.86 855.99 856.93 868.32 873.94
893.66 901.83 904.97 907.44 908.42 909.01
911.00 912.94 916.20 940.70 944.85 946.31
947.67 949.99 957.17 963.63 971.95 974.33
974.80 977.89 992.97 995.35 1008.47 1011.85
1020.75 1026.32 1029.11 1039.57 1046.18 1047.09
1060.80 1063.14 1073.02 1082.40 1088.45 1092.07
1094.12 1098.56 1102.80 1106.30 1108.83 1115.07
1123.26 1129.01 1133.19 1135.87 1145.07 1149.10
1149.47 1158.56 1165.67 1191.06 1191.60 1203.15
1204.51 1208.07 1216.41 1217.66 1219.38 1241.55
1256.50 1263.72 1285.74 1293.77 1295.71 1296.85
1300.27 1301.39 1309.05 1310.18 1311.43 1316.78
1319.99 1326.82 1337.08 1343.61 1349.17 1349.63
1351.20 1355.73 1363.95 1366.14 1368.38 1377.05
1378.29 1382.36 1390.30 1392.86 1394.68 1395.16
1398.01 1398.94 1403.86 1413.33 1415.36 1416.19
1434.92 1436.26 1437.57 1461.49 1463.27 1476.09
1492.21 1495.30 1497.58 1498.64 1499.25 1501.18
1501.53 1502.35 1503.30 1504.86 1505.96 1506.11
1507.58 1508.93 1510.16 1515.08 1518.41 1518.71
1521.48 1522.60 1524.08 1524.91 1526.44 1528.57
1529.28 1611.03 1613.90 1616.05 1622.64 1646.85
1651.95 1661.20 1661.23 3008.09 3012.43 3019.59
3019.73 3024.57 3032.29 3032.42 3033.29 3033.64
3034.42 3035.47 3037.72 3038.60 3039.69 3040.90
3045.67 3047.95 3064.03 3064.88 3065.56 3069.60
3070.78 3074.56 3079.48 3080.73 3091.18 3096.00
3103.06 3103.94 3104.78 3106.26 3110.77 3111.07
3113.70 3114.37 3114.55 3118.31 3118.81 3121.37
3128.06 3146.98 3151.93 3153.91 3165.13 3165.64
3173.70 3175.32 3178.48 3188.87 3193.07 3199.21
3207.47 3210.57 3217.42 3458.66 3597.08 3618.16

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14.17 17.18 26.44 28.92 30.66 38.45
41.11 45.72 53.11 58.14 60.81 63.57
70.49 75.39 75.85 81.56 84.64 89.11
92.59 100.68 106.48 110.55 116.09 117.06
123.79 138.58 146.90 151.79 162.78 168.51
172.04 184.14 193.46 199.79 205.93 220.34
226.63 232.41 234.16 243.09 244.12 249.33
254.11 257.15 264.65 269.03 276.35 278.51
281.68 285.91 291.57 303.33 307.63 316.39
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 3177.66 3181.59 3182.99 3183.72 3188.47 3194.26
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 901.65 901.83 907.03 907.49 908.69 910.33

913.20	913.89	919.15	920.00	923.80	940.83	117.91	123.13	128.04	129.01	137.22	139.53
943.44	946.07	946.40	946.91	949.06	949.54	148.28	151.52	153.97	156.89	161.42	166.14
949.61	951.60	953.51	962.68	970.58	973.39	166.41	174.13	180.81	183.11	188.90	192.05
974.52	975.07	978.92	986.78	993.31	994.31	196.75	200.09	213.03	215.38	223.01	224.28
998.04	1001.48	1005.58	1010.99	1014.55	1025.60	224.48	227.45	235.23	235.62	238.75	242.16
1027.57	1040.80	1041.58	1041.84	1042.53	1042.66	245.37	246.02	246.95	248.08	249.17	252.27
1044.10	1044.46	1045.19	1048.23	1048.84	1059.12	254.72	255.66	256.32	259.35	262.82	266.18
1061.05	1063.37	1070.08	1086.36	1086.84	1092.36	269.19	270.24	271.41	278.36	280.28	283.79
1094.31	1097.82	1103.22	1105.35	1110.24	1115.87	285.97	288.82	291.90	299.49	300.56	301.88
1126.56	1129.39	1131.42	1136.19	1146.35	1153.03	305.97	309.30	309.38	311.89	312.85	320.76
1154.03	1163.66	1188.51	1192.34	1202.82	1204.77	333.95	336.29	341.79	362.42	363.10	365.29
1206.75	1214.53	1215.35	1218.56	1226.99	1231.89	365.89	368.98	370.67	373.06	374.20	376.81
1233.69	1239.15	1241.17	1241.52	1241.96	1242.41	380.70	384.51	391.76	410.48	418.42	422.93
1243.49	1243.95	1250.78	1251.68	1252.30	1260.59	426.89	434.76	443.23	445.93	450.98	452.19
1262.22	1270.64	1286.56	1292.85	1296.67	1297.44	457.01	457.65	460.38	466.83	478.43	483.61
1301.30	1302.89	1308.16	1310.33	1311.34	1314.96	486.92	489.68	494.86	496.52	497.51	498.49
1324.05	1327.09	1336.11	1342.76	1350.37	1351.97	499.04	502.15	502.98	507.26	508.08	514.34
1353.37	1360.40	1362.87	1366.93	1368.99	1380.46	528.69	535.45	545.13	561.29	567.32	568.47
1381.83	1385.89	1389.29	1390.42	1391.73	1393.76	591.40	608.28	626.09	634.27	641.81	653.60
1393.98	1394.47	1394.75	1395.13	1396.39	1398.48	666.88	671.75	672.99	712.82	715.02	727.34
1399.14	1399.39	1401.60	1401.81	1414.39	1415.44	748.30	748.87	750.00	752.66	753.87	754.05
1416.51	1416.99	1419.06	1419.91	1427.37	1434.38	756.19	773.81	778.62	781.51	799.36	807.75
1435.12	1436.68	1437.46	1460.84	1465.40	1475.22	811.04	825.48	827.59	832.93	833.24	838.58
1485.29	1486.10	1486.99	1487.29	1487.68	1488.11	853.30	856.93	866.13	869.25	887.09	888.43
1488.56	1490.66	1492.07	1493.01	1494.30	1495.50	891.54	892.59	892.69	893.60	895.10	895.41
1497.08	1498.56	1499.45	1499.99	1500.55	1500.74	896.20	898.14	900.61	902.28	905.16	909.02
1502.42	1503.03	1503.71	1504.86	1505.62	1505.75	910.25	911.75	912.71	920.89	927.96	935.08
1506.67	1507.97	1508.24	1508.58	1509.05	1509.31	935.35	943.54	946.64	947.23	949.36	949.60
1509.68	1510.47	1511.63	1512.69	1514.55	1517.72	949.86	951.61	956.44	963.42	965.88	970.28
1518.27	1518.55	1519.15	1520.15	1520.97	1522.31	973.61	974.47	975.25	977.27	981.30	982.80
1522.73	1523.75	1525.45	1526.95	1528.42	1531.87	985.92	988.61	998.91	999.24	1005.98	1008.62
1535.64	1561.31	1611.87	1613.24	1617.86	1621.93	1010.02	1021.54	1025.17	1028.78	1040.80	1042.28
1643.37	1647.22	1659.70	2086.12	2998.64	3000.57	1043.35	1043.85	1043.95	1044.10	1045.89	1046.72
3001.51	3005.57	3006.64	3007.59	3008.88	3009.55	1048.86	1052.00	1056.68	1057.11	1058.36	1060.07
3011.70	3016.21	3017.27	3017.35	3019.78	3022.81	1064.59	1085.56	1086.71	1092.97	1095.34	1098.84
3024.42	3027.44	3027.86	3031.30	3032.82	3034.69	1102.88	1104.20	1106.36	1106.93	1110.89	1125.55
3035.47	3037.54	3038.31	3038.46	3039.26	3040.10	1129.89	1131.87	1134.92	1141.95	1147.45	1148.74
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3067.06	3067.67	3067.83	3070.58	3071.51	3072.38	1204.54	1205.51	1208.50	1210.67	1212.70	1218.49
3073.82	3075.21	3076.31	3076.65	3077.48	3078.32	1222.52	1229.94	1234.17	1237.34	1238.62	1241.30
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3092.31	3092.39	3094.34	3098.43	3098.95	3099.19	1255.06	1265.72	1266.65	1274.66	1284.52	1288.42
3100.67	3101.63	3102.38	3102.58	3105.69	3108.41	1289.32	1291.92	1297.83	1300.50	1303.53	1304.79
3110.58	3111.36	3112.10	3112.92	3113.34	3114.98	1307.32	1311.16	1311.55	1317.30	1328.93	1331.75
3115.34	3115.82	3116.66	3118.16	3119.94	3123.59	1341.73	1350.37	1353.32	1356.25	1360.62	1362.03
3127.23	3130.18	3130.70	3131.80	3145.48	3156.29	1363.66	1363.90	1369.14	1378.05	1380.60	1386.02
3163.28	3175.94	3176.67	3181.13	3187.25	3187.37	1390.81	1392.30	1394.32	1395.64	1396.32	1396.56
3187.74	3193.97	3200.85	3230.27	3439.91	3539.81	1397.35	1398.03	1398.08	1400.07	1400.84	1401.71
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10.65	15.86	19.22	21.53	22.84	24.13	1436.66	1445.38	1459.40	1466.00	1475.83	1479.89
24.80	27.82	29.58	35.38	35.50	37.86	1481.74	1484.67	1485.92	1486.35	1487.45	1487.72
41.36	44.23	45.57	48.28	50.24	53.01	1488.99	1490.23	1491.32	1491.81	1493.77	1495.11
54.94	57.70	60.78	61.64	66.30	69.45	1495.66	1496.15	1496.65	1498.61	1499.32	1500.37
71.39	75.07	75.95	79.64	83.40	84.93	1501.24	1502.69	1502.81	1504.25	1505.10	1506.87
87.07	88.47	90.78	93.25	95.08	96.06	1507.03	1507.68	1508.08	1508.58	1508.73	1509.20
98.35	98.87	102.21	105.99	109.57	112.45	1509.89	1510.52	1510.99	1512.32	1513.19	1515.22
						1516.02	1518.13	1518.17	1519.56	1520.14	1520.69

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811.89 824.02 826.12 833.98 857.13 858.43
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891.39 891.84 892.24 894.65 900.69 900.90
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1401.81 1412.74 1414.98 1415.65 1417.39 1421.57
1422.76 1433.52 1436.48 1437.11 1455.63 1464.19
1475.13 1483.06 1484.65 1486.96 1487.58 1487.74
1489.99 1491.61 1492.20 1493.60 1494.71 1495.99
1497.19 1497.91 1498.59 1499.33 1500.46 1501.16
1502.79 1503.43 1505.09 1505.53 1506.49 1506.95
1507.06 1507.77 1508.14 1508.35 1509.47 1510.92
1511.95 1513.01 1513.22 1514.04 1515.96 1517.55
1518.14 1519.29 1520.43 1522.75 1524.95 1525.08
1526.78 1527.57 1529.53 1530.27 1597.93 1613.11
1615.16 1618.76 1622.80 1631.87 1649.43 1658.93
2997.18 2997.65 3008.78 3009.60 3009.95 3013.17
3013.89 3014.19 3014.62 3017.02 3020.72 3021.35
3023.56 3029.15 3031.26 3032.34 3032.61 3035.31
3035.54 3038.50 3039.23 3040.98 3042.65 3046.14
3054.37 3058.18 3063.28 3065.18 3065.79 3067.99
3070.81 3071.46 3073.28 3074.84 3076.16 3078.16
3079.46 3079.77 3080.86 3081.50 3083.28 3083.49
3085.83 3088.93 3090.11 3091.88 3093.17 3096.06
3101.45 3101.86 3103.12 3103.16 3103.74 3104.56
3107.77 3108.47 3109.27 3112.13 3114.06 3115.86
3116.57 3117.07 3117.56 3120.02 3122.93 3124.26
3125.88 3139.68 3141.20 3158.30 3158.85 3163.69
3165.02 3165.61 3174.57 3175.98 3177.00 3179.34
3185.03 3187.66 3189.28 3194.95 3195.82 3196.73
3203.97 3206.68 3504.19

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1G

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17.59 27.17 35.12 38.80 43.05 46.00
51.67 60.34 63.53 67.16 70.79 75.22
78.81 85.55 88.44 95.69 98.15 103.61
114.49 128.30 137.36 141.63 148.42 152.73
158.01 172.78 175.31 181.73 191.07 198.26
201.73 216.03 227.04 240.67 245.91 249.17
253.95 261.78 264.14 266.41 268.89 270.58
274.95 282.70 284.55 290.89 302.98 312.74
330.55 335.43 341.22 363.06 380.41 383.99
389.00 414.55 417.29 435.12 447.45 451.98
452.84 466.21 474.74 486.43 490.45 499.81
509.33 529.71 535.09 546.56 558.25 559.62
590.06 608.06 625.30 641.84 653.43 667.01
668.01 672.60 707.42 726.23 733.66 749.49
753.04 754.87 775.12 781.72 787.81 799.80
808.41 810.82 826.11 827.41 833.15 854.93
856.82 867.07 869.18 896.59 900.60 902.61
903.65 907.04 908.65 911.73 912.39 913.31
934.48 941.31 945.79 946.95 948.91 955.66
964.71 971.62 973.38 975.08 979.37 985.33
990.29 1004.08 1008.92 1021.03 1023.85 1028.55
1039.61 1046.33 1049.16 1059.27 1060.62 1064.40
1082.91 1086.86 1094.20 1096.37 1100.49 1104.19
1105.55 1109.18 1109.53 1126.66 1129.42 1131.52
1135.59 1137.93 1146.44 1148.52 1163.22 1189.75
1192.71 1203.32 1205.87 1208.85 1211.24 1216.85
1218.75 1231.56 1242.41 1265.45 1283.94 1289.98
1292.16 1297.87 1300.26 1305.00 1306.00 1307.36
1309.38 1314.07 1314.32 1329.73 1333.63 1342.68
1351.76 1352.68 1354.12 1359.77 1361.81 1364.42
1369.60 1378.26 1382.34 1382.76 1390.48 1391.68
1392.44 1396.07 1397.84 1401.38 1401.90 1412.74
1415.77 1417.16 1434.88 1436.34 1437.28 1459.72
1464.85 1475.55 1494.01 1494.44 1496.32 1498.15
1498.97 1500.21 1500.46 1500.92 1502.39 1503.91
1505.19 1506.46 1507.16 1507.68 1508.15 1511.11
1517.74 1518.41 1520.53 1521.61 1522.68 1523.77
1524.55 1525.40 1529.91 1572.77 1613.49 1613.93
1618.72 1620.12 1643.82 1658.83 3011.76 3013.14
3014.82 3019.25 3020.08 3023.40 3023.84 3029.65
3033.48 3034.89 3035.64 3036.04 3037.04 3038.01
3038.64 3040.59 3044.57 3058.40 3066.22 3069.14
3069.44 3071.04 3071.22 3073.61 3076.12 3080.46
3092.94 3100.65 3102.38 3102.61 3106.87 3108.68
3109.02 3110.49 3116.03 3116.39 3119.52 3121.46
3126.14 3130.47 3134.64 3146.03 3161.58 3165.37
3166.22 3169.93 3179.38 3179.89 3181.13 3185.45
3191.73 3194.17 3204.31 3223.83 3446.22 3533.41

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1G'

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12.35 23.17 28.05 33.35 36.68 42.00
44.65 49.09 55.16 57.37 69.10 72.55
73.65 78.25 80.75 86.32 89.14 93.22
94.91 100.54 101.99 114.43 126.68 136.86

138.40	148.82	152.33	157.59	173.70	180.25
188.74	192.45	198.98	212.79	216.31	227.69
241.00	245.47	246.45	249.47	253.81	257.98
265.02	268.40	269.05	271.31	274.23	282.54
291.48	301.54	312.25	331.45	335.04	340.31
363.51	380.24	382.83	389.03	390.07	412.49
420.81	429.27	436.10	447.45	451.36	452.19
469.71	472.58	485.64	488.71	492.49	498.49
509.11	531.31	532.90	536.21	546.38	548.56
558.38	589.10	607.47	625.69	630.03	640.78
653.37	665.98	666.95	672.31	708.06	712.40
731.83	745.67	752.75	755.09	770.22	775.18
784.18	799.67	799.88	808.65	812.27	826.30
828.39	831.54	832.42	854.13	856.35	859.50
867.31	869.35	870.27	896.15	901.01	901.41
902.55	905.31	908.81	912.42	913.39	913.41
934.49	942.90	946.04	946.91	948.80	955.19
962.58	963.89	973.54	974.10	974.85	978.12
981.11	981.76	992.02	994.65	1003.28	1009.08
1019.04	1024.24	1029.23	1039.07	1043.31	1046.15
1049.69	1057.28	1060.31	1064.91	1082.95	1086.25
1092.73	1093.72	1097.02	1100.09	1104.04	1105.54
1109.44	1112.13	1126.30	1129.56	1131.27	1135.18
1140.58	1147.82	1148.85	1162.86	1175.07	1189.67
1191.77	1192.45	1201.00	1203.85	1205.55	1208.75
1211.20	1217.20	1218.58	1233.61	1243.77	1264.82
1284.06	1289.57	1291.71	1298.39	1299.98	1304.67
1306.47	1307.83	1311.03	1312.73	1316.04	1324.02
1330.21	1332.70	1342.92	1352.32	1352.87	1354.58
1355.05	1360.60	1361.31	1363.96	1370.29	1372.43
1377.77	1382.19	1385.11	1391.31	1392.81	1395.05
1396.59	1398.54	1401.61	1402.30	1413.63	1415.76
1417.13	1435.33	1436.23	1437.47	1459.72	1464.80
1475.68	1492.54	1494.93	1496.28	1496.89	1498.47
1499.00	1500.45	1500.82	1501.52	1503.84	1504.17
1505.55	1506.84	1507.22	1508.18	1508.72	1511.65
1514.18	1517.91	1518.43	1520.63	1521.82	1522.85
1523.83	1524.91	1525.77	1529.42	1598.48	1612.61
1613.69	1618.53	1620.05	1643.66	1645.48	1658.91
3011.39	3013.16	3014.02	3023.47	3029.71	3032.01
3033.97	3035.24	3035.39	3035.66	3036.71	3037.32
3038.53	3038.73	3040.32	3043.55	3043.85	3055.74
3066.01	3066.47	3067.08	3071.02	3071.43	3079.50
3080.26	3080.60	3097.39	3099.79	3102.37	3102.66
3104.62	3105.56	3108.86	3110.15	3115.61	3116.31
3118.59	3121.50	3126.01	3127.81	3131.18	3157.05
3157.63	3163.90	3165.03	3166.26	3169.67	3171.60
3176.08	3178.45	3180.36	3181.98	3182.08	3185.47
3190.84	3192.78	3202.67	3205.23	3210.23	3495.02

1H

22.18	32.19	39.03	44.40	48.38	49.97
55.18	58.96	64.49	66.46	73.46	78.21
83.67	85.75	90.78	93.77	95.11	100.06
112.55	124.96	139.93	140.68	147.98	150.44
164.98	169.80	178.18	182.99	185.18	195.44
211.62	217.01	224.94	232.12	236.85	248.38

253.94	255.12	257.16	267.29	268.96	274.14
277.25	278.44	283.81	289.80	298.19	316.24
331.98	335.26	341.69	362.02	381.64	383.61
398.14	412.87	421.94	432.76	450.65	451.98
452.07	457.44	480.12	485.27	489.84	499.81
511.26	519.55	524.63	538.59	544.03	563.63
589.40	608.99	626.13	639.27	648.95	660.04
670.29	678.72	715.96	731.56	745.42	748.29
753.47	771.23	779.49	786.34	787.36	809.19
817.99	827.55	829.07	834.57	845.52	857.75
860.41	869.23	872.59	895.12	901.69	901.92
905.16	907.30	909.92	910.52	911.29	914.99
941.43	945.26	945.97	947.51	951.79	959.82
965.33	973.19	974.42	974.91	975.45	979.52
989.90	1003.89	1009.08	1019.58	1026.80	1028.95
1041.34	1044.32	1049.01	1064.32	1064.94	1074.17
1086.41	1089.43	1094.96	1096.04	1098.59	1101.87
1104.68	1107.56	1113.69	1127.29	1128.21	1133.31
1138.50	1142.25	1151.30	1157.41	1164.08	1191.15
1192.25	1203.30	1203.96	1206.34	1211.84	1216.80
1218.95	1238.15	1249.09	1262.04	1288.67	1291.95
1298.52	1299.89	1301.11	1306.51	1307.13	1309.41
1310.49	1313.32	1320.48	1326.83	1336.60	1342.40
1347.51	1347.58	1348.64	1349.65	1360.61	1368.62
1370.08	1378.01	1382.96	1387.05	1390.31	1393.21
1395.25	1395.46	1398.95	1401.46	1403.09	1412.79
1414.13	1414.57	1431.90	1433.93	1434.46	1464.36
1468.14	1479.24	1491.98	1493.05	1495.06	1497.83
1499.89	1501.42	1501.56	1501.85	1503.86	1504.22
1505.08	1505.40	1506.56	1507.50	1508.80	1512.39
1514.32	1515.33	1516.06	1517.04	1520.99	1523.99
1525.27	1528.00	1529.15	1573.81	1605.80	1612.27
1615.67	1619.92	1642.16	1660.70	3008.99	3013.08
3014.90	3016.99	3020.67	3023.96	3026.03	3027.07
3028.25	3029.63	3033.57	3034.10	3034.84	3036.24
3039.48	3040.57	3043.16	3053.58	3064.94	3067.46
3068.35	3070.27	3072.98	3074.57	3075.38	3081.43
3085.87	3091.61	3095.30	3099.24	3101.47	3103.19
3104.67	3104.75	3109.42	3111.08	3113.21	3119.98
3124.00	3125.19	3131.85	3132.19	3139.57	3158.71
3164.28	3175.66	3178.34	3179.14	3183.25	3189.73
3190.44	3195.92	3201.64	3212.05	3420.13	3504.96

1H'

10.70	15.64	27.63	33.35	38.85	41.34
47.51	52.87	57.15	58.53	62.55	64.81
70.63	75.05	78.63	81.32	89.49	95.37
98.74	101.62	102.02	114.62	135.03	138.39
143.15	149.95	157.03	161.10	166.76	183.00
188.31	198.91	204.97	208.65	215.28	228.80
232.29	240.73	248.29	251.33	255.18	257.68
265.47	266.28	276.53	279.75	284.62	290.64
301.78	306.10	319.62	328.07	334.80	338.45
341.02	366.11	382.22	385.17	397.59	415.27
424.05	425.68	435.43	450.14	452.69	454.25
457.13	480.93	485.60	486.19	490.61	501.23
519.51	526.01	536.77	545.36	551.22	562.53

587.90 592.37 608.93 624.96 635.95 637.48
648.47 659.02 670.06 679.37 704.66 712.21
731.84 736.26 746.67 753.10 754.65 765.70
772.29 777.36 786.53 811.17 819.21 826.98
828.74 830.37 833.12 849.67 856.29 857.28
870.05 872.96 874.35 894.96 900.80 901.64
904.27 908.03 909.31 911.54 914.43 914.93
941.69 944.09 946.26 947.17 947.64 949.52
956.56 961.35 969.42 973.87 974.01 975.26
976.17 980.02 990.95 1004.23 1004.67 1009.48
1019.82 1026.92 1029.95 1040.64 1044.45 1047.88
1052.38 1063.30 1065.95 1074.44 1084.52 1087.66
1094.65 1097.25 1099.62 1100.90 1103.67 1105.02
1106.58 1113.01 1127.26 1128.28 1132.86 1137.13
1143.01 1152.68 1157.34 1163.64 1185.68 1190.88
1190.91 1203.14 1203.57 1206.17 1206.95 1214.40
1216.17 1217.50 1235.09 1244.23 1251.29 1260.75
1286.62 1290.11 1295.66 1296.66 1301.74 1306.15
1306.48 1308.71 1314.35 1315.57 1317.48 1319.31
1325.83 1337.25 1341.65 1346.00 1349.20 1351.30
1352.02 1362.70 1363.64 1368.33 1370.64 1377.27
1383.22 1385.08 1385.55 1390.18 1393.75 1395.11
1395.56 1399.12 1401.86 1403.61 1414.16 1415.20
1416.68 1433.93 1435.12 1437.64 1465.48 1468.11
1477.77 1489.97 1493.55 1497.81 1499.51 1500.26
1501.03 1501.33 1502.05 1504.07 1504.83 1504.84
1505.22 1506.48 1507.96 1508.43 1512.12 1512.72
1513.32 1516.60 1516.83 1516.98 1522.05 1523.91
1524.77 1527.37 1529.13 1532.42 1602.08 1612.07
1617.56 1618.26 1620.96 1641.62 1650.64 1656.76
3009.33 3013.77 3014.62 3017.46 3021.23 3022.57
3025.39 3028.39 3031.67 3032.50 3033.75 3035.68
3037.73 3038.19 3040.97 3042.08 3044.99 3046.01
3062.71 3068.88 3069.17 3070.23 3072.54 3075.15
3075.88 3087.00 3087.74 3091.65 3098.03 3099.43
3101.45 3102.74 3105.55 3108.28 3109.71 3112.08
3113.78 3118.23 3118.67 3121.82 3122.55 3144.66
3151.92 3158.43 3160.13 3164.63 3167.02 3172.73
3178.51 3179.95 3180.67 3185.70 3187.36 3190.07
3195.22 3197.12 3201.70 3213.19 3255.78 3503.21

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1H-TS
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-435.66 14.58 20.66 38.00 41.54 44.59
46.53 51.82 55.50 60.97 65.76 68.63
76.73 81.78 82.62 84.71 92.88 96.64
103.08 112.45 135.61 141.42 145.29 151.07
154.03 166.16 175.79 184.52 185.04 199.63
215.92 232.22 235.70 249.77 252.98 254.42
254.68 256.74 259.06 267.09 273.50 276.43
278.40 284.74 290.38 297.05 313.13 331.99
334.66 340.65 360.95 380.05 381.83 394.99
411.23 421.91 427.34 431.01 449.78 451.38
452.74 457.48 459.59 464.43 483.55 489.70
500.62 518.15 525.52 534.71 543.00 563.24
590.21 608.02 620.61 626.59 641.82 645.35
646.00 662.65 677.70 708.02 731.30 738.32
748.34 752.07 770.72 781.43 787.64 808.74

813.96 818.12 826.82 829.93 834.74 845.21
857.38 860.62 869.44 873.21 895.54 901.44
902.16 904.76 908.21 909.79 911.66 911.77
941.32 944.68 945.76 946.88 949.20 958.48
958.73 965.40 972.83 974.16 974.50 974.80
980.06 994.72 1002.82 1004.32 1020.44 1026.70
1028.95 1044.14 1048.96 1051.75 1063.61 1064.29
1073.65 1087.87 1095.25 1098.68 1099.87 1101.32
1103.82 1107.05 1113.46 1127.34 1130.09 1132.65
1136.73 1141.46 1150.55 1156.41 1163.79 1188.11
1191.12 1203.28 1203.74 1205.74 1206.43 1215.89
1218.81 1235.09 1247.67 1262.56 1287.25 1293.63
1297.20 1298.51 1300.12 1303.66 1306.00 1308.81
1312.09 1318.73 1319.91 1322.07 1334.37 1342.32
1348.86 1349.83 1352.25 1355.83 1359.67 1367.89
1369.56 1379.17 1381.21 1385.89 1390.15 1392.58
1394.29 1394.93 1398.56 1400.41 1403.41 1412.39
1413.32 1415.73 1431.55 1432.61 1435.30 1468.08
1471.77 1476.55 1488.37 1492.11 1493.65 1495.36
1497.72 1499.39 1500.68 1501.21 1501.68 1503.80
1504.64 1504.98 1505.87 1506.94 1507.89 1512.39
1514.43 1515.67 1516.77 1517.07 1520.56 1524.10
1524.94 1525.43 1527.95 1554.84 1600.58 1611.35
1611.87 1619.74 1642.56 1659.85 3007.64 3011.11
3014.55 3016.29 3019.56 3022.64 3023.34 3025.27
3027.38 3031.78 3032.14 3033.17 3034.15 3035.66
3038.73 3038.86 3040.70 3050.68 3062.14 3064.87
3066.58 3067.91 3071.49 3072.94 3075.70 3076.42
3085.23 3086.56 3099.48 3100.65 3101.12 3101.61
3101.95 3106.07 3109.43 3111.65 3113.06 3116.96
3121.19 3121.88 3121.93 3125.53 3130.26 3157.76
3162.53 3175.15 3176.72 3178.66 3184.01 3186.89
3188.09 3200.04 3200.89 3212.59 3556.76 3670.61

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1H'-TS
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-373.87 14.88 20.58 24.03 33.58 35.98
37.48 46.43 52.08 59.37 64.75 65.19
73.08 77.44 78.02 81.54 84.37 88.97
92.43 95.26 97.84 109.91 119.67 138.88
142.91 143.56 150.49 152.05 165.02 170.40
184.36 186.15 197.62 215.01 224.50 229.74
234.35 240.77 245.66 251.58 252.80 256.58
258.39 266.18 274.50 276.40 281.80 286.77
289.64 290.54 298.80 314.53 331.93 336.02
341.02 361.77 381.47 383.16 395.10 423.93
424.63 429.09 432.11 449.44 450.93 452.20
453.24 457.35 483.70 489.71 500.53 515.82
518.82 525.53 535.07 541.97 549.11 561.92
585.30 591.45 608.86 620.19 633.06 638.05
641.06 646.46 664.42 678.79 699.35 708.92
726.75 731.34 747.57 753.46 769.95 770.86
782.45 784.70 786.79 808.35 818.26 826.00
829.20 829.84 834.76 839.09 856.90 860.00
866.28 869.27 872.88 893.38 895.35 901.70
903.39 904.49 908.42 908.96 910.96 915.72
941.81 944.30 944.95 946.49 947.49 957.66
958.23 959.23 964.44 974.12 974.55 975.56

976.29 980.10 980.50 997.18 1001.66 1003.30
 1010.41 1021.49 1026.12 1029.22 1043.60 1049.26
 1052.86 1054.37 1063.39 1066.44 1072.80 1088.31
 1094.32 1098.62 1101.57 1101.69 1103.63 1106.49
 1110.58 1113.57 1127.88 1128.47 1133.39 1136.81
 1141.08 1151.27 1157.35 1164.32 1188.29 1190.07
 1190.67 1203.24 1203.52 1205.50 1207.71 1211.10
 1215.61 1218.14 1232.59 1248.58 1258.02 1262.64
 1287.03 1292.73 1296.84 1298.20 1300.50 1303.44
 1305.47 1306.31 1308.35 1312.63 1319.57 1321.09
 1324.01 1334.87 1341.43 1344.95 1350.66 1351.42
 1354.09 1362.78 1365.99 1367.81 1369.51 1379.68
 1380.85 1385.93 1389.06 1391.39 1392.70 1394.42
 1395.17 1398.42 1400.56 1402.79 1413.05 1413.69
 1415.72 1432.71 1433.02 1436.22 1467.92 1469.29
 1475.85 1490.70 1493.19 1494.33 1496.97 1498.33
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II

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45.71 46.80 50.19 55.44 61.11 64.53
69.09 72.21 74.06 76.69 81.53 82.26
84.47 90.70 94.36 95.22 99.64 102.72
105.70 109.99 112.01 120.31 122.15 126.36
133.19 135.64 138.01 140.93 148.73 149.09
152.60 156.11 157.11 158.81 162.30 167.80
178.72 185.30 187.16 187.80 190.12 192.13
202.86 210.19 212.95 218.51 219.63 222.52
225.72 228.48 230.95 231.49 233.47 235.98
239.08 241.99 242.72 246.97 248.68 249.36
250.58 252.32 252.78 259.49 260.25 262.37
263.62 267.82 270.29 272.66 275.05 282.56
284.35 293.77 300.23 301.45 305.57 310.43
310.92 315.02 316.36 318.78 326.22 328.15
336.72 342.01 351.25 353.74 357.04 364.04
366.43 367.61 368.94 371.06 371.91 373.90
375.11 379.07 386.76 390.80 396.80 406.20
410.75 430.84 451.68 454.47 456.68 460.39
462.18 465.49 474.27 476.22 491.59 493.48
495.16 496.16 497.49 500.11 501.07 505.59
506.61 510.76 534.35 559.05 584.73 601.00
606.98 613.78 627.31 631.95 646.84 658.44
659.06 672.42 675.52 708.50 715.55 743.73
748.65 750.45 752.06 755.13 786.10 794.02
824.36 824.89 831.28 855.39 858.83 868.03
887.50 889.82 890.55 891.21 891.44 893.01

893.72 895.28 901.04 904.91 906.09 917.86
934.21 944.14 946.47 948.11 949.35 949.72
951.08 953.57 955.08 956.55 960.30 968.66
969.56 973.80 974.23 975.06 975.52 986.46
990.62 997.60 1000.98 1008.02 1009.32 1035.32
1042.11 1042.44 1042.52 1042.75 1043.63 1044.52
1046.03 1046.24 1048.87 1057.03 1065.15 1072.98
1074.96 1080.90 1087.38 1089.93 1099.14 1101.62
1110.63 1116.60 1119.08 1121.75 1125.96 1127.92
1129.93 1141.06 1176.99 1183.36 1188.11 1190.52
1192.78 1198.23 1199.40 1210.00 1214.53 1224.07
1234.09 1235.15 1238.93 1241.15 1241.80 1243.37
1243.82 1247.01 1247.54 1251.22 1276.63 1283.63
1283.76 1287.60 1289.58 1292.85 1308.44 1317.41
1321.68 1344.16 1349.65 1350.00 1351.98 1357.22
1358.52 1374.98 1390.23 1392.37 1393.40 1395.14
1395.96 1398.58 1399.76 1406.13 1414.03 1415.72
1416.62 1417.28 1417.82 1418.18 1420.41 1420.53
1421.13 1422.64 1432.22 1435.65 1436.12 1436.69
1437.71 1439.52 1445.28 1464.37 1474.31 1479.95
1484.71 1485.23 1485.76 1486.15 1487.64 1488.16
1488.60 1490.49 1491.14 1491.66 1494.44 1494.79
1495.62 1496.86 1498.15 1499.22 1500.39 1500.71
1501.84 1502.39 1505.22 1505.97 1506.84 1507.19
1507.38 1507.87 1508.60 1508.70 1509.12 1509.97
1511.04 1512.26 1512.60 1517.60 1517.69 1518.32
1518.54 1519.13 1520.91 1523.65 1524.25 1524.67
1525.80 1527.16 1529.19 1529.53 1533.11 1533.95
1581.01 1589.01 1603.57 1609.37 1615.45 1622.32
1659.30 2998.79 3004.99 3005.53 3008.83 3010.78
3014.86 3018.84 3020.48 3026.59 3028.37 3030.25
3031.27 3031.30 3034.47 3034.58 3037.77 3038.77
3038.93 3042.19 3043.82 3045.20 3045.46 3053.78
3063.35 3064.92 3071.25 3072.40 3075.04 3075.65
3080.80 3081.88 3082.70 3083.16 3084.51 3087.88
3087.94 3089.58 3090.65 3091.71 3093.53 3093.70
3093.87 3094.77 3098.88 3101.43 3101.98 3103.75
3103.92 3105.07 3107.43 3109.90 3110.14 3112.17
3113.83 3114.07 3115.20 3115.42 3117.13 3120.07
3121.02 3128.90 3129.30 3136.02 3140.45 3143.82
3152.92 3153.26 3153.43 3156.68 3162.50 3163.58
3170.06 3174.18 3180.07 3183.57 3183.81 3188.64
3190.75 3194.31 3204.05 3224.56 3442.30 3520.01

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2E'
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10.13 15.72 19.68 22.88 25.01 28.20
29.42 32.30 36.32 37.36 39.85 42.51
43.75 44.40 49.53 50.18 53.40 54.94
58.00 64.50 70.29 72.81 75.90 76.94
82.74 83.52 86.01 89.77 90.45 92.69
94.43 96.71 101.31 103.04 105.43 106.82
112.27 120.20 127.69 128.99 134.42 137.70
139.68 144.05 149.45 150.76 154.38 157.45
157.64 160.17 166.39 170.14 176.24 183.70
184.36 189.68 196.45 203.97 207.95 211.89
215.90 219.07 222.04 225.41 226.77 229.09
230.86 232.99 234.07 234.58 238.79 242.85

245.80 246.63 250.72 251.65 252.15 256.07
 256.89 259.88 261.94 267.00 268.37 269.40
 271.52 273.51 277.95 281.00 283.55 287.28
 292.81 308.01 308.43 314.52 315.88 316.92
 320.51 322.71 325.24 326.30 329.54 330.16
 351.09 357.44 365.67 366.89 368.58 371.01
 372.24 373.60 374.54 377.38 382.10 383.12
 391.29 397.47 401.39 409.85 412.10 426.91
 432.18 452.48 456.34 457.95 460.26 463.10
 471.59 476.89 486.61 490.48 494.05 495.02
 497.22 499.69 501.16 502.89 504.86 505.45
 511.74 533.46 555.70 560.02 567.86 584.92
 597.87 606.17 614.09 626.95 630.87 636.20
 646.82 658.67 658.83 673.21 676.16 706.52
 710.32 714.54 746.06 749.51 750.49 751.40
 752.60 770.83 783.80 793.87 824.53 825.78
 830.87 837.72 854.11 858.32 867.17 885.52
 888.71 890.66 891.87 892.44 892.50 894.36
 894.56 896.56 900.65 904.56 907.37 917.96
 933.35 943.57 945.27 946.47 950.10 951.61
 952.07 953.18 953.91 957.02 959.44 965.57
 970.12 970.86 973.92 974.84 975.51 978.36
 985.44 986.73 991.23 996.55 999.69 1005.27
 1007.17 1010.02 1033.82 1040.67 1042.09 1042.20
 1042.40 1043.83 1045.32 1046.55 1047.38 1048.72
 1055.01 1055.94 1065.31 1071.03 1073.34 1080.75
 1087.54 1089.44 1099.50 1102.77 1108.15 1110.37
 1117.00 1119.77 1121.74 1126.90 1128.16 1130.69
 1141.81 1178.32 1182.98 1184.84 1190.09 1190.56
 1192.20 1198.32 1199.94 1212.44 1213.19 1214.56
 1224.48 1233.56 1234.78 1239.39 1241.87 1242.60
 1243.38 1243.63 1244.83 1246.93 1248.21 1251.07
 1279.61 1283.42 1284.29 1284.87 1287.81 1291.46
 1293.66 1310.90 1317.98 1326.70 1343.62 1350.55
 1351.90 1353.04 1357.01 1359.72 1363.61 1376.25
 1385.45 1386.57 1390.55 1392.69 1393.64 1394.17
 1396.74 1399.40 1412.12 1414.46 1415.96 1416.29
 1417.35 1418.02 1418.05 1419.55 1420.13 1420.78
 1422.75 1430.63 1435.91 1436.33 1437.03 1437.43
 1439.47 1445.56 1464.68 1475.14 1480.36 1484.22
 1487.45 1487.87 1488.02 1489.40 1491.35 1492.92
 1493.44 1494.49 1495.21 1496.01 1496.06 1496.29
 1496.57 1498.24 1499.52 1500.52 1500.75 1501.99
 1503.00 1505.34 1506.10 1506.24 1506.48 1507.70
 1509.25 1509.82 1510.33 1511.09 1511.53 1511.79
 1512.35 1513.85 1514.21 1517.62 1517.79 1518.67
 1518.90 1521.22 1523.94 1524.67 1524.80 1525.45
 1527.72 1528.51 1529.08 1529.23 1530.11 1533.80
 1534.75 1593.20 1607.39 1609.60 1615.45 1620.50
 1621.34 1648.63 1659.19 2996.29 2998.49 3001.45
 3007.33 3013.85 3014.24 3015.60 3021.56 3024.41
 3027.00 3028.60 3031.81 3032.94 3034.75 3037.44
 3037.71 3038.55 3038.84 3041.48 3042.01 3045.27
 3046.41 3056.00 3058.17 3063.16 3067.06 3071.92
 3075.43 3077.09 3081.04 3082.05 3082.45 3085.33
 3086.48 3088.74 3089.49 3090.00 3090.98 3091.50
 3091.97 3094.70 3096.34 3096.75 3100.34 3101.42
 3102.67 3104.12 3105.77 3106.42 3107.41 3110.13

3113.55 3113.91 3114.03 3114.42 3114.85 3115.17
 3116.09 3116.98 3117.67 3118.67 3130.02 3133.79
 3144.16 3144.20 3150.79 3151.60 3152.19 3156.70
 3157.17 3160.40 3162.13 3164.63 3167.97 3175.28
 3175.89 3180.51 3181.88 3187.31 3189.75 3190.59
 3194.83 3195.33 3203.22 3203.60 3229.38 3503.62

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 2F
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16.11 19.31 26.13 32.60 41.55 46.55
 49.38 56.80 66.61 73.56 76.29 89.33
 91.94 99.85 102.72 106.90 114.25 119.30
 129.08 130.04 139.55 141.48 146.69 152.90
 154.95 161.64 167.31 168.59 171.97 177.11
 181.84 190.82 196.74 205.70 210.13 220.98
 225.03 232.66 238.35 243.82 245.42 249.85
 253.78 258.70 261.38 266.24 269.08 272.22
 285.00 287.21 293.89 302.44 305.48 309.62
 321.60 326.36 339.68 353.52 359.07 366.87
 375.80 378.95 391.36 397.15 399.17 411.48
 415.23 428.77 436.11 459.20 468.50 475.42
 477.80 484.49 493.61 505.32 526.47 529.95
 549.93 564.57 601.10 607.44 616.84 624.71
 625.64 644.11 656.64 670.78 671.30 681.26
 714.70 719.18 729.46 743.78 781.92 786.12
 812.07 816.69 824.65 846.58 855.37 858.87
 888.58 899.37 901.92 905.14 908.97 916.45
 922.18 945.84 946.96 947.95 949.45 950.63
 953.48 955.34 970.69 971.16 973.45 974.87
 975.66 985.47 987.13 990.97 1009.13 1026.67
 1036.29 1042.49 1044.23 1047.28 1053.55 1071.45
 1075.51 1079.47 1080.27 1088.76 1095.58 1097.13
 1108.69 1118.12 1119.25 1122.87 1127.20 1128.81
 1137.53 1143.25 1170.44 1185.45 1190.65 1191.80
 1195.95 1197.75 1199.48 1206.94 1213.90 1223.16
 1243.70 1270.31 1279.11 1283.21 1284.89 1286.15
 1310.34 1314.08 1318.85 1338.92 1344.06 1348.73
 1350.04 1353.11 1361.28 1367.03 1370.66 1391.58
 1395.27 1411.07 1413.02 1416.38 1416.88 1417.66
 1418.22 1421.95 1422.82 1433.12 1435.71 1436.49
 1438.96 1440.92 1443.31 1464.87 1470.14 1484.84
 1490.32 1492.60 1496.80 1499.70 1499.92 1500.48
 1501.06 1502.70 1503.87 1504.82 1505.91 1506.57
 1507.02 1507.90 1508.31 1511.68 1513.28 1514.91
 1517.85 1518.65 1519.77 1520.51 1522.80 1525.08
 1526.25 1527.71 1530.10 1532.32 1534.74 1535.72
 1581.75 1587.06 1605.79 1608.61 1617.66 1622.75
 1658.75 2972.05 3012.31 3028.87 3028.97 3032.87
 3034.85 3039.01 3039.78 3040.46 3041.08 3042.81
 3043.01 3043.26 3043.53 3044.48 3047.35 3048.91
 3074.59 3075.65 3082.15 3087.40 3090.52 3100.24
 3101.87 3103.53 3103.92 3107.82 3109.88 3110.38
 3113.65 3115.32 3115.87 3116.28 3117.70 3122.64
 3126.87 3133.53 3134.35 3139.50 3152.40 3157.39
 3159.78 3166.01 3168.11 3171.57 3173.27 3175.23
 3176.95 3180.61 3187.57 3190.44 3197.40 3203.53
 3204.56 3426.56 3506.19

2F'

10.29	15.34	25.70	26.35	34.70	38.44
43.24	46.43	49.49	57.58	58.42	75.72
76.55	84.39	91.09	93.99	100.48	105.12
108.05	114.00	117.20	126.33	130.57	132.52
141.72	143.39	148.92	153.70	161.59	166.96
171.00	174.79	181.53	188.46	192.87	201.67
202.70	209.32	219.97	224.91	235.34	241.04
244.11	246.93	253.11	255.44	257.09	262.77
266.89	269.54	271.44	284.86	286.23	294.57
295.59	303.82	306.98	318.01	321.82	332.40
341.23	351.05	354.75	362.99	371.05	376.71
388.69	395.39	395.91	410.30	414.52	417.23
423.86	425.09	436.94	458.67	468.35	473.02
483.25	488.88	495.18	496.94	518.56	542.63
549.15	560.35	586.06	594.72	603.84	617.15
620.31	622.73	636.23	639.49	656.76	670.49
671.77	681.26	701.54	710.58	713.36	720.29
748.17	759.58	765.52	771.21	780.89	807.68
822.17	828.77	839.76	853.49	858.71	875.73
888.88	899.01	901.21	906.21	912.08	916.48
918.50	945.19	947.20	949.04	949.65	950.12
952.32	953.19	955.75	967.55	971.11	972.33
973.52	974.74	975.34	985.38	987.74	993.49
999.17	1009.02	1018.89	1032.39	1039.18	1041.89
1044.90	1051.44	1052.46	1071.72	1076.89	1079.54
1080.19	1086.73	1094.34	1101.83	1106.50	1107.97
1108.87	1118.59	1120.28	1126.82	1128.46	1134.88
1143.78	1168.82	1184.70	1189.28	1189.69	1192.77
1196.86	1197.96	1199.27	1201.08	1209.12	1216.44
1221.44	1236.24	1237.87	1267.40	1279.04	1280.65
1284.50	1285.77	1299.78	1302.10	1313.09	1316.55
1337.20	1342.75	1348.41	1352.34	1353.06	1358.93
1359.67	1365.76	1368.79	1381.70	1389.07	1390.62
1405.17	1407.64	1413.66	1416.72	1417.59	1418.21
1419.60	1423.86	1431.87	1435.79	1436.51	1439.71
1441.64	1444.21	1466.48	1467.53	1483.12	1489.06
1490.75	1496.69	1499.44	1499.79	1500.62	1500.99
1502.78	1503.02	1504.04	1504.79	1505.57	1506.47
1507.01	1507.37	1510.31	1510.85	1512.17	1514.06
1514.43	1518.57	1520.13	1520.43	1522.91	1524.67
1525.57	1526.65	1527.05	1531.12	1533.34	1535.59
1537.76	1584.26	1604.47	1606.84	1615.12	1618.67
1623.53	1644.16	1657.20	2960.85	3013.36	3028.93
3034.43	3035.03	3038.40	3039.06	3039.34	3041.01
3041.85	3042.97	3043.11	3043.76	3046.19	3047.56
3050.21	3050.43	3076.39	3078.54	3083.66	3086.55
3089.58	3101.15	3103.02	3103.54	3104.92	3106.83
3109.55	3110.61	3113.89	3114.59	3115.97	3117.02
3117.99	3124.11	3126.74	3133.02	3136.61	3141.42
3144.14	3146.02	3148.38	3159.94	3160.27	3164.75
3166.90	3167.37	3167.56	3168.60	3174.20	3177.04
3181.71	3185.46	3187.17	3187.21	3187.64	3194.94
3198.55	3204.77	3504.39			

2G

24.85	35.61	42.41	46.96	49.88	53.16
60.79	66.13	75.26	78.20	82.16	91.88
93.72	96.03	103.17	108.19	113.49	118.99
123.72	134.66	141.92	143.82	148.13	157.71
159.59	164.22	166.89	175.19	177.28	181.58
185.96	193.83	196.94	213.67	217.86	229.96
231.83	235.77	240.33	244.08	245.88	250.27
254.10	256.84	260.77	264.96	271.61	273.05
274.52	278.62	282.05	288.47	296.40	303.54
308.16	324.09	332.50	347.60	353.31	356.42
367.83	382.49	383.89	393.32	405.25	411.19
414.80	426.21	452.45	456.40	464.33	475.03
480.67	484.37	489.08	505.56	517.55	534.62
555.96	586.42	595.25	616.62	627.19	627.60
631.13	638.99	652.18	653.78	666.23	671.71
717.38	722.54	744.92	751.25	783.77	789.98
811.28	813.88	832.78	858.97	859.12	884.11
895.19	895.87	902.25	906.85	911.27	919.28
939.06	943.95	947.07	949.06	951.84	959.70
961.23	965.15	971.73	974.19	974.64	975.06
985.39	986.16	989.91	990.80	1009.92	1038.31
1040.43	1042.51	1045.61	1054.24	1058.79	1068.57
1071.56	1082.60	1086.91	1090.11	1096.85	1106.71
1115.77	1119.42	1124.09	1126.87	1129.24	1129.59
1132.21	1143.78	1175.47	1184.78	1190.66	1192.45
1195.75	1200.55	1201.51	1209.89	1214.17	1224.49
1251.96	1280.84	1282.75	1285.28	1293.86	1297.56
1306.06	1309.90	1326.37	1344.90	1348.19	1348.37
1349.78	1350.22	1358.43	1361.50	1376.86	1401.90
1411.80	1413.62	1414.47	1417.52	1418.88	1420.05
1422.84	1425.97	1430.93	1432.74	1433.39	1434.08
1437.61	1439.56	1445.40	1464.07	1478.85	1486.04
1488.69	1492.32	1495.60	1498.41	1498.96	1499.20
1499.86	1500.85	1502.55	1503.59	1504.70	1505.69
1506.02	1506.45	1508.62	1508.79	1511.36	1514.53
1514.89	1515.72	1517.50	1519.03	1520.99	1521.72
1524.52	1526.57	1527.37	1528.21	1530.59	1534.15
1579.01	1593.49	1598.85	1609.32	1616.91	1621.91
1657.76	3011.23	3025.80	3030.55	3032.39	3034.31
3036.55	3036.99	3037.21	3038.39	3039.82	3040.75
3041.26	3042.02	3044.74	3045.57	3052.47	3071.93
3084.32	3088.50	3091.15	3091.68	3096.51	3101.16
3102.15	3105.01	3106.51	3108.82	3109.08	3110.85
3113.67	3116.38	3118.92	3119.23	3122.24	3127.20
3128.89	3129.52	3135.33	3135.69	3139.27	3151.81
3155.30	3157.90	3160.04	3162.82	3164.51	3170.87
3172.08	3183.53	3184.64	3188.36	3190.71	3196.94
3197.07	3419.56	3505.18			

2G'

16.96	23.10	25.99	30.83	36.66	40.29
48.45	53.37	56.91	64.37	71.83	77.02
79.74	83.81	87.48	95.82	97.06	101.76
107.98	115.13	118.26	128.45	132.01	137.02
144.02	146.48	150.28	153.94	158.71	163.49
172.05	174.35	179.86	183.09	195.68	207.23
212.81	215.76	223.83	230.92	233.02	239.01

241.83	245.43	246.25	250.84	253.06	258.29
263.30	265.93	271.76	274.51	279.82	285.14
296.90	299.66	305.76	311.90	327.96	331.39
335.92	350.35	354.48	359.81	367.59	379.50
383.61	393.08	404.97	410.61	411.49	421.29
425.15	453.29	455.93	464.16	474.74	477.59
481.65	484.83	490.09	515.71	533.26	550.25
554.84	582.96	584.24	595.50	615.17	626.21
627.45	629.16	633.67	639.56	651.46	653.49
665.72	671.67	700.32	710.47	722.19	738.90
742.30	750.38	765.70	783.45	788.47	811.36
824.31	831.28	847.33	850.03	857.02	872.56
895.47	896.18	902.70	903.52	907.25	918.23
937.88	943.77	944.25	944.34	948.35	949.50
957.50	958.72	963.18	965.08	969.13	973.71
974.33	976.34	985.31	986.16	986.49	989.32
1003.49	1009.77	1037.94	1038.99	1042.06	1045.14
1052.54	1054.44	1059.05	1068.03	1071.27	1081.56
1085.97	1087.66	1099.77	1104.56	1105.99	1116.22
1119.27	1123.52	1128.15	1129.46	1130.25	1132.24
1141.05	1174.93	1184.63	1186.56	1189.13	1190.88
1195.92	1199.90	1201.73	1206.49	1209.59	1214.79
1222.54	1243.35	1251.78	1279.76	1282.33	1283.79
1292.32	1298.24	1303.93	1312.17	1313.43	1325.68
1345.10	1348.27	1349.42	1349.99	1350.61	1356.48
1362.33	1362.81	1375.52	1384.40	1400.43	1412.04
1414.60	1417.21	1417.65	1418.69	1419.89	1422.92
1426.21	1431.22	1433.18	1434.28	1437.80	1438.42
1439.71	1445.88	1465.05	1476.88	1485.65	1489.00
1491.54	1495.79	1497.69	1498.64	1498.95	1500.21
1501.28	1502.68	1503.36	1503.89	1504.82	1505.60
1505.64	1506.62	1508.07	1509.36	1510.97	1514.46
1515.86	1516.94	1517.48	1519.35	1521.24	1521.38
1523.21	1525.23	1526.77	1528.45	1530.25	1530.63
1534.19	1593.19	1595.71	1609.29	1618.64	1620.20
1621.60	1649.96	1654.23	3011.53	3023.20	3035.09
3035.76	3037.13	3037.31	3037.89	3039.31	3041.31
3042.05	3042.85	3043.14	3044.30	3045.69	3046.46
3054.05	3072.23	3085.37	3087.93	3089.44	3091.31
3102.01	3103.80	3105.38	3107.65	3109.55	3111.08
3111.63	3113.03	3115.42	3115.84	3121.70	3123.51
3124.09	3126.87	3128.65	3132.29	3136.78	3137.69
3150.50	3154.87	3156.68	3156.94	3158.35	3159.89
3161.49	3165.66	3167.72	3169.37	3172.09	3172.88
3180.88	3183.22	3189.62	3192.38	3196.23	3196.75
3205.32	3227.05	3498.94			

2G-TS

-413.44	24.90	35.41	38.21	47.87	49.74
53.30	54.57	59.59	68.48	75.98	81.90
84.73	94.07	97.92	100.46	107.76	116.75
117.66	127.78	133.27	142.77	144.40	147.78
152.91	161.08	162.73	165.07	168.02	173.58
179.53	182.72	195.20	217.82	232.33	233.53
235.33	238.20	244.91	247.30	248.78	250.04
255.22	256.83	259.73	267.55	271.55	276.05
279.81	282.61	289.57	297.48	299.72	308.42

319.22	331.37	347.87	355.15	356.65	366.36
380.18	382.70	385.71	393.14	406.67	411.07
424.30	425.48	428.77	451.84	454.44	464.77
468.71	475.69	482.99	487.96	514.25	534.09
556.68	586.38	594.53	616.07	622.74	626.62
629.10	636.87	639.81	650.00	655.12	672.32
684.35	718.08	720.85	750.88	770.37	782.67
788.00	812.53	833.76	833.98	859.25	872.62
881.53	895.91	896.26	901.91	905.39	916.41
938.77	943.71	947.03	949.52	949.65	956.76
959.64	961.62	965.84	973.10	974.02	974.08
976.16	985.10	985.59	989.76	999.46	1013.66
1038.57	1042.82	1045.46	1052.34	1056.51	1057.99
1068.16	1071.91	1083.78	1088.71	1099.83	1105.77
1112.74	1118.89	1123.74	1126.84	1127.84	1129.30
1132.59	1141.86	1176.80	1184.99	1188.58	1192.07
1195.15	1199.05	1202.00	1208.83	1209.60	1224.94
1249.42	1277.81	1280.45	1287.09	1290.43	1294.97
1300.03	1312.22	1326.31	1345.66	1346.85	1349.85
1350.97	1351.87	1357.73	1360.28	1376.08	1398.98
1411.02	1413.10	1415.24	1416.57	1417.75	1419.57
1421.60	1425.10	1429.88	1432.02	1432.57	1435.14
1436.56	1438.00	1444.05	1469.57	1475.87	1486.39
1489.35	1491.69	1495.28	1495.98	1497.39	1498.44
1499.08	1499.99	1500.48	1502.34	1504.20	1504.38
1505.72	1506.59	1507.79	1508.25	1510.83	1514.72
1515.23	1516.07	1517.25	1519.40	1520.18	1520.96
1524.49	1524.82	1526.36	1527.95	1530.47	1532.80
1568.25	1594.41	1602.86	1605.53	1608.59	1620.24
1657.02	3010.72	3024.28	3031.37	3032.28	3033.33
3035.63	3036.14	3036.31	3037.03	3037.09	3038.31
3040.26	3041.81	3044.82	3045.53	3050.53	3071.39
3081.47	3082.72	3087.89	3091.01	3098.29	3099.78
3099.99	3103.35	3105.79	3107.99	3109.03	3111.04
3112.71	3114.16	3116.24	3117.09	3123.68	3125.58
3130.90	3132.89	3134.54	3134.77	3139.20	3148.10
3151.62	3157.98	3159.54	3160.49	3163.26	3171.39
3172.00	3178.58	3181.93	3183.51	3186.44	3197.31
3197.88	3535.65	3639.41			

2G'-TS

-394.04	12.01	24.63	26.86	35.73	39.19
45.05	51.90	55.32	57.30	66.61	67.10
77.32	79.34	84.08	90.46	96.93	100.87
105.26	114.20	116.18	118.72	129.96	131.66
140.79	143.64	148.00	151.26	153.31	160.80
163.44	171.50	173.77	179.17	182.16	197.11
217.41	222.49	227.66	231.83	234.70	238.23
243.67	246.07	248.26	251.38	252.17	255.44
259.91	265.90	269.45	272.48	276.25	281.30
282.26	296.09	299.78	302.15	309.39	324.74
332.30	349.42	355.87	358.68	365.96	378.32
382.79	392.17	405.01	410.65	421.60	425.23
429.68	450.33	451.65	454.57	465.27	475.78
483.07	488.00	513.43	513.79	534.46	547.22
556.98	584.21	586.92	594.88	616.65	621.03
626.27	628.30	632.85	637.73	639.86	650.19

654.75 673.04 698.73 705.49 721.48 726.04
750.54 767.28 782.33 785.45 787.79 812.62
829.55 833.91 835.51 858.63 861.20 869.01
885.51 895.43 896.20 903.86 904.29 918.12
937.81 943.43 943.57 947.72 949.20 951.83
955.41 957.26 960.56 964.04 973.40 973.77
975.09 975.39 977.58 985.00 985.48 990.34
997.67 1000.27 1009.38 1038.28 1042.72 1045.36
1052.19 1054.00 1054.92 1057.79 1068.00 1071.73
1083.14 1087.24 1104.36 1104.94 1109.42 1113.08
1118.84 1123.18 1126.61 1127.97 1129.88 1132.22
1140.53 1176.25 1184.65 1188.81 1189.22 1190.18
1194.54 1198.28 1201.64 1206.62 1209.48 1212.25
1223.09 1249.50 1258.43 1277.83 1278.71 1285.75
1289.84 1294.46 1298.53 1306.26 1322.21 1323.81
1345.86 1346.36 1348.84 1349.74 1355.73 1357.14
1362.33 1364.34 1374.94 1392.15 1397.83 1410.40
1413.25 1416.58 1417.25 1417.87 1419.44 1421.85
1425.22 1429.92 1432.26 1432.92 1436.64 1438.13
1438.66 1444.27 1471.35 1473.37 1485.85 1489.37
1492.76 1494.40 1495.65 1496.56 1497.90 1499.09
1499.87 1500.96 1502.62 1503.35 1504.44 1505.57
1506.28 1507.45 1507.82 1508.44 1510.40 1514.23
1515.17 1516.84 1517.06 1519.08 1520.22 1521.12
1523.84 1524.57 1526.38 1528.15 1530.41 1533.28
1534.83 1594.19 1602.34 1603.80 1608.84 1619.07
1630.55 1654.24 1655.43 3010.94 3022.79 3032.84
3034.26 3035.27 3035.88 3036.62 3037.45 3038.35
3038.51 3041.17 3041.49 3043.71 3045.62 3046.36
3051.95 3071.59 3083.32 3084.92 3087.07 3091.45
3100.42 3102.03 3102.82 3103.22 3108.16 3108.24
3110.80 3111.26 3112.72 3113.88 3116.70 3122.19
3123.26 3127.18 3130.85 3131.65 3135.01 3138.68
3148.45 3151.74 3155.64 3158.64 3159.31 3159.69
3165.33 3165.58 3168.67 3168.90 3174.97 3179.23
3179.89 3179.97 3181.77 3197.36 3198.71 3199.37
3212.64 3214.36 3579.78

2H

13.67 26.05 30.66 37.60 42.25 45.40
45.70 61.73 65.52 67.73 71.48 73.98
79.82 82.94 92.66 98.20 100.69 106.04
111.01 117.70 130.47 133.94 136.34 144.39
145.84 159.31 161.47 167.36 173.31 182.01
187.62 190.64 197.04 220.39 227.45 228.63
239.20 241.28 245.45 251.35 253.10 258.29
260.99 263.82 272.49 276.04 280.59 290.98
293.40 297.14 303.87 310.22 322.65 336.97
339.63 353.95 359.24 367.87 373.81 377.49
384.93 386.48 395.10 409.79 414.84 417.05
436.88 449.94 452.13 467.06 476.00 479.73
487.38 515.34 517.71 533.20 544.26 549.57
556.48 586.28 592.39 615.17 621.55 628.47
634.96 636.21 650.99 652.59 672.51 703.43
718.75 747.57 761.40 780.91 786.42 808.53
823.05 833.56 836.89 857.36 885.21 895.62
896.26 903.24 904.32 916.08 924.74 937.41

945.08 947.23 948.14 949.22 953.90 959.78
960.55 964.85 972.91 974.49 975.90 980.96
984.30 984.39 988.00 1015.37 1039.09 1042.48
1044.48 1046.51 1056.96 1060.56 1067.15 1072.04
1079.92 1085.65 1094.60 1106.75 1108.39 1116.97
1120.48 1124.07 1128.93 1130.23 1133.36 1138.34
1155.64 1175.88 1185.49 1190.61 1192.75 1193.91
1197.64 1202.51 1209.04 1213.02 1222.56 1246.30
1268.13 1275.31 1278.63 1283.04 1287.22 1292.35
1294.65 1321.65 1342.38 1350.17 1351.80 1355.39
1359.13 1359.68 1367.38 1372.86 1375.40 1400.15
1408.59 1411.80 1411.97 1412.99 1417.27 1417.46
1418.77 1421.79 1429.44 1430.48 1431.55 1433.22
1435.14 1436.95 1439.16 1471.74 1486.26 1489.47
1491.13 1495.07 1495.74 1497.33 1499.42 1500.78
1501.31 1501.87 1502.66 1503.67 1505.92 1506.96
1507.54 1508.67 1512.48 1513.12 1514.59 1515.46
1517.41 1518.18 1519.32 1520.20 1521.85 1524.27
1526.48 1528.06 1528.16 1530.90 1532.38 1543.31
1592.69 1600.21 1607.71 1646.08 1648.61 1657.33
1667.29 3009.34 3019.01 3023.52 3025.88 3027.46
3030.74 3032.77 3033.40 3033.94 3035.21 3035.98
3037.15 3037.77 3038.42 3044.75 3054.35 3070.05
3079.57 3080.61 3084.06 3088.67 3092.42 3095.32
3096.63 3096.77 3098.76 3101.49 3104.90 3105.56
3107.88 3109.20 3112.65 3112.89 3117.01 3117.21
3119.40 3124.92 3128.68 3129.22 3131.90 3135.95
3138.61 3140.41 3147.68 3159.61 3164.51 3168.43
3170.95 3178.27 3188.41 3190.51 3192.29 3203.35
3218.48 3488.95 3593.13

2H'

10.23 17.53 27.83 33.11 35.38 39.33
45.09 46.76 50.01 56.83 64.22 67.80
70.97 76.28 78.77 83.26 86.81 94.77
100.56 103.51 110.52 115.51 117.39 128.33
131.40 134.36 143.12 148.54 154.04 156.44
165.71 170.64 173.95 185.58 190.82 193.07
217.41 223.95 235.19 236.31 241.65 245.76
246.57 252.25 253.56 256.02 264.95 269.06
270.88 273.12 278.53 289.41 291.96 292.92
301.90 303.30 310.36 313.41 322.52 333.94
349.47 355.62 366.62 371.18 381.40 389.70
396.85 409.56 413.22 417.82 426.49 433.21
451.58 453.90 464.90 468.21 473.37 479.18
481.38 486.74 514.78 532.50 536.72 556.79
577.42 582.23 591.55 615.37 619.07 626.83
629.69 633.57 636.31 638.43 648.72 651.62
671.89 704.75 712.99 719.34 748.28 762.25
766.69 779.64 786.80 809.10 815.62 833.79
840.30 856.71 862.65 864.89 894.21 896.25
899.23 904.21 905.13 918.48 924.87 937.52
942.73 945.94 946.37 949.96 953.29 956.64
961.00 962.26 963.48 973.85 974.58 975.60
980.08 982.36 984.73 986.07 988.84 1001.87
1015.62 1018.38 1039.18 1042.52 1044.55 1046.33
1054.50 1056.77 1060.02 1067.53 1071.93 1079.17

1088.69 1104.55 1105.37 1107.71 1115.63 1117.48
1120.79 1124.52 1127.49 1128.83 1133.33 1139.29
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1197.95 1200.99 1201.79 1209.45 1211.76 1223.77
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1286.33 1291.97 1297.92 1322.68 1324.74 1334.27
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1362.35 1365.92 1376.60 1399.17 1410.49 1410.83
1411.39 1414.37 1416.40 1417.44 1418.37 1421.80
1429.30 1430.33 1431.12 1431.77 1434.05 1435.33
1439.92 1440.22 1471.11 1486.49 1489.54 1490.89
1495.37 1495.88 1496.11 1497.08 1499.29 1500.52
1500.91 1501.64 1502.17 1504.41 1505.51 1506.56
1507.45 1508.88 1511.95 1514.60 1514.89 1516.58
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3206.70 3214.87 3451.35

2I

10.54 27.98 36.52 43.24 45.39 49.21
55.15 64.19 71.42 76.52 87.25 91.72
98.57 99.52 115.27 117.70 119.26 125.00
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166.23 168.11 174.79 180.23 184.12 190.63
193.69 205.47 207.20 212.18 213.25 220.57
230.85 238.16 244.97 248.82 252.16 255.08
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295.82 296.93 302.15 305.10 313.50 321.05
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424.02 446.92 457.54 460.63 469.54 482.08
483.63 488.84 497.16 504.25 529.06 550.09
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1094.93 1096.17 1100.78 1101.06 1105.26 1108.99
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1284.55 1289.25 1290.14 1306.96 1307.99 1312.78

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3174.54 3177.48 3179.63 3184.43 3190.23 3191.83
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15.93 23.35 30.86 37.97 40.80 43.53
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74.22 76.14 77.47 84.57 87.45 96.49
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248.99 250.14 257.32 265.73 269.31 272.76
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485.34 511.76 523.58 526.50 534.55 557.35
579.29 605.47 611.41 617.32 628.06 641.77
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1125.14 1126.53 1128.82 1131.69 1133.68 1141.21
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1397.43 1399.08 1400.86 1410.97 1413.84 1414.80

1418.19 1419.81 1421.03 1430.06 1431.28 1432.95
 1434.49 1436.25 1449.44 1470.34 1484.29 1487.13
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 1499.36 1499.68 1499.97 1500.52 1500.88 1501.72
 1502.70 1503.65 1504.70 1507.91 1508.60 1508.91
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3-TS

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3D

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3H-TS

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1508.51 1508.80 1510.92 1512.18 1512.42 1513.14
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1524.71 1528.16 1530.32 1534.27 1536.96 1594.41
1597.30 1604.56 1606.70 1619.36 1632.48 1657.77
1658.32 3008.16 3009.18 3011.36 3011.64 3011.79
3017.73 3019.16 3029.35 3030.50 3030.91 3034.79
3035.93 3037.23 3038.04 3039.73 3041.74 3043.35
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3098.89 3099.58 3106.53 3108.42 3108.60 3109.06
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3180.89 3182.97 3198.91 3199.27 3200.09 3207.96
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15.18 25.09 26.13 33.74 38.01 38.63
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417.78 419.36 432.35 449.97 452.02 455.11
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3J

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3197.67 3201.87 3225.58

3K

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 3227.07 3468.80 3584.48

3L

25.12	27.89	32.76	37.64	41.13	47.37
53.02	60.27	62.10	66.02	69.06	75.75
78.70	82.89	92.06	94.89	99.14	103.43
108.80	112.50	115.10	119.58	122.04	124.87
130.52	139.06	143.06	151.50	152.14	161.63
167.51	171.25	175.60	178.25	182.21	182.87
184.02	193.87	204.56	207.18	209.32	213.57
215.08	224.79	229.31	231.13	236.38	242.21
243.85	248.60	254.06	257.21	265.68	269.68
276.67	279.10	281.36	296.24	300.39	302.61
311.82	315.26	320.80	326.20	330.72	332.97
339.72	345.23	353.66	358.37	362.10	367.68
374.47	383.24	391.36	395.93	400.85	405.85
407.24	425.30	433.16	436.20	448.31	454.87
456.58	464.61	468.07	470.11	473.29	474.75
484.30	490.44	498.75	504.00	526.08	533.62
542.02	546.46	562.69	575.15	590.31	606.99
614.22	618.90	629.88	640.81	648.76	654.67
661.84	668.05	711.88	717.47	726.93	731.11
745.78	748.12	752.55	759.55	781.62	800.07
813.85	817.47	818.17	822.02	831.49	840.11
869.48	871.89	873.58	882.28	884.85	888.69
898.40	899.32	906.37	910.86	914.93	915.92
916.36	928.32	934.20	940.84	941.18	944.24
946.94	947.14	949.96	962.22	970.34	971.27
973.41	977.66	984.64	987.53	1005.95	1014.25
1021.69	1029.91	1030.01	1035.21	1037.31	1039.51
1041.36	1042.72	1043.27	1048.59	1055.11	1059.26
1062.30	1068.01	1071.80	1078.47	1082.08	1087.95
1091.44	1096.01	1098.88	1099.89	1108.26	1111.74
1113.01	1119.29	1130.62	1131.57	1132.76	1146.19
1155.43	1160.14	1177.24	1184.40	1187.07	1190.26
1195.23	1201.99	1204.94	1213.52	1216.73	1221.51
1224.78	1232.04	1234.24	1241.00	1251.85	1256.51
1260.21	1268.33	1278.71	1282.38	1294.69	1299.41
1301.55	1303.56	1307.00	1309.55	1317.69	1321.05
1331.77	1335.45	1337.03	1345.22	1354.35	1355.15
1356.78	1363.35	1365.35	1368.22	1375.27	1381.39
1386.49	1388.80	1391.81	1392.83	1394.29	1395.95
1396.57	1398.78	1401.63	1403.71	1409.99	1411.23
1413.43	1417.21	1419.97	1423.32	1430.74	1433.35
1435.59	1436.17	1440.00	1462.03	1463.36	1477.87
1481.00	1483.99	1487.75	1488.84	1490.30	1491.98
1492.92	1496.95	1497.77	1499.27	1499.66	1500.68
1501.08	1501.87	1502.41	1504.12	1504.94	1505.38
1506.04	1507.29	1510.35	1511.28	1512.06	1512.84
1514.93	1516.13	1516.87	1517.78	1517.93	1521.12
1522.13	1524.23	1527.63	1530.20	1530.86	1533.74
1540.45	1548.27	1584.05	1601.39	1608.54	1612.86
1624.43	1649.89	1653.93	1663.56	3006.95	3009.23
3010.66	3011.06	3020.73	3021.09	3021.24	3021.99
3025.73	3027.72	3029.67	3030.73	3036.05	3036.83
3038.04	3038.42	3038.44	3040.07	3041.03	3041.44
3044.06	3047.40	3061.57	3063.18	3064.55	3066.00
3069.58	3071.21	3073.34	3085.01	3085.44	3088.93
3092.13	3094.71	3096.07	3096.93	3099.05	3099.31

3100.53	3105.07	3105.64	3108.44	3108.75	3109.56
3112.45	3117.35	3117.65	3121.71	3122.43	3122.70
3131.52	3134.31	3134.63	3137.11	3142.75	3143.69
3144.25	3152.84	3154.21	3156.73	3160.53	3164.44
3166.91	3170.38	3174.58	3181.14	3191.05	3191.51
3197.44	3201.21	3264.76	3454.55	3577.76	3622.13

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15.22	19.97	22.75	30.72	35.53	37.55
42.73	44.40	50.59	57.25	64.97	66.01
68.08	70.18	78.94	83.42	90.25	91.55
95.44	98.18	105.57	109.71	110.80	113.97
115.84	119.47	123.26	126.40	134.02	141.78
144.49	150.47	156.21	158.41	162.51	167.92
172.45	176.77	184.61	187.99	191.14	198.56
207.74	216.50	221.04	223.30	231.41	236.98
243.41	248.80	252.05	253.98	256.45	257.07
265.36	269.27	269.68	277.06	284.84	291.62
303.71	307.56	309.63	319.50	322.27	327.12
329.46	331.49	338.24	343.61	346.12	357.88
359.82	363.75	366.53	370.08	384.72	393.46
398.62	403.65	407.47	409.72	412.69	420.83
424.43	437.34	440.99	450.91	457.09	458.86
463.16	466.57	468.31	472.41	483.78	488.59
491.14	495.41	520.28	524.30	537.51	538.43
541.10	548.51	552.68	579.19	587.38	607.11
614.02	628.13	628.88	629.59	642.74	650.72
661.14	667.57	674.07	708.35	710.98	719.47
726.07	737.37	743.34	749.09	750.09	770.42
782.09	791.96	809.03	813.62	816.47	818.40
824.14	832.69	835.13	847.52	857.59	867.46
869.56	872.13	889.36	894.62	896.94	901.93
902.87	904.73	907.17	909.29	909.52	919.01
932.42	935.98	941.97	944.43	945.88	946.94
947.72	949.30	952.04	958.72	965.79	966.50
972.25	974.17	974.66	975.45	979.01	988.39
989.37	1009.71	1016.81	1017.23	1023.03	1027.56
1037.85	1040.08	1041.14	1042.07	1042.38	1045.39
1045.45	1047.91	1057.72	1058.08	1058.28	1066.84
1070.27	1073.66	1084.04	1088.22	1089.20	1093.21
1098.31	1100.62	1101.22	1107.52	1109.79	1117.90
1119.21	1122.85	1129.01	1133.78	1140.48	1148.26
1155.15	1160.96	1172.96	1184.93	1189.66	1192.90
1195.08	1199.30	1204.09	1204.85	1210.53	1215.15
1220.30	1222.63	1223.63	1237.22	1239.94	1247.37
1255.63	1267.47	1270.31	1272.43	1284.32	1285.82
1287.62	1299.16	1302.27	1303.12	1306.27	1307.21
1312.46	1314.85	1321.02	1324.83	1334.50	1338.67
1347.99	1350.86	1351.68	1357.17	1365.05	1366.63
1368.00	1372.30	1373.96	1378.47	1385.14	1388.15
1391.23	1391.47	1394.05	1394.97	1396.59	1399.17
1400.00	1400.92	1405.68	1409.59	1412.55	1413.90
1418.52	1420.34	1424.32	1430.27	1434.29	1434.97
1437.23	1438.22	1462.30	1471.57	1478.14	1484.15
1485.30	1488.82	1493.13	1494.13	1494.65	1498.06
1499.13	1499.19	1500.98	1501.83	1502.26	1502.78
1502.99	1503.85	1504.51	1506.88	1507.49	1508.22

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3067.58 3070.15 3073.26 3073.82 3074.11 3077.59
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3097.25 3098.73 3101.27 3102.35 3103.44 3107.82
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3154.59 3156.45 3157.61 3160.16 3161.73 3163.34
 3168.77 3174.66 3178.74 3185.43 3194.57 3195.71
 3204.41 3269.18 3272.80

6.3. Computed energies of DFT-optimized structures

	E(SCF)/(eV)	ZPE/(kcal mol ⁻¹)	S(gas)/(cal mol ⁻¹)	G(solv)/(kcal mol ⁻¹)
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
PhCl	-18829.236	57.19	74.832	-1.16
NH₃	-1539.719	21.61	45.977	-3.44
NH₂Ph	-7828.959	73.65	75.469	-3.37
NHPh₂	-14118.159	124.45	101.41	-3.07
NaO^tBu	-10761.67	78.01	88.598	-19.04
(NaO^tBu)₄	-43054.637	315.12	222.23	-5.83
Na₄(O^tBu)₃Cl	-49234.625	237.55	200.79	-12.79
HO^tBu	-6361.349	85.47	76.633	-2.47
NaCl	-16941.986	0.51	54.88	-22.69
1,4-dioxane	-8375.044	76.98	72.58	-2.58
L1_0	-66607.352	530.09	257.78	-6.05
L1_10	-66607.352	529.97	258.37	-6.05
L1_20	-66607.313	529.89	258.64	-6.04
L1_30	-66607.336	529.90	257.61	-6.19
L1_40	-66607.234	529.85	259.33	-6.17
L1_50	-66607.141	530.28	257.01	-6.11
L1_60	-66607.023	530.57	255.75	-5.70
L1_70	-66606.844	529.70	258.89	-6.96
L1_80	-66606.867	529.80	258.32	-7.04
L1_90	-66606.922	529.61	259.96	-7.17
L1_100	-66606.906	529.65	260.22	-7.24
L1_110	-66606.906	530.11	262.26	-7.96
L1_120	-66606.938	529.97	261.85	-8.13
L1_130	-66606.898	530.13	259.34	-7.74
L1_140	-66606.945	530.07	260.60	-7.73
L1_150	-66606.898	529.81	260.78	-7.57
L1_160	-66606.891	529.79	259.71	-7.53
L1_170	-66606.859	529.81	260.27	-7.48
L1_180	-66606.91	529.85	260.41	-7.34

L2_0	-66579.820	519.77	269.14	-6.51
L2_10	-66579.766	519.78	270.34	-6.53
L2_20	-66579.703	519.70	269.93	-6.68
L2_30	-66579.563	519.53	272.35	-6.49
L2_40	-66579.469	519.50	271.80	-6.70
L2_50	-66579.305	519.45	273.08	-6.61
L2_60	-66579.148	519.40	268.59	-6.49
L2_70	-66579.047	519.46	269.97	-6.71
L2_70^a	-3243.364	-	-	-
L2_70^b	-63368.340	-	-	-
L2_80	-66579.016	519.64	272.21	-7.58
L2_90	-66579.016	519.46	273.15	-7.66
L2_100	-66579.109	519.01	277.38	-7.75
L2_110	-66579.141	519.08	278.64	-7.96
L2_120	-66579.141	519.04	275.94	-8.30
L2_130	-66579.148	519.15	275.07	-8.28
L2_140	-66579.172	519.52	272.34	-8.30
L2_150	-66579.234	519.65	271.12	-8.33
L2_160	-66579.133	519.47	274.01	-8.21
L2_170	-66579.172	519.42	272.30	-8.39
L2_180	-66579.211	519.37	272.06	-8.34
L3_0	-72935.414	603.43	286.11	-6.40
L3_10	-72935.414	603.41	285.46	-6.44
L3_20	-72935.336	603.30	286.01	-6.44
L3_30	-72935.258	603.13	287.76	-6.16
L3_40	-72935.070	603.04	288.77	-6.21
L3_50	-72934.875	603.04	288.63	-6.00
L3_60	-72934.758	602.79	288.41	-6.01
L3_70	-72934.477	602.56	287.81	-6.61
L3_70^a	-6421.101	-	-	-
L3_70^b	-66545.961	-	-	-
L3_80	-72934.633	603.66	284.71	-7.49
L3_90	-72934.641	603.71	284.33	-7.49
L3_100	-72934.625	603.54	286.80	-7.44

L3_110	-72934.719	602.84	287.48	-7.66
L3_120	-72934.836	603.18	287.04	-7.73
L3_130	-72934.914	603.17	288.37	-7.73
L3_140	-72934.805	602.83	290.78	-8.11
L3_150	-72934.945	603.35	286.36	-7.75
L3_160	-72934.891	603.35	286.18	-7.80
L3_170	-72934.750	603.45	286.75	-7.93
L3_180	-72934.719	603.70	286.27	-7.96
L4_0	-68626.602	523.21	269.44	-6.98
L4_10	-68626.547	522.89	270.25	-7.01
L4_20	-68626.445	522.78	270.86	-6.94
L4_30	-68626.281	522.68	272.70	-6.83
L4_40	-68626.063	522.73	271.55	-6.52
L4_50	-68626.016	522.95	270.03	-7.04
L4_60	-68625.813	522.84	271.98	-7.03
L4_70	-68625.563	522.65	274.29	-7.22
L4_80	-68625.289	522.65	274.82	-7.64
L4_90	-68625.391	522.68	273.56	-8.26
L4_100	-68625.500	522.84	271.01	-8.31
L4_110	-68625.813	522.94	274.64	-8.18
L4_120	-68625.953	522.93	273.34	-8.33
L4_130	-68626.070	523.10	266.33	-8.40
L4_140	-68626.148	523.30	272.37	-8.37
L4_150	-68626.164	523.36	272.52	-8.51
L4_160	-68626.141	523.37	271.90	-8.43
L4_170	-68626.102	523.73	262.78	-8.28
L4_180	-68626.000	523.78	268.79	-8.17
1	-66606.650	528.77	263.283	-2.3
1-TS	-66606.203	528.40	261.235	-2.81
1A	-66607.492	530.08	256.55	-6.34
1B	-66607.086	530.439	257.986	-7.26
1C	-68147.945	555.15	269.89	-7.33
1C'	-74437.234	606.09	290.43	-6.50
1D	-111203.906	871.32	444.26	-7.99

1D'	-117493.305	922.54	460.86	-6.03
1D-TS	-111203.477	868.48	439.98	-8.39
1D'-TS	-117493.031	919.29	460.38	-5.94
1E	-111203.461	870.16	446.08	-8.36
1E'	-117493.078	921.28	461.68	-6.48
1F	-104841.719	784.03	404.52	-6.50
1F'	-111131.383	835.05	429.05	-6.96
1G	-55605.180	545.00	259.25	-5.98
1G'	-61894.832	596.15	280.39	-5.61
1H	-55605.586	544.91	257.30	-3.12
1H'	-61895.311	596.30	280.85	-3.78
1H-TS	-55604.932	544.43	256.779	-2.90
1H'-TS	-61894.589	595.80	277.65	-3.52
1I	-55606.592	546.71	261.03	-3.40
1I'	-61895.863	597.20	282.87	-2.98
1J	-66606.977	530.502	256.373	-5.97
1K	-74982.938	608.97	285.05	-7.04
2	-66579.164	518.29	270.42	-2.80
2-TS	-66578.695	518.21	271.38	-3.15
2A	-66579.836	519.74	269.49	-6.49
2A^a	-3243.407	-	-	-
2A^b	-63368.879	-	-	-
2B	-66579.297	519.821	271.11	-7.76
2C	-68120.195	544.018	284.134	-7.99
2C'	-74409.516	595.284	305.666	-7.11
2D	-111176.195	861.32	455.90	-8.70
2D'	-117465.523	912.51	463.66	-7.38
2E	-104814.039	773.83	416.41	-6.76
2E'	-111103.742	825.09	439.08	-6.86
2F	-55577.332	534.20	273.60	-6.43
2F'	-61866.969	584.68	296.77	-6.01
2G	-55578.031	534.77	267.20	-3.84
2G'	-61867.715	585.66	292.22	-4.36
2G-TS	-55577.441	534.21	265.83	-3.30

2G'-TS	-61867.074	585.22	289.72	-4.01
2H	-55579.063	536.30	272.39	-3.51
2H'	-61868.227	586.62	295.91	-3.29
2I	-66579.109	519.603	266.499	-6.36
3	-72934.726	601.80	289.23	-2.78
3-TS	-72934.304	601.72	287.63	-3.54
3A	-72935.453	603.35	286.88	-6.32
3A^a	-6421.110	-	-	-
3A^b	-66546.586	-	-	-
3B	-72934.656	603.962	286.054	-6.15
3C	-74475.531	629.03	288.55	-5.75
3C'	-80764.797	680.07	307.65	-5.09
3D	-117531.414	944.49	461.23	-8.54
3D'	-123820.727	996.72	479.49	-7.60
3D-TS	-117531.352	943.87	448.09	-6.48
3D'-TS	-123820.461	995.28	470.33	-6.34
3E	-117531.352	945.50	456.16	-5.90
3E'	-123820.500	996.23	478.65	-6.20
3F	-111169.266	858.72	427.95	-5.31
3F'	-117458.602	909.84	445.68	-6.66
3G	-111169.578	856.75	435.55	-8.89
3G'	-117459.000	908.72	451.15	-9.81
3H	-61933.608	618.52	283.97	-4.02
3H'	-68223.227	669.50	308.86	-4.15
3H-TS	-61933.017	617.94	281.64	-3.49
3H'-TS	-68222.656	669.21	298.02	-3.86
3I	-61934.592	619.80	290.34	-3.47
3I'	-68223.870	670.25	313.25	-3.40
3J	-72934.922	603.36	287.72	-6.89
3K	-74475.844	627.66	299.20	-6.91
3K'	-80765.117	678.64	322.36	-5.63
3L	-68295.242	706.51	310.21	-3.36
3L'	-74584.422	758.62	332.54	-3.32
3L-TS	-68294.852	703.37	310.01	-2.95

3L'-TS	-74584.281	755.40	329.24	-3.56
3M	-117531.836	945.31	466.72	-7.91
3M'	-123821.164	996.59	479.85	-6.91
3M-TS	-117531.398	941.61	463.41	-8.67
3M'-TS	-123820.836	992.48	483.44	-7.72
3N	-81310.641	683.08	307.75	-6.09

^aR₁ fragment in Figure S3, ^bCatalyst fragment in Figure S3.

6. References

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