

Supporting Information

The Origin of the Ligand-Controlled Regioselectivity in Rh-Catalyzed [(2+2)+2] Carbocyclizations: Steric vs. Stereoelectronic Effects

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Computational Details

All calculations were carried out using DFT¹ as implemented in the Jaguar 8.1 suite of ab initio quantum chemistry programs.² Structures were optimized with the B3LYP³⁻⁷ functional including Grimme's D3 dispersion correction⁸ and the 6-31G** basis set. The Los Alamos LACVP⁹⁻¹¹ basis that includes relativistic effective core potentials was used to represent Rh. Additional single point calculations were performed on each optimized geometry using Dunning's correlation consistent triple- ζ basis set cc-pVTZ(-f)¹² that includes a double set of polarization functions to improve the electronic energy. For Rh, we used a modified version of LACVP, designated as LACV3P, in which the exponents were decontracted to match the effective core potential with triple- ζ quality. Solvation energies were evaluated by a self-consistent reaction field (SCRf)¹³⁻¹⁵ approach based on accurate numerical solutions of the Poisson-Boltzmann equation. Solvation calculations were carried out with the 6-31G**/LACVP basis at the optimized gas-phase geometry employing the dielectric constants of $\epsilon = 7.6$ for THF and 2.284 for benzene. Reactions using PPh₃ as the ligand were performed in benzene and those using xylbinap were done in THF for solubility of the ligand.¹⁶ As is the case for all continuum models, the solvation energies are subject to empirical parameterization of the atomic radii that are used to generate the solute surface. We employed the standard set of optimized radii in Jaguar for H (1.150 Å), C (1.900 Å), P (2.074 Å), O (1.600 Å), and Rh (1.464 Å). Analytical vibrational frequencies within the harmonic approximation were computed with the 6-31G**/LACVP basis to confirm that all intermediates had no imaginary frequencies except for transition states, which possessed one imaginary frequency.

The energy components have been computed with the following protocol. The change in Gibbs free energy in solution phase $\Delta G(\text{Sol})$ has been calculated as follows:

$$\Delta G(\text{Sol}) = \Delta G(\text{gas}) + \Delta G^{\text{solv}} \quad (1)$$

$$\Delta G(\text{gas}) = \Delta H(\text{gas}) - T\Delta S(\text{gas}) \quad (2)$$

$$\Delta H(\text{gas}) = \Delta E(\text{SCF}) + \Delta ZPE + \Delta C_v T + \Delta PV \quad (3)$$

$$\Delta H(\text{gas}) \approx \Delta E(\text{SCF}) + \Delta ZPE \quad (4)$$

$G(\text{gas})$ is the Gibbs free energy in gas phase; $G(\text{solv})$ is the free energy of solvation as computed using the continuum solvation model; $H(\text{gas})$ is the enthalpy in gas phase; T is the temperature (333 K); $S(\text{gas})$ is the entropy in gas phase; $E(\text{SCF})$ is the self-consistent field energy, i.e. "raw" electronic energy as computed from the SCF procedure and ZPE is the zero point energy. Note that by entropy here we refer specifically to the vibrational/rotational/translational entropy of the solute(s); the entropy of the solvent is incorporated implicitly in the continuum solvation model. As the contributions from the last two terms in equation 3 are negligibly small, this equation can be essentially reduced to equation 4.

To locate transition states, the potential energy surface was first explored approximately using the linear synchronous transit (LST) method,¹⁷ followed by a quadratic synchronous transit (QST)¹⁸ search using the LST geometry as an initial guess.

References

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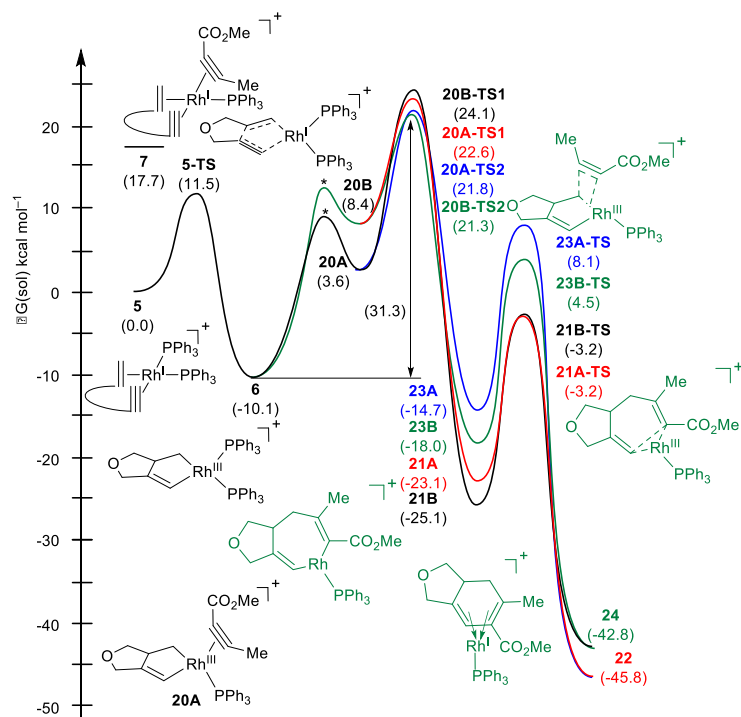


Figure S1. Regiodivergent reaction energy profiles for the Rh-catalyzed [2 + 2 + 2] carbocyclization with one PPh₃ ligand bound during alkyne insertion. Transition states indicated by * were not explicitly located and are shown for illustration only.

The reaction profile for alkyne insertion and subsequent product generation with only one monodentate phosphine ligand bound to Rh is shown in Figure S1. Our calculations indicate that the alkyne bound intermediates **20A** and **20B** with only one phosphine attached are 7.5 and 12.3 kcal mol⁻¹ higher in energy

than **8C**, respectively. These intermediates are still accessible under the experimental conditions and dissociation of a phosphine ligand provided a sensible hypothesis for the observed change in regioselectivity when a bulky bidentate ligand such as xyl-binap was used. The calculated activation barriers for alkyne insertion with only one phosphine ligand attached, however, are much too high to be accomplished with the lowest barrier height **20B-TS2** being 31.33 kcal mol⁻¹ uphill with respect to **6**. Moreover, **20B-TS2** is expected to generate the wrong regioisomer compared to experiments with monodentate phosphine. Whereas the lowest energy pathway **20A-TS2** leading to the expected regioisomeric product is only 0.5 kcal mol⁻¹ higher in energy, the calculated energy differences are too small to explain the experimentally observed product ratios.

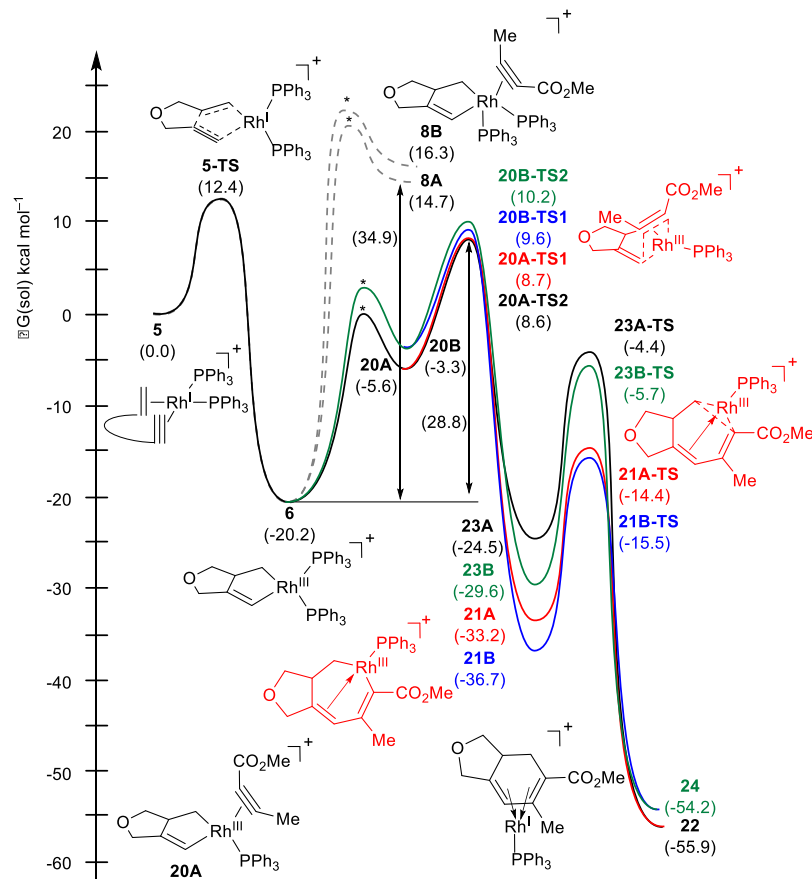


Figure S2. Regiodivergent reaction energy profiles for the Rh-catalyzed [2 + 2 + 2] carbocyclization calculated with B3LYP without Grimme's D3 dispersion correction.^[S1] Transition states indicated by * were not explicitly located and are shown for illustration only.

When the reaction profile is computed with B3LYP without including Grimme's D3 correction to account for noncovalent interactions, dissociation of a PPh₃ ligand prior to alkyne binding is computed to be favorable by 5.6 kcal mol⁻¹. B3LYP and B3LYP-D3 give a less than 1 kcal mol⁻¹ energy difference (Figure 1 and Figure S1) for the barrier of **5-TS**. Intermediates **8A** and **8B** are substantially higher in energy than intermediates **20A** and **20B** where only one phosphine ligand remains bound to Rh. Surprisingly, insertion into the Rh–alkyl bond through **20A-TS2** is calculated to be essentially isoenergetic with insertion into the Rh–alkenyl bond. Transition states **20A-TS1** and **20A-TS2** both lead to the correct experimentally observed regioisomer with an activation barrier of about 28.8 kcal mol⁻¹.

However, when (S)-xyl-binap is used as the ancillary ligand the lowest calculated barrier to alkyne insertion increases to 37.0 kcal mol⁻¹. Utilizing dispersion corrections to account for noncovalent actions seems to be critical to properly assess ligand binding energies and accurately predict the correct regioisomeric products.

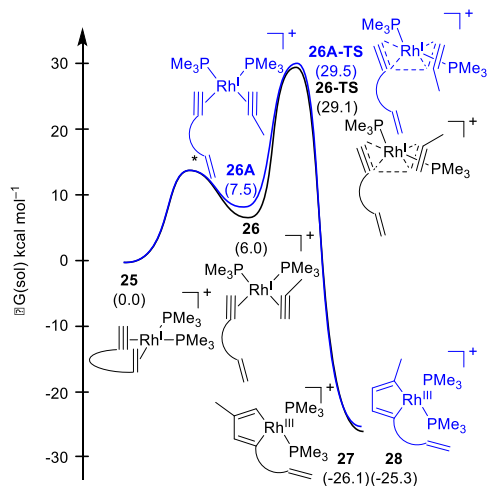


Figure S3. Reaction profile for coupling of alkyne of 1,6-ene-yne with methyl substituted alkyne substrate to produce the rhodacyclopentadiene with a dangling tethered alkyne computed with B3LYP.

A small model was used to explore the above pathway in Figure S3, which shows coupling of the alkyne of the 1,6-ene-yne with the methyl-substituted alkyne substrate. In this slightly truncated model the PPh₃ ligand was replaced by PMe₃ and the ester moiety of the alkyne substrate was replaced by hydrogen. Binding an equivalent of alkyne in place of the alkene fragment of the 1,6-ene-yne is uphill by 6.0 kcal mol⁻¹. The oxidative addition has a barrier of 29.1 kcal mol⁻¹ compared to only 12.4 kcal mol⁻¹ for the coupling of the alkyne and alkene shown in Figure S1. As such, this pathway was not explored any further.

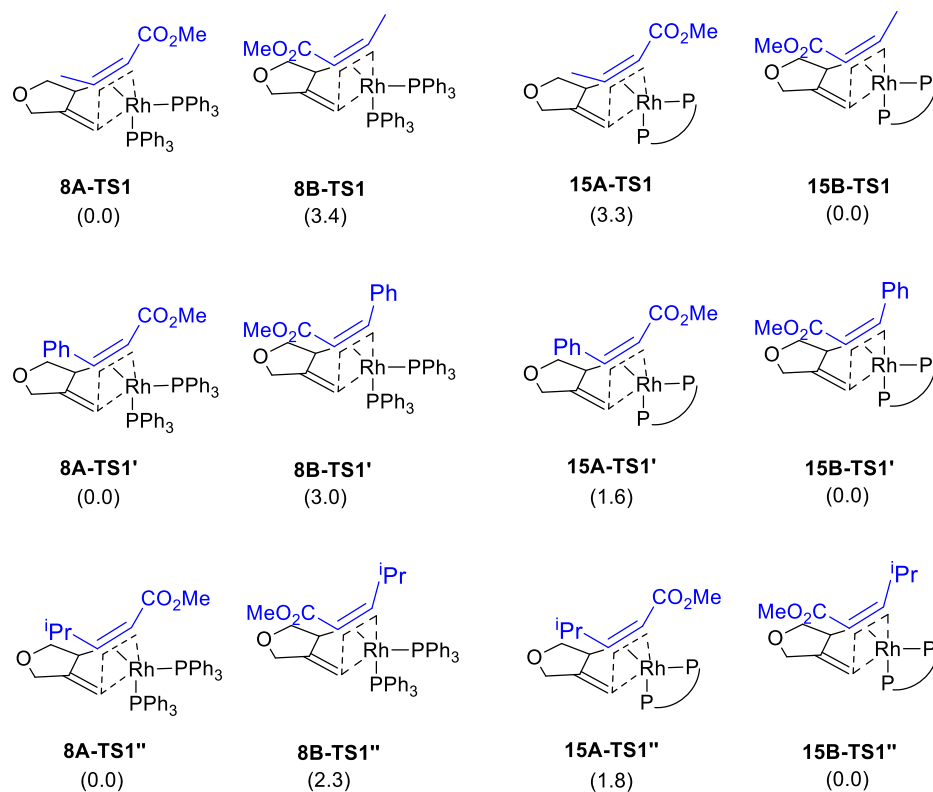


Figure S4. Relative energies of the key transition states using different substrates in kcal mol⁻¹

Unlike the ester moiety, the aryl and isopropyl fragments are able to rotate away to avoid a steric clash with the phosphine ligands bound to Rh. This flexibility of the aryl and alkyl substituents results in the change in regioselectivity being observed when the ancillary ligand is changed from L = PPh₃ to L = (*S*)-xyl-binap despite an increase in the steric bulk attached to the alkyne substrate.

Table S1. Energy components of optimized structures (L = PPh₃) in kcal/mol

Structure	E(SCF) (kcal/mol) cc-pVTZ(-f)	ZPE	TS (333 K)	G (solv) $\epsilon = 2.284$	G(sol) $\epsilon = 2.284$
1	-216276.66	62.56	31.04	-3.64	-216248.79
2	-193696.82	76.94	30.63	-2.65	-193653.16
PPh₃	-650459.05	171.99	46.57	-3.10	-650336.73
3	-410066.85	146.68	40.88	-4.04	-409965.09
4	-410067.77	146.76	40.62	-4.08	-409965.71
5	-1563305.48	426.77	88.09	-21.05	-1562987.85
5-TS	-1563292.70	426.82	89.04	-21.43	-1562976.35
6	-1129099.66	317.46	75.81	-24.18	-1128882.19
6-TS	-1129081.09	316.66	75.68	-23.82	-1128863.94
7	-1563313.85	427.03	89.48	-21.60	-1562997.90
8A	-1779603.20	492.68	103.61	-23.13	-1779237.26
8B	-1779605.27	492.54	103.51	-23.42	-1779239.66
8C	-1779608.45	492.83	101.81	-23.10	-1779240.53
8C-BPR	-1779601.74	492.14	103.48	-22.40	-1779235.48
8A-TS1	-1779599.16	491.94	102.74	-23.73	-1779233.69
8A-TS2	-1779591.57	491.68	103.29	-22.89	-1779226.07
8B-TS1	-1779599.67	491.77	98.67	-23.71	-1779230.28
8B-TS2	-1779589.80	491.59	102.15	-22.93	-1779223.29
9A	-1779642.21	493.91	101.32	-22.09	-1779271.71
9B	-1779639.10	494.35	103.62	-23.11	-1779271.48
11A	-1779638.09	493.36	103.75	-22.72	-1779271.19
11B	-1779648.42	493.80	101.71	-21.55	-1779277.88
9A-TS	-1779632.97	493.98	100.91	-21.88	-1779261.78
9B-TS	-1779633.91	493.83	98.00	-22.76	-1779260.84
11A-TS	-1779623.37	493.28	101.61	-22.17	-1779253.88
11B-TS	-1779624.04	493.32	103.32	-21.74	-1779255.78
10	-1779677.08	495.97	97.90	-21.78	-1779300.79
12	-1779671.18	496.16	98.43	-21.85	-1779295.30
20A	-1129112.11	317.86	77.61	-24.45	-1128896.31
20B	-1129107.71	317.54	76.64	-24.73	-1128891.54
20A-TS1	-1129092.62	317.11	77.28	-24.50	-1128877.29
20A-TS2	-1129095.92	317.63	76.36	-23.47	-1128878.12
20B-TS1	-1129090.99	316.96	76.81	-24.96	-1128875.79
20B-TS2	-1129095.58	317.62	76.60	-24.07	-1128878.63
21A	-1129143.66	319.91	75.02	-24.21	-1128922.98
21B	-1129143.54	319.58	76.31	-24.70	-1128924.97
23A	-1129131.44	319.84	75.47	-27.53	-1128914.59
23B	-1129140.38	320.73	71.77	-26.46	-1128917.89
21A-TS	-1129124.40	319.06	73.99	-23.73	-1128903.06
21B-TS	-1129124.15	319.15	74.02	-24.08	-1128903.09
23A-TS	-1129111.30	318.86	74.86	-24.53	-1128891.84
23B-TS	-1129117.25	319.02	73.57	-23.57	-1128895.37
22	-1129169.53	321.06	74.19	-23.07	-1128945.73
24	-1129167.34	321.38	73.70	-23.03	-1128942.70
25	-841139.81	224.03	57.47	-28.99	-841002.24
26	-914376.54	258.84	69.75	-26.84	-914214.29
26A	-914375.27	258.82	69.56	-26.76	-914212.76
26-TS	-914356.80	258.89	66.97	-26.31	-914191.19
26A-TS	-914355.81	259.01	67.50	-26.48	-914190.78
27	-39652.677	261.74	66.93	-28.98	-914246.41
28	-39652.706	261.88	66.47	-28.13	-914245.63

Table S2. Energy components of optimized structures (L = Xyl-binap) in kcal/mol

Structure	E(SCF) (kcal/mol) cc-pVTZ(-f)	ZPE	TS (333 K)	G (solv) $\epsilon = 7.6$	G(sol) $\epsilon = 7.6$
1	-216276.66	62.56	31.04	-6.52	-216251.67
13	-1952897.71	609.62	121.97	-31.87	-1952441.92
13-TS	-1952891.25	609.18	118.47	-31.83	-1952432.37
14	-1952900.63	610.76	122.98	-33.24	-1952446.10
15A	-2169194.75	675.28	133.53	-34.13	-2168687.14
15B	-2169193.58	675.64	134.06	-34.24	-2168686.23
15A-TS1	-2169184.84	675.70	132.53	-34.34	-2168676.01
15A-TS2	-2169178.15	675.17	132.50	-34.44	-2168669.92
15B-TS1	-2169185.90	675.03	134.75	-33.72	-2168679.34
15B-TS2	-2169176.05	675.13	131.30	-34.57	-2168666.79
16A	-2169239.49	676.82	131.82	-34.18	-2168728.67
16B	-2169234.40	677.18	131.62	-33.88	-2168722.71
18A	-2169223.44	676.78	133.35	-36.18	-2168716.20
18B	-2169229.02	677.23	133.90	-33.40	-2168719.09
16A-TS	-2169221.46	677.21	127.20	-33.89	-2168705.34
16B-TS	-2169221.37	676.95	129.61	-33.60	-2168707.63
18A-TS	-2169202.76	676.09	125.91	-34.18	-2168686.76
18B-TS	-2169206.72	676.91	129.97	-33.86	-2168693.64
17	-2169269.01	679.49	131.16	-32.49	-2168753.17
19	-2169261.31	680.03	129.40	-32.45	-2168743.13

Table S3. Energy components of optimized structures with (R = C₆H₅ or C₃H₇)

Structure	E(SCF) (kcal/mol) cc-pVTZ(-f)	ZPE	-TS (333 K)	G (solv) ^a $\epsilon = 2.284$ ^b $\epsilon = 7.6$	G(sol) ^a $\epsilon = 2.284$ ^b $\epsilon = 7.6$
8A-TS1'	-1899959.79	525.45	108.43	-22.39 ^a	-1899565.16 ^a
8B-TS1'	-1899958.06	525.34	106.91	-22.45 ^a	-1899562.08 ^a
8A-TS1''	-1828964.31	528.10	106.83	-22.29 ^a	-1828565.33 ^a
8B-TS1''	-1828961.57	528.10	107.18	-22.38 ^a	-1828563.03 ^a
15A-TS1'	-2289543.80	709.34	135.37	-34.20 ^b	-2289004.04 ^b
15B-TS1'	-2289542.65	708.52	137.69	-33.83 ^b	-2289005.65 ^b
15A-TS1''	-2218547.13	711.58	132.56	-33.65 ^b	-2218001.92 ^b
15B-TS1''	-2218547.13	711.35	134.72	-33.19 ^b	-2218003.68 ^b

Table S4. Cartesian coordinates of optimized geometries

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Rh(PPh₃)₂

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H 4.786329917 -2.131915737 2.017233909
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5

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5-TS

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6

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7

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C 5.570060881 -2.529612709 4.970671816
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7-TS

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8A

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8B

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8C

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C 3.705967907 -0.851446556 3.054860331
H 3.800320688 -1.545752195 2.229101654
C 3.727417030 0.052197575 -0.065997711
C 4.696829462 0.512147048 -0.969767693
H 5.058123773 1.533057040 -0.913620966
C 5.210685414 -0.340156427 -1.949750396
H 5.958742947 0.032348686 -2.643312596
C 4.771718686 -1.660535307 -2.036503598
H 5.174480773 -2.321171187 -2.798276161
C 3.807712349 -2.128128038 -1.140885643
H 3.455816468 -3.153674154 -1.203402429
C 3.277010551 -1.275665387 -0.175921080
H 2.501744341 -1.648072536 0.482051445

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8C-BPR

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C 1.074541205 0.482752594 0.231309233
C 2.752070957 -1.311007715 -0.971195453
Rh 1.653741129 -1.354926600 0.841250194
P 3.782292864 -2.107693838 2.067269215
P -0.206385253 -2.067027418 -0.289044139
C 1.836145397 0.991627026 -0.733084145
C 2.947916161 0.166354985 -1.316170075
C 2.886829321 0.643411296 -2.780922326
C 1.701174733 2.240837898 -1.583168059
O 2.620283191 2.044399521 -2.664147793
H 3.697252539 -1.833847826 -0.843843355
H 2.184569305 -1.827442731 -1.744761286
H 0.206935283 0.970414684 0.665698277
H 0.668655345 2.336093135 -1.954919212
H 1.972161753 3.170463591 -1.069907213
H 3.821956590 0.527818258 -3.334918704
H 2.079176074 0.124093818 -3.319813095
H 3.904199332 0.517938868 -0.901603460
C 0.630552551 -0.822934010 3.180176116
C 0.224937962 -1.967366716 3.282993330
C -0.263761823 -3.321590598 3.481913144
C 0.884259091 0.595884108 3.377060385
H -0.876193187 -3.648210675 2.635661456

H 0.566356783 -4.019740707 3.630393042
H -0.892057739 -3.342483237 4.379995893
O 2.089436481 0.787075241 3.930185446
O 0.098669372 1.471785199 3.078611637
C 2.466854767 2.164680082 4.159500866
H 3.486539128 2.119350552 4.537150230
H 2.427364843 2.723343255 3.221640967
H 1.792141227 2.623274894 4.886670718
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C 0.076592272 -1.940420236 -3.113342346
C -1.326294359 -0.252580135 -2.094745021
C -0.113936907 -1.341531742 -4.359942993
C -1.504238920 0.347411613 -3.340529939
C -0.896951979 -0.192412063 -4.476914875
H 0.693550572 -2.830510106 -3.045628424
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H 0.357502991 -1.773126143 -5.237980477
H -2.122192229 1.236621338 -3.422764558
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C -1.811512757 -1.860837451 0.584140676
C -2.829038408 -2.814667930 0.413078802
C -2.063504689 -0.724119993 1.368147240
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C -3.312228877 -0.543357131 1.962087311
C -4.318831504 -1.492722189 1.784548510
H -2.655477170 -3.704856159 -0.181341834
H -1.296674376 0.016262589 1.546472029
H -4.852040164 -3.373339618 0.872204026
H -3.488552224 0.340215621 2.567862958
H -5.290163861 -1.350616452 2.248959850
C 0.017174985 -3.883566320 -0.470353471
C 0.801398085 -4.561339110 0.479065127
C -0.594078625 -4.629634253 -1.492466693
C 0.986217825 -5.941346340 0.402704004
C -0.408889507 -6.011269352 -1.565826571
C 0.384061864 -6.671211957 -0.623671073
H 1.278171540 -4.013275950 1.286121841
H -1.212075048 -4.135608515 -2.235452059
H 1.601894630 -6.440206161 1.145824378
H -0.887007079 -6.572120437 -2.363635792
H 0.526854022 -7.745636372 -0.687882240
C 3.422142062 -3.143886706 3.541187097
C 3.005253045 -2.539113337 4.739768183
C 3.449669714 -4.546116873 3.458984317
C 2.631710357 -3.323895433 5.830435264
C 3.067227496 -5.325802617 4.552981672
C 2.654970271 -4.718640323 5.741028180
H 2.969889019 -1.457192006 4.818402398
H 3.787350543 -5.034156970 2.549785972
H 2.319917793 -2.843040319 6.753355266
H 3.103887840 -6.409038729 4.477934984
H 2.362828370 -5.325938549 6.592504788
C 4.935109473 -3.143621290 1.084317615
C 6.324041273 -3.110645159 1.274738401
C 4.395761214 -4.039140157 0.145312686
C 7.152594365 -3.964831099 0.546558983
C 5.226114280 -4.899508797 -0.571636361
C 6.607191615 -4.864247956 -0.371306834
H 6.763908482 -2.419084549 1.985668223
H 3.325256019 -4.065343962 -0.030462762
H 8.227294474 -3.928456107 0.699514886

H 4.793987995 -5.589927632 -1.290588184
H 7.256845472 -5.528558796 -0.933838685
C 4.777692464 -0.703143435 2.678102934
C 5.656346289 -0.823578472 3.766346503
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C 5.483297542 1.598474883 2.381770924
C 6.362891398 1.470232624 3.459051303
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H 7.118660586 0.161436061 4.999040470
H 5.409715034 2.540200570 1.845474956
H 6.981778894 2.310732685 3.759843007

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8A-TS1
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C 2.608104503 -0.170979936 0.546676629
C 0.613070864 -0.016179601 2.668546959
Rh 0.945723220 -1.358791965 1.045344166
P 1.857811392 -3.095734182 2.632505410
P 1.080875372 -2.732825941 -0.918300401
C 0.768445634 1.037775633 -0.576178830
C 2.121339141 1.182243806 0.066129797
C 2.899963908 1.856866502 -1.089391622
C 0.685845740 2.025694510 -1.719060087
O 1.940948749 2.713855204 -1.702014840
H 3.179754292 -0.110593245 1.468875810
H 3.145710949 -0.724026317 -0.223745584
H -0.999664966 -0.157017577 -0.657469218
H 0.529015558 1.502614486 -2.673303300
H -0.112972236 2.766795012 -1.593752624
H 3.743183150 2.470417918 -0.763115414
H 3.264281031 1.091636802 -1.795771386
H 2.050556915 1.885396177 0.907534479
C -1.758361652 0.875052929 1.869779791
H -2.458466998 0.146098708 1.448475431
H -2.091043762 1.141419239 2.880070817
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C 1.237755733 0.233108804 3.975774220
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H 3.282853617 1.095439682 5.490273000
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H 4.217009543 -0.385213578 5.075600935
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C 1.812265153 -1.222464688 -3.162458751
C -0.546242282 -1.740176273 -3.032238381
C 1.589887547 -0.491421515 -4.328285356
C -0.765602953 -1.002495779 -4.198339707
C 0.298445251 -0.376297348 -4.849976336
H 2.823646278 -1.314472295 -2.777775943
H -1.383634694 -2.233044703 -2.548151967
H 2.425683902 -0.010621062 -4.828153971
H -1.771407767 -0.926764966 -4.601711730
H 0.124854605 0.191755703 -5.758826968
C 2.652651187 -3.581408108 -1.315781474
C 2.784509868 -4.345494010 -2.489016144
C 3.771476678 -3.407484793 -0.492537492

C 3.994649221 -4.965778929 -2.791515510
C 4.987684202 -4.017811661 -0.802331481
C 5.097538597 -4.806914964 -1.947008950
H 1.947409863 -4.441552467 -3.173860980
H 3.697386547 -2.806800006 0.403227380
H 4.081646223 -5.564134475 -3.693695597
H 5.840339499 -3.875555928 -0.144359632
H 6.040821953 -5.287227006 -2.190411775
C -0.262066311 -3.972699816 -0.782133710
C -1.468055566 -3.526573065 -0.210302638
C -0.169958675 -5.298238459 -1.222499301
C -2.565547823 -4.379291578 -0.107528514
C -1.270116717 -6.149262508 -1.116471473
C -2.469052982 -5.693375248 -0.568123398
H -1.554356230 -2.501327214 0.145396937
H 0.760164926 -5.680683086 -1.624941982
H -3.492192966 -4.019185760 0.330422486
H -1.184530741 -7.177098917 -1.456444200
H -3.321812068 -6.361385587 -0.490425653
C 1.399346949 -4.833095451 2.164026220
C 0.156253062 -5.374326475 2.526351607
C 2.295590693 -5.637656755 1.439960247
C -0.172816869 -6.686400968 2.188424788
C 1.964514698 -6.950306665 1.108188518
C 0.731206319 -7.481481621 1.484919126
H -0.555426826 -4.790492598 3.097657185
H 3.268276822 -5.258330972 1.154676236
H -1.137261730 -7.087537117 2.485744294
H 2.679911172 -7.558428916 0.561856072
H 0.476530652 -8.507173948 1.233662369
C 3.634369092 -3.269982904 3.082073077
C 4.112014492 -4.442621729 3.695342672
C 4.535180310 -2.224231847 2.838812904
C 5.456152135 -4.562299226 4.045122321
C 5.882274411 -2.348208106 3.182663831
C 6.346132904 -3.517863529 3.785659663
H 3.435193424 -5.266446108 3.896395819
H 4.185405686 -1.307581697 2.387595277
H 5.808060908 -5.474386674 4.518554044
H 6.566541037 -1.529576113 2.978679699
H 7.394274183 -3.616360915 4.053006282
C 0.991951229 -2.901497567 4.251233540
C -0.376735542 -2.582233187 4.245962581
C 1.638372468 -3.075229814 5.483006280
C -1.082966320 -2.451803489 5.440115748
C 0.930496866 -2.935019016 6.677607851
C -0.429067918 -2.624665835 6.660335646
H -0.896877513 -2.424246050 3.305049158
H 2.695404272 -3.313374373 5.519136578
H -2.139827860 -2.203201975 5.417261668
H 1.446859002 -3.069396945 7.623891136
H -0.975020671 -2.512399895 7.592094086

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8A-TS2
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C -0.636012362 -0.092945386 0.737502056
C 0.562318952 -0.588941853 2.573637586
Rh 1.628626251 -0.022949525 0.776870348
P 1.637346998 2.478907402 1.418598970
P 3.822978160 0.034408862 -0.157016380
C 1.315075146 -1.839276314 -0.120130012

C 0.049655590 -2.257384200 -0.213185378
C -1.081836512 -1.484414225 0.411186712
C -2.137310329 -1.646164446 -0.713545951
C -0.576335765 -3.316289045 -1.105253719
O -1.973510987 -2.997418613 -1.131531690
H -1.235478484 0.492126198 1.425227494
H -0.413921171 0.491622125 -0.163648796
H 2.139651334 -2.390766331 -0.565654844
H -0.145682968 -3.292266911 -2.117174370
H -0.466401884 -4.333569326 -0.709478375
H -3.168099044 -1.516439418 -0.375331676
H -1.935720887 -0.936244698 -1.534230057
H -1.464588258 -2.003636727 1.298851597
C 1.635155814 -1.276958101 2.390201136
C 2.567098696 -2.303571718 2.887211271
H 3.569089130 -1.877819737 3.009978293
H 2.216597028 -2.688288773 3.850657524
H 2.639659328 -3.127835847 2.170834247
C -0.284852244 -0.077437721 3.657445928
O -1.133574092 0.787361595 3.563185489
O 0.063445339 -0.674825767 4.813716322
C -0.630136967 -0.185644973 5.985205706
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C 4.904057068 -2.535834714 -0.137217399
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H 4.980486639 -2.385189692 0.935921331
H 3.991505571 -0.923136508 -2.999778950
H 5.673435563 -4.541289658 -0.044803767
H 4.693139976 -3.077162279 -3.968664741
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C 3.776314016 1.282575284 -1.496809140
C 2.655805059 1.240659021 -2.347926008
C 4.755341756 2.261283912 -1.702321100
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C 6.525305602 0.459165760 0.525386626
C 4.940612541 0.629042435 2.345535319
C 7.565021910 0.738604521 1.410821012
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C 7.297246635 0.963037758 2.765047738
H 6.746199844 0.256571421 -0.518690429
H 3.920528585 0.594547245 2.706805917
H 8.587061926 0.772838677 1.045041608
H 5.765715691 1.065327240 4.283559313
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C 2.831542862 3.739729121 0.771278955
C 2.511666826 4.677488656 -0.219308754
C 4.110194772 3.782628379 1.352596190

C 3.452444963 5.625573104 -0.625525048
C 5.047841579 4.726343358 0.941502081
C 4.722408373 5.652447858 -0.052100974
H 1.527803985 4.694119185 -0.670824502
H 4.373602682 3.092023097 2.144842995
H 3.182774138 6.348431408 -1.390414028
H 6.029512896 4.743133369 1.406604394
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C 1.704753427 2.887020922 3.211402990
C 1.473226650 4.208327305 3.631337405
C 2.055991922 1.928785934 4.169358936
C 1.565324330 4.550339602 4.978398822
C 2.157399451 2.273413558 5.519552020
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H 1.225474659 4.971158286 2.899629777
H 2.238111476 0.904746605 3.872640624
H 1.377679570 5.574894798 5.286218071
H 2.432304322 1.514248303 6.246479545
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C -1.488318459 3.352780502 -1.080058384
C -2.301713239 3.736168292 1.160904628
C -2.524334423 3.716701935 -0.215260641
H 0.553456517 2.710503553 -1.246126288
H -0.904107944 3.394718480 2.755192334
H -1.655890407 3.325929099 -2.153259681
H -3.107787289 4.000475622 1.839024115
H -3.501197099 3.974629525 -0.613874169

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8B-TS1

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C 1.294293373 0.060936000 2.721961877
Rh 1.350033149 -1.258348401 1.014627647
P 3.131876985 -2.608698810 1.971046595
P 0.823315233 -2.690929523 -0.952490607
C 0.420554393 1.056461228 -0.434830515
C 1.839994203 1.425307618 -0.078137497
C 2.223650300 2.278288870 -1.313554429
C -0.060940527 2.040267030 -1.482247288
O 1.020612953 2.959394386 -1.651344880
H 3.466983631 0.294700273 0.878943845
H 2.980064588 -0.302055469 -0.742833857
H -1.125215980 -0.412582271 -0.186832291
H -0.291308008 1.515326250 -2.421966353
H -0.947156066 2.605079591 -1.172624854
H 2.993372645 3.027767764 -1.114893490
H 2.557371007 1.622733118 -2.134766486
H 1.832405544 2.069244719 0.812174414
C 2.194078505 0.686774426 3.710407287
H 3.128774328 1.021856865 3.253680240
H 1.676588574 1.542163345 4.156904921
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O -2.206039036 -0.451508089 2.031901445
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H -3.847932789 0.841091874 2.136550711
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C -0.565616117 -0.603470014 -4.242218833
C 0.608409046 -0.097603106 -4.800432321
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C 1.748790805 -4.204662107 -1.450651694
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C 2.360946869 -4.381196579 -2.698055944
C 2.503072755 -6.414517205 -0.788240616
C 3.053809438 -5.560497338 -2.977581836
C 3.137007413 -6.573403468 -2.022786472
H 1.296561963 -5.141199517 0.442682362
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C 4.499332034 -3.229193209 0.927479800
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C 4.538061459 -2.935209131 -0.438743412
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C 5.591112231 -3.384946432 -1.234305142
C 6.624300533 -4.127323424 -0.664949932
H 5.575022233 -4.146666538 2.568499993
H 3.737701974 -2.359155350 -0.881037093
H 7.421476098 -4.970767874 1.154715318
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C 2.250815579 -4.054840407 2.682893240
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C 2.749375540 -5.365395020 2.649520571
C 0.248228287 -4.870374053 3.797607754
C 2.001918621 -6.414788883 3.183493035
C 0.751871959 -6.171263476 3.757278701
H 0.595280453 -2.806679582 3.313018035
H 3.703729659 -5.576467381 2.180920447
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8B-TS2
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P 2.417849770 2.625724487 1.011091076
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9A

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C 0.164069927 1.834953673 -3.429000272
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H -0.647606393 3.262293395 -0.545878241
H 1.008870854 3.024326881 -1.194503327
H -0.114864280 -1.676528350 -0.710429720

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H 1.036297834 -1.244810732 -3.033969093
H -0.535443686 2.285661660 -4.135778953
H 1.065204712 2.467663183 -3.368614090
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H	5.298361397	-3.999037895	-1.008105053	C	2.901291849	2.929798965	2.295365378
C	2.545555572	-0.582394167	3.555832651	C	3.661431892	3.480136287	1.249753916
C	2.049330055	-0.952081706	4.812337936	H	3.189037086	4.061834016	0.468006914
C	3.849513888	-0.063115545	3.468784574	C	5.045098066	3.305567723	1.212796844
C	2.841325953	-0.807280355	5.954045729	H	5.615977391	3.743014761	0.398822372
C	4.634599641	0.080770453	4.610203552	C	5.694211073	2.583976151	2.217194240
C	4.133933272	-0.292288849	5.860301052	H	6.770901409	2.447536119	2.183958885
H	1.051659520	-1.365469309	4.909319610	C	4.948222173	2.050065335	3.268426683
H	4.265662712	0.212318576	2.505203106	H	5.434118811	1.490085903	4.061534103
H	2.441240138	-1.104231625	6.919315388	C	3.564352243	2.218286094	3.308411873
H	5.642297748	0.476838995	4.520382609	H	3.009162894	1.783483999	4.129010112
H	4.748544345	-0.189014988	6.749783512	C	0.592285780	4.650262917	1.677795552
C	0.213162710	-1.918866826	2.434751032	C	-0.055849492	5.531985371	2.557835662
C	0.148392993	-3.262211120	2.037816300	H	-0.273394239	5.231611204	3.576051192
C	-0.853779259	-1.372600552	3.167727036	C	-0.435252470	6.806386782	2.133945201
C	-0.951810425	-4.046249257	2.392346430	H	-0.936361009	7.471598542	2.830959036
C	-1.946323410	-2.158130663	3.525184909	C	-0.176961943	7.223805938	0.828674988
C	-1.996460330	-3.499843554	3.139584366	H	-0.474765167	8.215275797	0.501714134
H	0.953588899	-3.704703910	1.460979618	C	0.464585170	6.354280392	-0.055808524
H	-0.837864600	-0.328511073	3.455578748	H	0.668890101	6.665403718	-1.076065926
H	-0.989014171	-5.087328846	2.084446947	C	0.840479169	5.078452255	0.361108345
H	-2.764856468	-1.712560361	4.082035714	H	1.317476080	4.422024034	-0.354758010
H	-2.850517450	-4.113296741	3.411677301	O	-4.420496812	1.024285732	0.749495105
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9B							
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Rh	0.336743628	1.120461713	1.065590700	O	-3.835353529	-1.038408488	0.029258897
C	-1.182179574	-0.592937237	-0.028767691	C	-5.224028888	-1.418439455	0.095393624
C	0.737520480	1.883363028	-0.829082827	H	-5.257929131	-2.459461781	-0.224913794
C	-0.088126400	-0.494186949	-0.837850808	H	-5.601399530	-1.313529167	1.116120415
C	0.339824918	0.706695360	-1.700558047	H	-5.823294380	-0.790010059	-0.567979810
C	1.485305239	0.077235062	-2.531760406	P	1.708791171	-0.703251107	2.402402935
C	0.749528770	-1.677708506	-1.290638308	C	3.166391387	-1.233468972	1.428795773
O	1.194920654	-1.312379351	-2.592151577	C	3.766147195	-2.501104509	1.543115336
H	0.191452328	2.797294144	-1.053083425	C	3.737979974	-0.293026279	0.556901133
H	1.816027893	2.073346077	-0.810152501	C	4.873438121	-2.831615986	0.762036887
H	-1.432225729	-1.576923899	0.357791539	C	4.853779498	-0.622044189	-0.213145508
H	1.603425220	-1.849438645	-0.619743131	C	5.414663539	-1.896895500	-0.124957065
H	0.170168873	-2.602403071	-1.361118055	H	3.380712002	-3.225280574	2.253793463
H	1.543797238	0.460563108	-3.552803394	H	3.318271870	0.705599426	0.491790462
H	2.450725739	0.250220169	-2.027741804	H	5.317913559	-3.818409674	0.852018369
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C	-2.103170202	0.511085070	0.317611576	H	6.275201127	-2.158719868	-0.733078565
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C	-3.565797773	0.235992069	0.391685287	C	1.438084375	-0.352167216	5.185989844
C	-2.174859984	3.030427099	0.830757688	C	3.647704102	-1.015822739	4.476834354
H	-2.095758843	3.387961092	1.862702942	C	1.867093605	-0.337059121	6.512058249
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C	0.461346972	2.870518339	3.958018905	H	4.359881298	-1.270150559	3.700791423
C	1.147913187	3.488182478	5.015607378	H	1.165075935	-0.065945967	7.294754872
H	2.087209805	3.999879722	4.831393833	H	5.105999586	-1.246232899	6.037807991
C	0.628911119	3.444555524	6.309051673	H	3.522593375	-0.647716770	7.862775492
H	1.172455198	3.916538844	7.122012153	C	0.462860086	-2.068709989	2.404537058
C	-0.587062063	2.803783819	6.557918940	C	0.597771742	-3.285327566	1.722557160
H	-0.990940067	2.777231168	7.565821695	C	-0.752571011	-1.796450879	3.060359027
C	-1.284849425	2.201694222	5.509144241	C	-0.448179237	-4.211857803	1.713526756
H	-2.234546022	1.708600746	5.695547645	C	-1.789331679	-2.725967735	3.059380856
				C	-1.639877691	-3.939821109	2.384382795
				H	1.503590859	-3.516264723	1.176283117
				H	-0.909296396	-0.839019637	3.548029028

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H -2.449639483 -4.663150049 2.374356356

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11A
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C -0.306225447 -0.265290563 -0.231779904
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C 1.158818797 -0.994835232 -1.919907337
C -0.394338531 -1.781112899 -0.446773821
O 0.186453553 -2.014816787 -1.722903211
C 0.369432757 1.121286594 4.149030125
C -0.116193344 1.541596213 5.396442544
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C -0.619779462 0.606412472 6.304177513
H -0.989655336 0.943269252 7.268361223
C -0.640378051 -0.751540850 5.980940673
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H -0.146384541 -2.233340974 4.490865626
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H 0.721488682 -0.588282155 2.868129103
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H 1.406516183 -0.956742668 -2.983512652
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11B
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P 1.070829781 2.292536057 3.103472238
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C -1.408475669 -1.659250325 0.467912421
O -1.091656606 -2.184267708 -0.817254848
C 0.888019950 0.852719778 4.216178854
C 0.805361755 1.009875284 5.608506788
H 0.868701844 1.997715491 6.052546232
C 0.643175508 -0.105853867 6.431471735
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C 0.567776524 -1.385728795 5.879663187
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9A-TS

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9B-TS

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C 0.721719009 -1.880041414 -0.389189953
C -0.427443393 -1.023884277 -0.916788719
C 0.002084243 -0.849955902 -2.387416484
C 1.462448796 -2.432497256 -1.592498784
O 0.662080960 -2.064794742 -2.715426500
H -1.511845942 0.454228464 0.311506965
H -0.167035607 1.138443199 -0.591578248
H 1.543094805 -3.010893459 1.216301659
H 2.471505343 -2.007162606 -1.670937847
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H -1.935131709 0.033945150 3.115341308
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H	0.620899225	-4.193549968	5.053481732	H	2.610780619	2.591427939	-2.596404782
H	-1.088325737	-4.488100478	4.647285465	C	0.751253175	3.458837691	-3.222547959
P	3.817504805	-0.591782427	1.271900524	H	1.066391834	3.542083155	-4.258621409
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C	2.817553591	-1.408618812	3.783604399	H	-1.187312022	4.333666612	-3.572339173
C	4.983769860	-2.303893699	3.194677802	C	-0.904359022	3.803930085	-1.500328962
C	2.854193028	-2.107131878	4.990923407	H	-1.883445008	4.156799003	-1.189999416
C	5.023722955	-2.994557301	4.404001010	C	-0.036658958	3.256108115	-0.557639742
C	3.957767965	-2.900568161	5.303354586	H	-0.349315031	3.197671265	0.480070470
H	1.951415503	-0.806519363	3.547761395	C	2.245907180	3.194030725	1.747388972
H	5.812920281	-2.393501929	2.499231627	C	2.116895510	4.578140026	1.532597005
H	2.012745267	-2.030534713	5.673165170	H	2.016616646	4.966769271	0.523853719
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H	3.990744024	-3.446795938	6.241740403	H	2.014028840	6.525977101	2.435996370
C	4.425039519	-1.846868391	0.052873490	C	2.242444502	4.971677074	3.915894860
C	5.045008222	-1.455774902	-1.145183778	H	2.240971335	5.661159307	4.755314165
C	4.185427454	-3.215853091	0.262680771	C	2.366810983	3.599998663	4.136076417
C	5.407460992	-2.403057484	-2.104056267	H	2.464602345	3.211934036	5.145686489
C	4.555893904	-4.160439564	-0.694554167	C	2.365053796	2.712970009	3.059766409
C	5.161725879	-3.759122739	-1.886083633	H	2.441245867	1.649641835	3.252951693
H	5.266134163	-0.413425283	-1.337754755	H	-0.201501252	0.674436964	-0.782867053
H	3.727645591	-3.557483190	1.184583269	H	-2.550534073	-1.213352589	-1.313215615
H	5.888591153	-2.076236901	-3.021492842	H	-1.230018646	-1.376409766	-2.497597423
H	4.371384399	-5.213803504	-0.503971009	H	-1.369451086	-4.586792192	-0.123263177
H	5.446584342	-4.494381868	-2.632278946	H	-2.529429967	-3.335767452	0.397105379
C	5.199654016	0.620857720	1.374575954	H	0.510952705	-3.106130806	0.227505470
C	6.044201851	0.694850305	2.491868268	C	0.376843513	-1.341892878	2.522471628
C	5.439216877	1.484937707	0.292994265	C	-0.566448546	-2.407527857	1.960782770
C	7.121971774	1.580542790	2.504304427	C	-0.595265560	1.123073155	2.755686825
C	6.519721271	2.363977300	0.305630024	C	0.979095799	-1.506134512	3.872108669
C	7.372071790	2.407542866	1.409689195	H	-1.604104872	-2.137000973	2.201878605
H	5.864508834	0.073965630	3.361092150	H	-0.357323598	-3.341780115	2.486027359
H	4.775375158	1.494515891	-0.561145040	H	-0.498208154	1.100506639	3.848294590
H	7.765789492	1.622940661	3.378038371	H	-0.319279435	2.108597934	2.384608138
H	6.687569632	3.017329920	-0.545796212	H	-1.645482959	0.909309585	2.510080581
H	8.216830741	3.090150162	1.422272851	O	0.728587875	-2.700447668	4.423499861

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11A-TS
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C	0.022389582	-0.208179722	-0.190547093	H	1.007626365	-3.931345943	6.008416960
C	0.229793959	0.036207664	2.212731090	H	2.444004737	-2.946161984	5.579637408
Rh	1.679972268	-0.158811209	1.088332619	H	1.065870383	-2.183629592	6.423055920
P	2.331541784	2.032178448	0.326708281	P	3.891166777	-0.880065357	1.893164756
C	-0.595210843	-1.372797353	-0.387220241	C	3.913133945	-2.436675583	2.875605367
C	-0.457757745	-2.637019012	0.446762790	C	4.884261617	-2.697294730	3.853563619
C	-1.583695353	-3.515753631	-0.144200879	C	3.034893843	-3.460880620	2.495840360
C	-1.576366150	-1.694420620	-1.510240533	C	4.955822523	-3.955994631	4.452325948
O	-1.695049397	-3.111337169	-1.503248378	C	3.112148207	-4.717720591	3.091795638
C	4.012204597	2.251605350	-0.369416208	C	4.071349918	-4.967612222	4.074992662
C	4.854672717	3.311529317	-0.004070083	H	5.589059876	-1.928092190	4.148435898
H	4.533717161	4.040040358	0.731790359	H	2.284445169	-3.273596345	1.734160829
C	6.126296828	3.419350517	-0.566890616	H	5.709003112	-4.145162456	5.211812460
H	6.773482270	4.241258749	-0.273901626	H	2.420048481	-5.499171616	2.792320334
C	6.572469670	2.472802534	-1.492006555	H	4.131024960	-5.946279602	4.542387624
H	7.568611786	2.555026824	-1.917193926	C	4.942749415	0.302455284	2.798800933
C	5.735043302	1.420495829	-1.868596735	C	4.684698337	0.506059878	4.167462546
H	6.073050368	0.673163569	-2.579830857	C	5.904793732	1.092261605	2.153290180
C	4.461540029	1.314309655	-1.311503761	C	5.400453835	1.467637795	4.876535487
H	3.823306302	0.487779927	-1.602048547	C	6.611117167	2.057454474	2.871840699
C	1.241034407	2.809611612	-0.935796460	C	6.365994732	2.244507812	4.231724695
				H	3.913488035	-0.071701543	4.667370081

H 6.102533619 0.970871292 1.094775840
H 5.199190110 1.614043014 5.933899860
H 7.351244272 2.664647330 2.359345813
H 6.920615650 2.995273393 4.787321060
C 4.799922492 -1.471091793 0.411038762
C 6.191918323 -1.629281761 0.382424046
C 4.041823319 -1.898401156 -0.690724035
C 6.815135030 -2.155577950 -0.749129671
C 4.665276554 -2.433559508 -1.817945385
C 6.056981288 -2.551510183 -1.854222447
H 6.792575764 -1.342259677 1.239712287
H 2.954722479 -1.811486534 -0.678633539
H 7.895808340 -2.264252327 -0.763502373
H 4.066319087 -2.755634184 -2.664886311
H 6.546353029 -2.965374720 -2.730800593

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11B-TS

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C 0.706572772 -0.998346687 0.214972616
C -0.028703393 0.609878045 1.407109281
Rh 1.978103125 0.063684599 1.463580092
P 3.075438012 1.170759268 -0.176469633
C 0.397525836 -2.135811830 0.838700764
C 0.334373035 -2.180659101 2.359440406
C 0.203161129 -3.703061652 2.625326035
C 0.160128839 -3.543868241 0.341923154
O 0.638985766 -4.344518607 1.426421658
C 4.640141304 0.309472836 -0.631663880
C 5.788154170 1.001054289 -1.047441126
H 5.795250124 2.084036123 -1.086087601
C 6.948514145 0.300252131 -1.378236055
H 7.831833895 0.849115280 -1.692406971
C 6.984889009 -1.093821088 -1.290186310
H 7.895918371 -1.632327409 -1.533779538
C 5.843807157 -1.789435180 -0.884608332
H 5.859862397 -2.872011155 -0.799986656
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H 3.800317296 -1.638512390 -0.236698748
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H 2.948396116 -0.630096028 -2.505394314
C 1.600527525 0.265179354 -3.912326379
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C 0.783785149 1.358931641 -4.205177221
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C 0.668374113 2.403335534 -3.286356973
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H 1.257806952 3.170619350 -1.365432229
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H 4.678644404 5.742105686 -1.260676972
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H 3.818517332 4.984228661 2.886468916
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H -0.909496143 -3.738653617 0.152714899
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H 0.829772246 -4.063717693 3.443760749
H -0.846931188 -3.959497537 2.841523794
H 1.277741655 -1.821894675 2.810086069
C -0.875119514 0.101914673 2.334451284
C -0.795412685 -1.299410245 2.906883150
C -0.311937660 1.921105100 0.750992943
C -2.043440836 0.893248844 2.881785729
H -1.766817977 -1.778824546 2.710401844
H -0.707524913 -1.239173889 4.000305251
H -1.987010546 0.933483174 3.976493199
H -2.989289407 0.399066785 2.626198763
H -2.085800058 1.916547701 2.508482932
O -1.444204737 1.860364040 0.021968631
O 0.370365384 2.925252477 0.848048139
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H -1.160489410 3.433819535 -1.327561501
H -1.988637590 3.873263603 0.185100239
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P 3.885387058 -0.238249581 2.897551479
C 2.995334816 -0.238300435 4.507571908
C 2.041793145 0.768966021 4.750594765
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C 1.315346626 0.778819822 5.941065580
C 2.463084913 -1.226762306 6.655713321
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H 0.951122983 -0.219566711 7.816982573
C 4.607162052 -1.916781176 2.755321882
C 5.863272849 -2.219275646 3.304559481
C 3.853804695 -2.945477658 2.165156842
C 6.352804351 -3.525208089 3.255784023
C 4.339383415 -4.250562189 2.131256410
C 5.592708648 -4.542435247 2.674628243
H 6.461079418 -1.439909626 3.766077581
H 2.889559453 -2.741911378 1.714890989
H 7.328140927 -3.747387829 3.679305648
H 3.730554129 -5.029062734 1.680690192
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C 6.375085317 0.829377224 2.203835009
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C 7.407364721 1.762425491 2.273222351
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C 0.141545738 -0.267720376 1.014534034
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C 1.114204498 -2.390085715 1.653145863

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C -0.806880137 0.815743843 1.410033633
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C 2.687158155 4.256995220 3.297211644
H 2.937385801 4.676865068 2.327740646
C 2.481745394 5.110039375 4.380400552
H 2.590028507 6.182460929 4.245827333
C 2.132650134 4.591482606 5.630321355
H 1.970788932 5.259199980 6.471256740
C 1.980955118 3.213711185 5.787797351
H 1.702338829 2.798197020 6.751688347
C 2.185065037 2.359179164 4.704735421
H 2.067586753 1.293418344 4.848998813
C 4.687296927 1.683661406 1.809254938
C 5.261728842 0.574179002 1.170524940
H 4.646540692 -0.248881760 0.834779849
C 6.639611213 0.507460720 0.960396544
H 7.058665502 -0.359720862 0.458402856
C 7.465264190 1.545550947 1.396626585
H 8.539150297 1.493640644 1.243665008
C 6.899078460 2.657136116 2.026624879
H 7.533008802 3.471845195 2.365340493
C 5.520390746 2.730581967 2.230071609
H 5.105189509 3.592473816 2.740332225
C 2.291662225 2.678105864 0.596364146
C 3.055989436 2.749904719 -0.577943650
H 4.040007020 2.294660528 -0.618955812
C 2.568789241 3.427342532 -1.696973753
H 3.171039896 3.474806496 -2.599718312
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H 0.946395085 4.582227721 -2.521936188
C 0.567081360 4.003931312 -0.478623462
H -0.395957384 4.503665787 -0.433207911
C 1.042983372 3.319265364 0.637433107
H 0.452528626 3.293025436 1.548159166
O -1.461719442 1.328581703 0.355750259
O -0.978720380 1.199808293 2.557778064
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12

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C 0.420848785 -2.236992924 -0.516870626
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O 0.627641551 -3.562274920 -0.019983944
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H 0.432764737 0.471296533 0.069696716
H 0.325308954 -2.318667351 3.994209655
H 2.115384014 -3.527282252 1.431063346
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H -0.220560851 -2.306254123 -1.398582308
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H -0.227356594 2.481752277 3.189228165
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C 3.993664301 4.016102642 2.285157789

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H 9.202344906 1.090261788 1.331399033
C 7.520525711 1.425385168 2.644561773
H 8.130029435 1.614313361 3.523021247
C 6.132203121 1.478598568 2.755872713
H 5.691297465 1.720703803 3.715246833
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C 2.283678537 2.700241392 -0.300352748
H 2.206628731 3.560164365 0.356721987
C 1.808550757 2.789635402 -1.611359032
H 1.358410309 3.716421399 -1.955333482
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H 1.553185692 1.779270697 -3.498308106
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H 0.013712979 -0.172267628 7.292210742
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13-TS

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C 7.585686948 1.591256504 2.190553496
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C 8.807421044 1.935427634 2.725217423
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15B

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15A-TS1

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15A-TS2

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C 2.742622766 -1.615223671 6.764547152
H 2.706003365 -2.167520614 7.701457885
C 3.856031073 -1.773096705 5.927262675
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C 3.897428669 -1.053854375 4.731725403
H 4.763816421 -1.157469463 4.085468220
C 3.748264389 2.385455666 3.788489157
C 5.026370751 2.329306290 4.348671699

H 5.646527603 1.448503260 4.208142339
C 5.532001426 3.413358379 5.073332692
C 6.943070646 3.380802659 5.607207669
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H 5.093198781 5.375012678 5.833551998
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C -0.477367025 2.865555833 0.863247110
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C -2.808256904 0.696859958 2.883914191
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H -3.562041308 2.565262169 0.346828384
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O -0.268240333 2.563694888 -2.157388918
O -0.066838975 0.338074416 -2.529386195
C -0.246390346 0.594951497 -3.940670852
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H 0.816242365 6.692167002 -3.487271636
H -0.453279490 5.545208037 -3.056484128
H 2.234757434 7.622854297 2.668340499
H 1.224948101 8.703614471 1.695164352
H 0.477559537 7.458310661 2.695064138

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15B-TS1
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C 0.157059726 -0.181297861 1.964679238
C 2.688906757 -0.065377318 4.289849300

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H	0.864821486	0.948269273	4.839266437	C	1.841431298	5.378401272	0.598721583
C	1.382154529	-0.547078192	6.286839201	H	2.234780051	5.204701200	1.596402745
C	0.175276487	-0.295754321	7.160682565	C	3.594463080	2.292492202	-1.680155527
C	2.331749266	-1.513641908	6.639141904	C	4.402833856	3.155171307	-2.438896311
H	2.196246471	-2.076442400	7.561003876	H	4.615800438	4.156873641	-2.074768373
C	3.459025696	-1.766307617	5.849294571	C	4.930371977	2.744848437	-3.663343450
C	4.469220376	-2.809340559	6.267739433	C	5.784264059	3.669820287	-4.498079821
C	3.630214524	-1.030234338	4.670850072	C	4.640989604	1.448498424	-4.115805669
H	4.509183326	-1.210726069	4.058888981	H	5.043803509	1.122606019	-5.072837714
C	3.658931834	2.512046575	3.751629406	C	3.864596459	0.561588772	-3.368896239
C	4.853840740	2.461533859	4.472146941	C	3.598474699	-0.847279532	-3.841263473
H	5.474297727	1.570147386	4.440030230	C	3.352461593	0.996711160	-2.138769041
C	5.270223470	3.560887915	5.232510905	H	2.768939427	0.305660014	-1.539187810
C	6.593748361	3.525086265	5.958091903	P	2.961899323	1.069684317	2.883080517
C	4.447232323	4.691687538	5.279676127	P	2.950740768	2.877998500	-0.061701998
H	4.757993798	5.545072110	5.879451892	Rh	1.517020344	1.255725272	0.987581131
C	3.230384231	4.755572690	4.588850368	C	-0.027412699	2.606061409	1.448769611
C	2.359564952	5.986321901	4.681088555	C	-0.714592279	2.051389219	2.677006839
C	2.847936045	3.653256851	3.821219676	C	-0.685812277	0.548304014	2.704481197
H	1.905785756	3.671889779	3.281447667	H	0.301228387	-1.243311765	2.116837909
C	4.119624510	0.210068678	1.736953795	C	-1.753344786	0.126728630	3.690774887
C	3.776830394	-1.149338674	1.443445305	H	-0.159521334	2.386467082	3.570849391
H	2.985379355	-1.637284243	2.000782756	C	-2.204736076	2.300434527	2.966994133
C	4.424167694	-1.839100029	0.450567117	H	0.426226283	3.583678414	1.597503439
H	4.149272968	-2.869613891	0.243617049	H	-0.687670160	2.646645034	0.580413815
C	5.435959890	-1.219262027	-0.325816144	H	-2.397405227	-0.653741366	3.258290022
C	6.117495664	-1.919847253	-1.354949640	H	-1.346827570	-0.251834879	4.637209215
H	5.879173262	-2.968010004	-1.516517727	H	-2.433398089	3.283230223	3.387763266
C	7.056771160	-1.286045494	-2.136497027	H	-2.807527649	2.148576494	2.055993386
H	7.569434149	-1.832720114	-2.922562433	O	-2.503180359	1.319412846	3.967744299
C	7.350737223	0.082338459	-1.923729055	C	0.387191339	0.831038946	-0.742442048
H	8.078130773	0.581699343	-2.556647842	C	0.034423483	1.481645161	-2.019022335
C	6.722669792	0.783119493	-0.919795954	C	0.233105183	-1.692038550	-0.284802592
H	6.950740182	1.831720569	-0.771535125	H	-0.354409355	2.492668918	-1.843440916
C	5.757074106	0.156524625	-0.082577523	H	0.920435998	1.587852994	-2.652549085
C	5.080303311	0.865089885	0.964804211	H	-0.717297073	0.891223172	-2.551481384
C	5.413660073	2.306779073	1.184128933	O	0.829599882	-2.533960297	0.356979699
C	6.667893865	2.631610788	1.796089930	O	-0.492948588	-1.947541512	-1.387485827
C	7.562932335	1.631924129	2.271683621	C	-0.537571885	-3.337932829	-1.781655137
H	7.295521124	0.586326126	2.166969023	H	-1.182827651	-3.368808146	-2.658759032
C	8.760620706	1.979027441	2.856686428	H	0.465678680	-3.697711691	-2.023972225
H	9.431245059	1.201960289	3.211869916	H	-0.950023653	-3.948027278	-0.974278602
C	9.131058583	3.339358027	2.997933216	H	5.362054475	-2.783758569	5.636545885
H	10.082976284	3.596166758	3.453013873	H	4.784750637	-2.659510132	7.306024767
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H	8.552323731	5.377494765	2.663804551	H	0.460609333	-0.199903421	8.213663064
C	7.036553762	4.006105528	1.956982888	H	-0.352731627	0.616488448	6.867744426
C	6.148092540	5.007924047	1.496247261	H	-0.536590280	-1.127671120	7.096335200
H	6.433226390	6.051947695	1.598302438	H	6.644251095	4.284664556	6.743375929
C	4.945061593	4.679403082	0.922022374	H	6.770210141	2.547007941	6.417270076
H	4.298364568	5.471565573	0.567220815	H	7.415775056	3.709028856	5.256944295
C	4.552083967	3.321625132	0.770820512	H	1.425693463	5.862320705	4.125070808
C	2.102648444	4.458385298	-0.431643107	H	2.101551262	6.212856318	5.721665996
C	1.597732120	4.707491174	-1.713448988	H	2.876531124	6.867103892	4.281187660
H	1.801138582	4.014907572	-2.523707528	H	2.613941898	-1.197609857	-3.513172169
C	0.845038024	5.859205503	-1.979700361	H	3.640815731	-0.922218106	-4.931620525
C	0.282988567	6.098743640	-3.361284492	H	4.347028026	-1.533109367	-3.428826819
C	0.616429820	6.763890487	-0.940284286	H	6.707146939	3.173386367	-4.817153261
H	0.047512493	7.669310984	-1.141076229	H	5.255242339	3.979964203	-5.406975299
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H 1.583248516 7.475488300 2.249036677
H 0.816705975 8.560884657 1.077563757
H -0.146438823 7.344868873 1.916052627

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15B-TS2
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C 1.511051482 -0.989752081 6.128304843
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H 4.143717655 -4.307855150 5.541088462
H 0.662750969 -0.805054196 8.110829128
H -0.099368016 0.236948690 6.898403948
H -0.433273801 -1.499745771 6.916165181

H 6.683555947 3.780088684 6.631162259
H 6.919469988 2.127265834 6.034245205
H 7.387216579 3.501280281 5.031104732
H 1.215541728 5.306621047 4.716766222
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C 2.399611877 6.270557399 11.432043708
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H 1.838542935 7.536652968 20.902918433
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H -2.120698221 2.956793519 19.933737707
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H	6.538081991	5.848808761	18.551241544	C	7.395168507	7.279048037	13.996473743
H	7.411421757	6.211634693	17.065004441	H	7.764057194	8.131344670	13.431353499
C	-0.766134585	4.171265832	14.325359344	C	8.060971883	6.838089419	15.116222437
C	-0.655539124	6.984624585	14.816562829	H	8.964975569	7.340023499	15.448776967
C	-1.671483437	4.508373277	13.156100720	C	7.562717460	5.728816915	15.839811286
C	-1.115373214	7.585939987	13.692540030	H	8.080168893	5.395401329	16.734700879
C	-0.976561454	5.519302054	12.226490427	C	6.428033389	5.070829023	15.425774989
C	-0.820303559	6.860850772	12.436815500	H	6.054161276	4.233714969	16.001676721
H	-0.472184175	7.458381354	11.592225739	C	5.715759051	5.495031680	14.268854010
C	-0.828358509	4.827418722	10.884891335	C	4.523566786	4.830832237	13.816107542
C	-1.794149921	8.929853300	13.596107933	C	4.175757031	3.533013234	14.475122513
C	-1.980775418	3.347958234	12.170388104	C	5.062829198	2.424863468	14.225116152
H	-2.592665294	4.973236344	13.525173869	C	6.138554077	2.507061278	13.294776167
C	-0.824473304	7.497780199	16.189347063	H	6.293509806	3.423858699	12.738023661
H	-0.260814975	3.206483464	14.269488051	C	6.982116526	1.438986087	13.088330015
H	-1.266190478	4.294757845	15.280117154	H	7.794025275	1.526533232	12.371989171
O	-1.922828559	3.916261420	10.866442352	C	6.805338898	0.230089719	13.802269916
H	-0.916227235	5.508450920	10.034843407	H	7.486707227	-0.599479759	13.637565326
H	0.125684071	4.286582864	10.807132167	C	5.765353476	0.107451785	14.694236713
H	-1.230886890	2.548087195	12.275772849	H	5.610775753	-0.818636064	15.241731483
H	-2.975222270	2.917768934	12.309547987	C	4.869245364	1.186286733	14.915798348
H	-1.235456580	9.592559756	12.922595277	C	3.785023017	1.079867430	15.817039449
H	-2.806608221	8.833401514	13.186103709	H	3.637290545	0.149698848	16.359899915
H	-1.862021046	9.415992856	14.572399330	C	2.927595435	2.130495183	16.016207420
O	0.012220313	8.147597524	16.790847517	H	2.123222970	2.007117137	16.725995968
O	-2.013335001	7.141111988	16.713474074	C	3.099784672	3.375411995	15.341702149
C	-2.250052841	7.595334920	18.063702374	C	0.780637933	4.013585652	16.901928172
H	-3.231740730	7.206621339	18.333749470	C	0.544913536	4.422305984	18.214659840
H	-1.481386504	7.205401997	18.732335880	H	1.138969269	5.216554686	18.656118286
H	-2.244950147	8.687615527	18.103885221	C	-0.459096112	3.807718218	18.984605717

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C	1.788798589	5.460072192	10.626412085	C	-1.990847721	2.303434006	18.998213768
C	1.608926134	6.827327555	10.374228283	C	-0.992084473	2.351069497	17.090846512
H	1.626908070	7.533302429	11.199831213	C	-1.819473443	1.233764079	16.499587425
C	1.404836451	7.306797632	9.074966811	C	0.004346364	2.976679758	16.347717681
C	1.235238764	8.787833745	8.828631735	H	0.189213651	2.648362283	15.327273981
C	1.373819104	6.382603068	8.026412427	C	3.155692255	5.810669738	16.794774579
H	1.206911033	6.738577608	7.011684277	C	3.762788958	5.253012117	17.928864241
C	1.548558730	5.009411836	8.245650332	H	3.493373690	4.250983987	18.253505718
C	1.507483138	4.041579323	7.086505042	C	4.725295057	5.971040155	18.645569685
C	1.754387980	4.558151195	9.553482795	C	5.351488262	5.381439844	19.887646529
H	1.883448062	3.495714938	9.732232686	C	5.088257304	7.243925229	18.186865251
C	1.762775342	3.097902266	12.249634418	H	5.848653982	7.802417908	18.728837083
C	2.743391406	2.139073045	11.997182271	C	4.520952958	7.810841317	17.040922261
H	3.777975816	2.436230011	11.861528020	C	4.983657846	9.147335909	16.513343775
C	2.404306401	0.779192408	11.918296798	C	3.543383068	7.081983490	16.355408209
C	3.484274518	-0.251584568	11.688932479	H	3.092719319	7.512225640	15.464595336
C	1.063396089	0.415181911	12.069352620	P	2.049949110	4.893730672	12.355897124
H	0.791956461	-0.636986677	12.007550645	P	1.995840181	4.810198972	15.792503622
C	0.052835097	1.367383144	12.275762483	Rh	0.857713915	6.088720484	14.194080964
C	-1.392900719	0.943966494	12.390667728	H	-2.050875455	1.803768480	12.546614229
C	0.416285184	2.711198257	12.367959998	H	-1.726269527	0.429235014	11.482489968
H	-0.357347146	3.466765076	12.479046849	H	-1.537918064	0.246267794	13.224188849
C	3.815124191	5.340588968	12.725705766	H	3.063475311	-1.236103779	11.466323326
C	4.352885981	6.452423496	12.012280757	H	4.135620239	0.036615250	10.856461813
H	3.851061495	6.812468343	11.124598797	H	4.123940724	-0.346697923	12.574214406
C	5.515069233	7.065094128	12.403585583	H	1.714468609	3.017414925	7.408615582
H	5.911924464	7.896577739	11.826298819	H	0.523653122	4.049571361	6.603250511
C	6.212185097	6.629882571	13.554586300	H	2.244579910	4.311475104	6.321852872
				H	0.804588323	8.986022713	7.843520277

H	0.583382828	9.246471070	9.580748758	C	4.440207528	4.144434566	4.781276119
H	2.200331134	9.306619899	8.877777339	C	5.608461676	4.121448669	5.737218024
H	-1.571700903	3.776118915	20.844853209	C	3.724448183	5.326195577	4.540372497
H	0.170551452	4.009474895	21.041534709	H	4.000159955	6.226634907	5.085403966
H	-0.832519105	5.340081082	20.465210381	C	2.666854876	5.382809743	3.627778961
H	-1.563373923	1.057501885	15.450917401	C	1.930861514	6.669726320	3.345373997
H	-1.664400433	0.296273537	17.046144055	C	2.320998083	4.215650632	2.939671346
H	-2.889713280	1.463501325	16.552927013	H	1.493531149	4.226274400	2.239710961
H	4.155020341	9.712448168	16.074014152	C	3.707739629	0.698668404	1.237786349
H	5.433437340	9.758487499	17.301217676	C	3.361276537	-0.631428934	0.837472515
H	5.740160727	9.000171563	15.732532161	H	2.464863596	-1.092818187	1.236896686
H	6.286475653	5.887408224	20.144268247	C	4.142746062	-1.328184822	-0.047850383
H	4.679413535	5.475637814	20.749396784	H	3.869128584	-2.339269899	-0.337166397
H	5.565628411	4.315285902	19.758279617	C	5.313508505	-0.746542704	-0.590795157
C	-1.013425730	5.266893563	14.645824722	C	6.155074445	-1.471996180	-1.472422849
C	0.264931626	7.578179086	15.450262365	H	5.895464212	-2.499509669	-1.712928646
C	-1.947511764	6.208947429	13.920412007	C	7.282432770	-0.891210809	-2.004174528
C	-0.015966159	8.540985841	14.524970677	H	7.926876921	-1.457234289	-2.670221852
C	-1.086097319	6.961689995	12.897498625	C	7.603643902	0.448843692	-1.685865100
C	-0.268020147	8.030019718	13.156897265	H	8.490982942	0.905294223	-2.114535235
H	0.137472288	8.586017142	12.314764900	C	6.798437860	1.184301880	-0.847815019
C	-1.489873403	6.431357663	11.533971701	H	7.054758340	2.212794456	-0.626936990
C	-0.021889261	10.001448975	14.796348628	C	5.637662090	0.610757998	-0.256483599
C	-2.955991067	5.496195236	12.998776382	C	4.794609683	1.345716522	0.643913061
H	-2.412849742	6.915089487	14.616066960	C	5.056604076	2.809134666	0.838647233
C	0.244786639	7.717376754	16.933366338	C	6.196540011	3.231451311	1.591945912
H	-0.979656190	4.269894405	14.210014235	C	7.051230806	2.308811192	2.255498750
H	-1.160960058	5.222010371	15.721277391	H	6.833563450	1.247634950	2.194798647
O	-2.226576703	5.240245239	11.798163423	C	8.149289084	2.744985857	2.961604884
H	-2.128969130	7.184914924	11.038979178	H	8.792819456	2.024584194	3.458225727
H	-0.662326064	6.191292904	10.869295791	C	8.450058364	4.126229977	3.045122936
H	-3.311144304	4.540367987	13.392534768	H	9.324597399	4.455166515	3.598844842
H	-3.823398655	6.145513949	12.796871713	C	7.631067679	5.047108302	2.432889481
O	0.207009608	10.520902224	15.872582016	H	7.847656193	6.110027268	2.500292112
O	-0.291033186	10.707621114	13.670821418	C	6.489294902	4.629835758	1.699515216
C	-0.284124519	12.140195577	13.831853665	C	5.630361366	5.559977739	1.066562293
H	0.694008218	12.482175052	14.181104169	H	5.855206252	6.620727191	1.143392019
H	-1.042414908	12.446100340	14.557299822	C	4.525680115	5.138880532	0.368254378
H	-0.507159398	12.548374482	12.846158332	H	3.878040394	5.870744978	-0.100208166
H	-0.256712695	6.850695534	17.378042284	C	4.222386824	3.757261100	0.244792524
H	1.260573332	7.736869045	17.340046914	C	1.971799427	4.808090053	-1.260556696
H	-0.258339955	8.636313714	17.241662673	C	2.250503166	5.342511255	-2.524564110
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18A							
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C	-1.276964682	3.153338386	1.733763441	C	2.019603098	7.135983577	-4.283110512
C	-0.087609886	0.212182111	1.313408686	C	0.830678991	7.230649739	-2.044102596
C	2.268687487	0.403413582	3.819514633	H	0.382583029	8.171973319	-2.354336733
C	1.546829315	0.927793405	4.901433762	C	0.525574103	6.714141852	-0.778877590
H	1.142429094	1.933224913	4.854101643	C	-0.423445835	7.417333753	0.161878996
C	1.361467853	0.188175981	6.073630745	C	1.105931465	5.500039882	-0.400398402
C	0.532099919	0.755103593	7.200822963	H	0.842348766	5.073868119	0.560548241
C	1.942641509	-1.079785185	6.159613574	C	3.375798660	2.345527195	-2.096219170
H	1.815293733	-1.661228472	7.070339490	C	4.538958835	2.799118895	-2.734922639
C	2.706146231	-1.612243529	5.113939101	H	5.014227366	3.718741995	-2.403090324
C	3.349202476	-2.972265726	5.252701305	C	5.130233730	2.056276239	-3.759800748
C	2.861847261	-0.862443276	3.944883193	C	6.386177260	2.540641004	-4.444099399
H	3.480660709	-1.267863466	3.154668448	C	4.542050696	0.838656811	-4.123009527
C	3.024063893	3.029437661	3.158252237	H	5.013844130	0.236450456	-4.896749617
C	4.069387741	2.989425610	4.091248636	C	3.384791912	0.358363449	-3.502639022
H	4.599293262	2.060388689	4.281857460	C	2.833009766	-1.002019803	-3.853084578
				C	2.799480568	1.131946453	-2.493463630

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18B

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16A-TS

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H	5.836674060	1.391313916	15.267621029	H	-1.280775586	7.968386255	14.225788004
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H	2.167811928	-0.111570666	19.757142090	H	3.037535821	4.174368164	10.199733566
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C	3.813699779	7.510988870	13.146470848	H	-0.792900456	0.059218233	15.981450638
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C	4.139474886	4.385902884	15.389282269	H	0.186090156	9.004445739	8.372546973
C	5.349786766	3.610421004	15.303022741	H	-0.079384457	9.188783220	10.115861275
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C	7.727977902	2.068767609	15.212266299	C	-2.091630258	3.949770225	14.267459744
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C	-0.957356395	1.706913362	17.380971901	H	-4.434562183	4.544734676	15.692361625
C	-1.291811535	0.306963567	16.922429230	H	-3.333468241	3.765394305	16.830546938
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C	1.910704562	6.264545166	17.124069904	C	-1.062486013	9.343837624	16.866028343
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H	2.480483114	5.156913298	18.887691243	H	-0.688617073	10.201720336	16.306975455
C	2.945592617	7.247568488	19.092718280	H	-2.065073259	9.542160585	17.252879997
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C	1.272503204	4.692788445	8.324174201	C	4.178571598	6.200141768	18.679357586
C	1.404661450	3.707787571	7.186289375	C	4.954907686	5.730828862	19.887455551
C	1.546829814	4.312195860	9.639849405	C	4.220413810	7.549831924	18.292126364
H	1.867930360	3.295828356	9.834705300	H	4.810916601	8.247685934	18.882653216
C	2.098658362	2.946276025	12.295788658	C	3.548807285	8.015615608	17.161885292
C	3.285429235	2.366418828	11.846169671	C	3.647529819	9.453300160	16.713876353
H	4.146017139	2.989609587	11.621078698	C	2.784461531	7.106281968	16.416487704
C	3.386006404	0.976008538	11.696196551	H	2.254008807	7.449991091	15.533898075
C	4.690986120	0.360106754	11.253882925	P	1.870824145	4.749603789	12.419381838
C	2.263563694	0.193895505	11.979698581	P	1.814804592	4.568937581	15.730952571
H	2.329069003	-0.885643303	11.859698332	H	2.674195211	9.827273694	16.378125578
C	1.050726784	0.756098891	12.404473889	H	4.008985966	10.104617572	17.514649569
C	-0.141824922	-0.129443095	12.676653783	H	4.344910468	9.540806268	15.872089180
C	0.982248048	2.140702062	12.565867967	H	4.680564820	6.301424595	20.781840345
H	0.056923800	2.604219424	12.900675527	H	4.778243544	4.672070014	20.096042880
C	3.477007036	5.606704251	12.776617597	H	6.032348391	5.867929046	19.737500662
C	3.717567356	6.834450319	12.097173865	H	-1.277527263	0.362426232	15.302818077
H	3.138899508	7.081427955	11.217408820	H	-0.721605558	-0.588734626	16.683331998
C	4.686250583	7.709129594	12.517534660	H	-2.300912120	0.191712473	16.737827113
H	4.858907674	8.632224180	11.971150333	H	-1.170293494	2.598153328	20.881102892
C	5.466399828	7.429830172	13.663580128	H	0.451201803	3.302474653	20.973757444
C	6.433118979	8.347939635	14.149993883	H	-0.915326151	4.309054727	20.491838155
H	6.570799218	9.288226187	13.622331950	H	4.578709074	-0.701826258	11.018794213
C	7.179083154	8.054627610	15.267603728	H	5.086909766	0.865464207	10.366264529
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C	6.070287030	5.908489068	15.483214185	H	0.043736067	-0.790261270	13.531324662
H	5.924275705	4.980186135	16.020449605	H	1.745217042	2.729627794	7.536626172
C	5.278628458	6.177009601	14.331778212	H	0.445721667	3.567173677	6.674634917
C	4.296587492	5.246442947	13.848694552	H	2.119593082	4.066023318	6.437026628
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C	5.376545820	3.014007602	14.204204533	H	-0.667678801	8.575331311	9.263042364
C	6.444130172	3.383439675	13.336288928	H	1.022043516	9.087438885	9.247569020
H	6.414901343	4.341873032	12.833372663	C	-0.731475029	8.157395164	14.560066135
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19

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20A
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C 1.315423020 0.402472490 -3.203528789
C 1.123381115 -1.597202498 -2.045439592
O 1.141457795 -1.006790077 -3.349803974
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H 1.810228692 2.323765492 -1.330834387
H 1.095608158 -1.069332960 0.931813606
H 2.114319608 -1.996960548 -1.779080068
H 0.409910572 -2.429022397 -2.059563246
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C -1.860136304 2.100833182 0.831954263
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20B
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C 5.923568845 0.733425156 -1.640103883
H 6.689039885 0.551660901 -2.388585240
C 4.924037293 -0.218180145 -1.416796513
H 4.909680352 -1.140394986 -1.990576562
C 3.935127483 0.015883387 -0.463909476
H 3.151565723 -0.717798536 -0.316568314
O -3.147328669 0.094674678 2.487360798
O -0.875951835 0.184107539 2.623862210
C -0.890816662 -0.899854603 3.593650237
H 0.152113228 -1.159867056 3.753469834
H -1.354244852 -0.555769911 4.520787857
H -1.457171088 -1.741578002 3.191405810

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20A-TS1

=====

C 0.163677715 0.112595736 -0.120738196
C -0.314576304 0.443682054 1.864561668
Rh 1.933422712 0.050330533 0.896419898
P 3.181486763 -1.133046408 -0.761345796
C 2.275291028 1.887385488 -0.008683892
C 0.004929830 1.305646940 -0.741471715
C 0.906809359 2.449003929 -0.372061511
C 0.783780057 3.325453814 -1.645506736
C -0.839750879 1.732160673 -1.915677266
O -0.562107624 3.119557769 -2.071898681
H 2.813472524 2.465858056 0.748892166
H 2.891393112 1.733238600 -0.895350481
H -0.362085417 -0.796654519 -0.405890826
H -0.547383741 1.158103525 -2.810821694
H -1.915600623 1.598158222 -1.755137868
H 0.923737858 4.392730885 -1.465781044
H 1.501383603 2.985535568 -2.410645571
H 0.465594152 2.984489417 0.480861288
C 0.746938892 0.893276936 2.400374621
C -1.699725655 -0.051145754 1.957637671
C 1.305412626 1.538810655 3.595516194
H -2.366063263 0.503083399 1.291001751
H -1.764427954 -1.115217694 1.709361573
H -2.028480472 0.087300538 2.993930089
O 0.694128346 2.267129254 4.340487616
O 2.613830810 1.221059933 3.712058543
C 3.293255226 1.791017729 4.858140542
H 4.317050179 1.424634391 4.799057872
H 3.264672349 2.881968854 4.808258908
H 2.815414197 1.459506071 5.782492927
C 4.997686877 -0.955035066 -0.643644057
C 5.540248258 0.191197735 -0.040617485

H 4.886451994 0.954913717 0.371667425
C 6.923728191 0.362240526 0.028072764
H 7.335070069 1.252833782 0.493868565
C 7.774967157 -0.611484607 -0.497659090
H 8.851307125 -0.480401567 -0.441626255
C 7.240562706 -1.758368972 -1.091518379
H 7.900706033 -2.519942348 -1.496039021
C 5.859709459 -1.932740204 -1.165731593
H 5.453600843 -2.830451904 -1.621920221
C 2.845813633 -2.925051201 -0.658331209
C 2.675704758 -3.480871526 0.621038088
H 2.737459359 -2.847815016 1.504863670
C 2.447494280 -4.847440475 0.772612344
H 2.319949766 -5.268117567 1.765577868
C 2.384600827 -5.671695494 -0.353271726
H 2.203586816 -6.736041111 -0.237084137
C 2.556266684 -5.127912032 -1.627878416
H 2.512369871 -5.768923940 -2.503431687
C 2.788225472 -3.760936191 -1.784452614
H 2.920379630 -3.348010968 -2.779427266
C 2.721536909 -0.607305350 -2.450931122
C 3.518432068 0.299574536 -3.165370331
H 4.484320724 0.603158404 -2.772473295
C 3.080385026 0.805515988 -4.391789735
H 3.707504104 1.503165110 -4.938412090
C 1.850911437 0.408329030 -4.919474473
H 1.515633129 0.798727637 -5.875234666
C 1.056832369 -0.503120146 -4.216839707
H 0.106942190 -0.830435283 -4.630100350
C 1.481636200 -0.999383737 -2.985084308
H 0.858520876 -1.709667798 -2.4449601828

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20A-TS2

=====

C -0.161487218 -0.066312725 -0.040574695
C 0.015214855 0.046617195 2.225481198
Rh 1.823487450 0.040044079 1.065464314
P 4.113534419 0.412300465 1.359223506
C 2.116020476 -1.776149014 0.348544050
C 1.055506459 -2.244390776 -0.318721512
C -0.271936149 -1.526665215 -0.351705939
C -0.749724080 -1.925674565 -1.775269365
C 0.959383434 -3.400864779 -1.304421770
O -0.341708999 -3.283643801 -1.878259417
H -1.098338835 0.435410911 0.161962453
H 0.443606866 0.508912272 -0.756899226
H 3.075040984 -2.279824167 0.436727596
H 1.743830853 -3.320118328 -2.072713185
H 1.042051263 -4.383909283 -0.828600224
H -1.833097976 -1.880427200 -1.899052142
H -0.266947604 -1.293430986 -2.539231106
H -0.959596328 -1.994136617 0.364233192
C 1.111745780 -0.083928435 2.909123615
C 1.668039974 -0.214043834 4.269567290
C -1.426022853 0.060388326 2.570119056
H 2.020887091 -1.236032149 4.441965094
H 2.514189386 0.464505944 4.412029291
H 0.883309002 0.016882527 4.997188067
C 4.835104763 1.059350125 -0.188470129
C 5.645755319 2.203866908 -0.212632724
H 5.846999124 2.752216642 0.702087638

C 6.198253570 2.637964268 -1.418455003
H 6.827030880 3.523217827 -1.432980520
C 5.947050409 1.937903064 -2.599792790
H 6.379184793 2.280124644 -3.535381512
C 5.139996954 0.797369565 -2.579947007
H 4.944949446 0.251109287 -3.497965177
C 4.582357031 0.359152162 -1.380932383
H 3.957301183 -0.530243508 -1.369931020
C 4.300656818 1.724293076 2.612262417
C 3.545419453 2.900138237 2.454103095
H 2.918411928 3.033083396 1.574918495
C 3.611976362 3.908994968 3.412149001
H 3.031852087 4.817497955 3.281186971
C 4.426112912 3.750222519 4.537584150
H 4.476372911 4.536131103 5.285191676
C 5.177041959 2.584997281 4.698848205
H 5.813669662 2.463369068 5.570143351
C 5.117763183 1.570604472 3.740674591
H 5.706002289 0.667810826 3.870808959
C 5.181118800 -0.968997164 1.876321773
C 6.543675573 -0.990133471 1.538756111
H 6.965100877 -0.204444928 0.918970598
C 7.358057550 -2.023908607 1.999150514
H 8.411411714 -2.037029009 1.735932067
C 6.821724262 -3.040248813 2.793296806
H 7.459304939 -3.844567613 3.147929682
C 5.465485564 -3.027589151 3.125903834
H 5.045869671 -3.821620272 3.736326353
C 4.645832485 -1.997170350 2.667403368
H 3.588310151 -1.995419401 2.911234381
O -2.345737205 -0.240641386 1.838017517
O -1.559455845 0.435578976 3.852821633
C -2.919616572 0.448141012 4.354825225
H -2.841928266 0.795700767 5.383662375
H -3.534440031 1.125688482 3.758926324
H -3.344945630 -0.556985897 4.312925308

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20B-TS1

=====

C 0.116776787 -0.124578693 -0.090506964
C -0.122415748 0.099439719 1.838285749
C 2.864260636 -0.103247398 0.253221752
C 0.947601927 0.044161018 2.547811133
Rh 1.369746783 -1.336904461 1.002445866
P 1.574207854 -3.014365944 -0.716313398
C 0.823840122 0.873575279 -0.667017764
C 2.194994403 1.196593993 -0.155647512
C 2.776365847 1.977179021 -1.365080490
C 0.558933686 1.719370732 -1.888066057
O 1.643872026 2.642344335 -1.918594890
H 3.571999912 -0.011274356 1.083723154
H 3.305553172 -0.621485934 -0.598513883
H -0.825627355 -0.522016590 -0.454514119
H 0.544772800 1.087640053 -2.791166629
H -0.382822831 2.277143824 -1.839083570
H 3.515086263 2.733032430 -1.092498487
H 3.221978983 1.274897448 -2.088534690
H 2.095139290 1.868972031 0.710708905
C 1.649567706 0.401862047 3.797252380
C -1.593225994 -0.005566642 2.017761312
H 2.390256018 1.186844217 3.604802585

H 0.935712691 0.778020048 4.538220962
H 2.180758432 -0.457408941 4.217001447
O -2.307169371 -0.769325409 1.400672893
O -1.984754409 0.825525178 2.985156853
C -3.397193959 0.775966959 3.315833596
H -3.533238922 1.520433414 4.098401303
H -3.996633737 1.019283873 2.435971966
H -3.663812350 -0.221002107 3.673596610
C 2.737063754 -4.314864610 -0.173046412
C 3.893937791 -3.899099959 0.512301108
H 4.082246251 -2.839151851 0.675223844
C 4.819276488 -4.835497387 0.970429047
H 5.712506356 -4.504270998 1.491611446
C 4.590424352 -6.197056410 0.761619380
H 5.306538404 -6.928953005 1.122653664
C 3.438209506 -6.617204647 0.094376083
H 3.257096586 -7.676271962 -0.062354556
C 2.512294153 -5.683884915 -0.372937140
H 1.616451743 -6.023104721 -0.882193864
C -0.016840279 -3.792816758 -1.146259278
C -1.138315453 -3.577044295 -0.330274343
H -1.079970924 -2.930815485 0.541592453
C -2.362481514 -4.166018146 -0.650081400
H -3.225287872 -3.982193439 -0.017443592
C -2.476104191 -4.973959288 -1.782250251
H -3.429032392 -5.431313139 -2.030527366
C -1.365573236 -5.184184968 -2.605658299
H -1.454381249 -5.803461130 -3.493220484
C -0.142340857 -4.592849976 -2.296235512
H 0.710741440 -4.741934721 -2.952074021
C 2.214694436 -2.342870085 -2.295414312
C 1.328437468 -1.661998509 -3.147992420
H 0.263711656 -1.656078028 -2.933888762
C 1.806493205 -1.006941524 -4.282364837
H 1.110734118 -0.496255901 -4.941892560
C 3.173772521 -1.009870044 -4.574061479
H 3.544289370 -0.495403560 -5.455275000
C 4.057332781 -1.689931127 -3.734641486
H 5.118824143 -1.710719453 -3.963055788
C 3.583492703 -2.355209752 -2.600858272
H 4.282048386 -2.889372268 -1.964026309

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20B-TS2

=====

C -0.213899808 -0.127039776 0.033517850
C -0.017610923 0.001137792 2.323890093
Rh 1.824371013 -0.015037807 1.052670851
P 4.131151951 0.281011567 1.361513387
C 2.085182540 -1.831334040 0.333111604
C 1.007529453 -2.300173694 -0.302597749
C -0.325733125 -1.589127465 -0.290533565
C -0.840172874 -1.983282265 -1.701856864
C 0.883515547 -3.458353019 -1.282771873
O -0.432751886 -3.338463875 -1.825145819
H -1.147871939 0.381139964 0.245935378
H 0.337931469 0.448827122 -0.723679263
H 3.044994925 -2.335689714 0.403453172
H 1.647719977 -3.383850770 -2.070993216
H 0.973459237 -4.440249036 -0.806030474
H -1.926637933 -1.940744164 -1.802463921
H -0.378432800 -1.342255435 -2.471350647

H -0.977007757 -2.090736037 0.438904929
C 1.136779241 -0.143586176 2.884832565
C -1.459417108 0.100074417 2.635807188
C 1.787135737 -0.249658216 4.206839406
H -1.887393842 1.038916631 2.269653668
H -2.026188275 -0.727764839 2.195811458
H -1.571382311 0.064533133 3.724374323
C 4.442172796 1.389112767 2.773762067
C 5.373091712 1.072413468 3.770611228
H 5.951826320 0.157335159 3.706444400
C 5.546749489 1.931929311 4.856300988
H 6.272780094 1.684321463 5.625009255
C 4.792378469 3.102207130 4.956190669
H 4.933088485 3.768815883 5.802013801
C 3.859776617 3.420786182 3.964289556
H 3.275850460 4.333571488 4.035714114
C 3.683154989 2.567452800 2.877274591
H 2.965828035 2.827311149 2.101571670
C 5.232419178 -1.159448547 1.536929243
C 4.855029295 -2.221751233 2.375683357
H 3.913626578 -2.178795275 2.911310439
C 5.710470414 -3.310000420 2.542267024
H 5.418362019 -4.126875319 3.195441122
C 6.937229396 -3.349637636 1.875583666
H 7.599522204 -4.200275496 2.007401499
C 7.313336098 -2.296110677 1.040404866
H 8.267196300 -2.323929774 0.522490211
C 6.465885967 -1.202322455 0.867387300
H 6.765938575 -0.387407719 0.216722370
C 4.702571604 1.158532467 -0.137419720
C 5.439719894 2.349489194 -0.081735923
H 5.691611718 2.792897651 0.876043231
C 5.858625610 2.963345518 -1.263180256
H 6.432863523 3.883718822 -1.215147321
C 5.547766719 2.396570581 -2.500211809
H 5.877300699 2.878072482 -3.415897444
C 4.815937111 1.207541709 -2.561209847
H 4.578901242 0.760997641 -3.522258663
C 4.392151150 0.590568816 -1.386458418
H 3.834286431 -0.341868100 -1.438102414
O 2.846388615 -0.806958628 4.402413987
O 1.061151184 0.379535935 5.138026958
C 1.654601317 0.412082203 6.461482774
H 0.949528408 0.966052985 7.078994675
H 1.792585410 -0.603457319 6.839668589
H 2.621022181 0.919776654 6.417639362

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21A

=====
Rh 0.559018909 1.354067581 0.975842941
C -0.479022585 -0.539612224 -0.290857704
C 0.752363575 2.495277634 -0.718325770
C 0.488862164 0.039209046 -1.066505481
C 0.458323851 1.425499650 -1.754831555
C 1.548082706 1.237069139 -2.850389033
C 1.654011115 -0.710520531 -1.684646180
O 1.733863612 -0.166336318 -2.991992243
H 0.041965681 3.320101454 -0.681207228
H 1.789424906 2.848438660 -0.725917475
H -0.382337288 -1.606252813 -0.080687668
H 2.585837485 -0.531284774 -1.117657165

H 1.491160165 -1.788968579 -1.757110371
H 1.256980410 1.640318631 -3.822205965
H 2.487572077 1.719369409 -2.532902236
H -0.535942140 1.572857438 -2.190815449
C -1.684627983 0.136238443 0.249561777
C -1.397807599 1.326416294 0.830417926
C -3.016771534 -0.553958338 0.145254414
C -2.361211979 2.323372268 1.355398386
P 1.049076564 2.930410707 2.555131970
H -3.800253118 0.024642471 0.633138740
H -3.279400806 -0.721637144 -0.905811143
H -2.959513575 -1.540358386 0.622422849
C 0.617197343 2.356737868 4.228665550
C 1.530399272 2.499618761 5.287016669
H 2.512554110 2.926569551 5.108728153
C 1.174831310 2.090475659 6.570625373
H 1.883083595 2.202417767 7.386042255
C -0.087025527 1.539198737 6.806719268
H -0.359474337 1.220357273 7.808306261
C -0.997220403 1.395794872 5.757908405
H -1.978037169 0.967189407 5.939574344
C -0.649624505 1.799781915 4.469283094
H -1.369240628 1.681796211 3.665784766
C 2.860301571 2.746091414 2.392703359
C 3.695330178 3.770383936 1.922346491
H 3.303226797 4.770206084 1.769170026
C 5.041456939 3.508864588 1.668093129
H 5.685697372 4.309486666 1.317166556
C 5.563945205 2.228528171 1.868309821
H 6.612596505 2.032749850 1.666135805
C 4.741239726 1.204415946 2.341816163
H 5.147709060 0.213029795 2.517631951
C 3.395210124 1.457943226 2.605535133
H 2.770525565 0.667269845 3.015656399
C 0.639834991 4.700667417 2.467603086
C 0.162366188 5.375854179 3.600781055
H 0.023148961 4.845753549 4.536831513
C -0.135257699 6.737324057 3.528246257
H -0.501776322 7.253476155 4.410342351
C 0.037735559 7.432023178 2.330752879
H -0.193601644 8.491639965 2.278202541
C 0.508835086 6.762433856 1.197429915
H 0.644317489 7.299157105 0.263266745
C 0.804545885 5.402601223 1.261662961
H 1.168553679 4.896273287 0.376025485
O -1.918042143 3.581660191 1.185211869
O -3.413213091 2.036916784 1.894600154
C -2.771740393 4.626025077 1.704885831
H -3.725809428 4.633758410 1.172948700
H -2.221497616 5.551400583 1.542831379
H -2.955636545 4.467167842 2.769851645

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21B

=====
Rh 0.429295715 1.322757464 1.066960889
C -0.980007080 -0.325519325 -0.163502171
C 0.932478680 2.307623000 -0.659846652
C 0.115599090 -0.034265347 -0.927773874
C 0.445989486 1.283744372 -1.669885620
C 1.514815741 0.790870053 -2.688996812
C 1.085000797 -1.072144381 -1.461489173

O 1.360058624 -0.619653876 -2.777534052
H 0.439860131 3.279071056 -0.706187800
H 2.021599516 2.421749913 -0.621510782
H -1.152114586 -1.369286441 0.093939334
H 2.006348071 -1.109274740 -0.851363769
H 0.660504623 -2.078236746 -1.512179722
H 1.384013785 1.209990342 -3.688485448
H 2.524913445 1.045997870 -2.326884226
H -0.461801281 1.633078770 -2.173617794
C -1.983390395 0.656102127 0.314158923
C -1.478495032 1.776056646 0.891769771
C -3.441487644 0.340881911 0.213693198
C -2.148865899 3.032101956 1.321881997
H -2.050807526 3.192827544 2.400323542
H -1.680435386 3.895294115 0.836447866
H -3.210650358 2.993199239 1.065187167
P 1.199346474 2.881077839 2.568721108
C 0.858291462 2.290527819 4.260686849
C 1.792691814 2.487499390 5.290197898
H 2.732437782 2.991377279 5.086053052
C 1.516085732 2.025880326 6.575750754
H 2.240988668 2.178192260 7.369615271
C 0.313616609 1.365803197 6.841743504
H 0.105261840 1.003696551 7.844004941
C -0.618603567 1.166809754 5.821660935
H -1.552385507 0.652525074 6.027542136
C -0.349106140 1.625168039 4.532433502
H -1.079325926 1.465385469 3.743133613
C 3.012408918 2.815534423 2.370793175
C 3.817287107 3.946212415 2.180244886
H 3.381631195 4.939443128 2.195066179
C 5.190710286 3.794570191 1.978349958
H 5.811477929 4.673981308 1.836022152
C 5.766563492 2.523429924 1.963076647
H 6.834835560 2.413082837 1.803322649
C 4.970655392 1.391981091 2.162571877
H 5.417444447 0.402349931 2.165313543
C 3.600591283 1.535857751 2.367433480
H 2.992919921 0.651674999 2.556915078
C 0.667455193 4.617271929 2.463911503
C -0.031923749 5.219250901 3.519806429
H -0.213935070 4.670737806 4.438368296
C -0.497122576 6.528984334 3.390740920
H -1.038106784 6.988333087 4.212378244
C -0.267454892 7.245535177 2.215549272
H -0.631174305 8.263774044 2.119174626
C 0.437274175 6.652403537 1.163674853
H 0.627220363 7.209791370 0.251388646
C 0.899547474 5.343324410 1.282011617
H 1.454607579 4.896800020 0.463078931
O -4.343969221 1.075796853 0.560822438
O -3.623879682 -0.887445149 -0.306312746
C -5.000312157 -1.312455726 -0.428701904
H -4.958778648 -2.310890303 -0.861879467
H -5.478546395 -1.333210403 0.553558181
H -5.549861347 -0.628141700 -1.079100636

=====
23A

=====
Rh -0.568687356 1.994153272 1.000605922
P 0.795487008 2.247131181 2.787598270

C -0.095595233 0.120854759 0.653693154
C 0.351971817 -0.362083138 -0.506870590
C 0.975824271 0.356211888 -1.691566026
C 1.703313331 -0.820832033 -2.378082049
C 0.393817273 -1.859037674 -0.834264611
O 0.859309283 -1.944115808 -2.170961153
C 0.071971617 1.427104459 4.248997330
C 0.562461825 1.789846922 5.516813820
H 1.343877023 2.538687374 5.606658152
C 0.044030036 1.191639200 6.661842482
H 0.430950198 1.472445653 7.636672011
C -0.974844156 0.240335663 6.556973080
H -1.380698974 -0.219562478 7.452839460
C -1.475313596 -0.113151302 5.303872053
H -2.272565997 -0.845153709 5.220239928
C -0.953472211 0.475179879 4.150780317
H -1.360285677 0.187985236 3.187193918
C 2.502397087 1.656147598 2.602756197
C 2.974911357 0.584121825 3.374114250
H 2.330650274 0.102000450 4.101412978
C 4.285869974 0.136148783 3.209874308
H 4.646966107 -0.694009516 3.809187414
C 5.129241286 0.752503689 2.285161841
H 6.149708518 0.402129081 2.163385846
C 4.660318644 1.818387438 1.512285288
H 5.312386056 2.296192933 0.787522692
C 3.349727022 2.265151178 1.660647266
H 2.983488575 3.075652454 1.038162164
C 0.824452091 4.010289254 3.249216125
C 1.987977302 4.792047493 3.267354283
H 2.952676735 4.356605778 3.035463044
C 1.909995731 6.143633389 3.607917516
H 2.814784883 6.743502239 3.623503632
C 0.681386351 6.719957792 3.932067916
H 0.627772810 7.772093235 4.194379084
C -0.479358516 5.940425470 3.929779503
H -1.434946655 6.382182856 4.195002547
C -0.410460358 4.592852201 3.590317824
H -1.314229404 3.988158603 3.605050740
H -0.389910523 -0.554529386 1.462039595
H 1.081905175 -2.364873111 -0.134695995
H -0.583082857 -2.348045495 -0.771091108
H 1.835731240 -0.681366355 -3.453168493
H 2.694090071 -0.974695007 -1.914788813
H 0.180522807 0.702944843 -2.365866846
C 0.380460368 3.194719578 -0.207029317
C 1.264261963 2.879409332 -1.171747209
C 1.917429319 1.515804280 -1.330854910
C -0.319959876 4.490852156 0.093908601
C 1.588804495 3.959343058 -2.168780381
H 2.435366434 1.251265137 -0.403817643
H 2.677251073 1.597811894 -2.109716768
H -1.161582437 4.350443256 0.799593265
H 0.363777570 5.204668793 0.560911269
H -0.723936735 4.938636581 -0.817355159
O 1.396186333 5.149496223 -1.999784231
O 2.112248377 3.446090932 -3.298139295
C 2.434547452 4.407763376 -4.325963912
H 2.838588527 3.824409139 -5.152499802
H 1.535841328 4.947549824 -4.633682245
H 3.171826653 5.124959943 -3.957491905

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=====
23B
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Rh -0.32800000 2.22910000 0.98380000
P 0.99670000 2.28040000 2.81280000
C -0.22070000 0.30480000 0.60370000
C 0.22730000 -0.30710000 -0.49660000
C 1.18410000 0.18460000 -1.56580000
C 1.75200000 -1.16040000 -2.06150000
C -0.10750000 -1.75480000 -0.86410000
O 0.64300000 -2.04620000 -2.03810000
C 0.06110000 1.37820000 4.09570000
C -0.47660000 2.04720000 5.20760000
H -0.31920000 3.11130000 5.34040000
C -1.20730000 1.33800000 6.16020000
H -1.61680000 1.86220000 7.01810000
C -1.40530000 -0.03570000 6.01720000
H -1.97480000 -0.58240000 6.76240000
C -0.86700000 -0.70890000 4.91700000
H -1.01160000 -1.77910000 4.80690000
C -0.14320000 -0.00820000 3.95630000
H 0.27680000 -0.53910000 3.10900000
C 2.67030000 1.57170000 2.69810000
C 3.08900000 0.50370000 3.50460000
H 2.40990000 0.04540000 4.21360000
C 4.39930000 0.03170000 3.40980000
H 4.71470000 -0.79750000 4.03550000
C 5.30080000 0.62610000 2.52740000
H 6.31930000 0.25650000 2.45970000
C 4.89430000 1.70510000 1.73750000
H 5.59560000 2.17890000 1.05740000
C 3.58690000 2.17540000 1.81840000
H 3.27740000 3.01440000 1.20420000
C 1.22750000 3.99000000 3.41900000
C 2.47400000 4.43320000 3.89260000
H 3.33280000 3.77260000 3.88970000
C 2.61520000 5.73260000 4.37910000
H 3.58280000 6.06520000 4.74210000
C 1.52040000 6.59710000 4.40490000
H 1.63570000 7.60840000 4.78310000
C 0.27420000 6.15800000 3.95010000
H -0.58340000 6.82320000 3.97660000
C 0.12530000 4.86300000 3.45820000
H -0.84520000 4.53880000 3.10150000
H -0.85740000 -0.25230000 1.30220000
H 0.17150000 -2.42540000 -0.03480000
H -1.16870000 -1.90920000 -1.08630000
H 2.13950000 -1.12140000 -3.08260000
H 2.55910000 -1.50190000 -1.38920000
H 0.59780000 0.61720000 -2.39000000
C 0.92270000 3.12560000 -0.28150000
C 1.84110000 2.63090000 -1.13550000
C 2.26230000 1.17370000 -1.09850000
C 0.39290000 4.48030000 -0.08000000
C 2.50900000 3.45760000 -2.20770000
H 2.56040000 0.89830000 -0.08290000
H 3.14580000 1.05910000 -1.73630000
H 3.59090000 3.48640000 -2.02260000
H 2.37430000 2.96270000 -3.17740000
H 2.13780000 4.47740000 -2.27270000
O 0.98820000 5.53230000 -0.61300000

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O -0.59950000 4.56810000 0.67070000
C 0.42990000 6.83280000 -0.27790000
H 0.45930000 6.97750000 0.80390000
H -0.60030000 6.90040000 -0.63220000
H 1.06630000 7.55320000 -0.78850000

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21A-TS
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C -0.336425994 0.229028048 0.102433452
C -0.008296671 -0.015671624 2.117656258
Rh 1.694568737 0.009382272 1.056100558
C 0.847150749 -2.143226167 1.544158942
C 0.830780393 -1.958704339 0.175442417
C -0.212632599 -1.125376281 -0.572560221
C 0.402155985 -1.134366875 -1.987460461
C 1.611403038 -2.742220816 -0.864913082
O 1.008799222 -2.414431681 -2.112449263
H -1.337350402 0.470634604 0.445179174
H 0.036390140 1.090074967 -0.452954021
H 1.445777271 -2.955431601 1.957396959
H 2.676128110 -2.462327030 -0.849468799
H 1.538731647 -3.825902591 -0.717825525
H -0.333984269 -1.028529476 -2.786993861
H 1.151675623 -0.328522732 -2.077413181
H -1.165113375 -1.671446670 -0.582207301
C 0.068949975 -1.335760627 2.500495036
C -0.404692449 -1.957060848 3.783130808
C -0.593824005 1.117124936 2.877618669
P 2.577265143 2.092250015 1.145485759
H -0.775997160 -1.205277824 4.476416777
H -1.203044302 -2.680309256 3.574553896
H 0.414186909 -2.515504230 4.252206852
C 3.200614637 2.790208817 2.697622137
C 4.330829129 3.626244634 2.697527307
H 4.847601567 3.848660681 1.767774844
C 4.786058132 4.175641351 3.893999220
H 5.660312837 4.819598924 3.893882428
C 4.118610086 3.897673817 5.090656636
H 4.475052063 4.330358279 6.020647845
C 3.000069009 3.062491791 5.094959455
H 2.485754050 2.842219144 6.025429694
C 2.540418670 2.503131914 3.902120470
H 1.679594267 1.843002287 3.915282589
C 3.888997582 1.145161787 0.301525312
C 4.291335884 1.303902278 -1.040118331
H 4.027909066 2.206568168 -1.581305995
C 5.031632535 0.308237041 -1.664504563
H 5.353013453 0.445587140 -2.692698940
C 5.366794844 -0.874180130 -0.982922293
H 5.938284100 -1.645647956 -1.489359831
C 4.998086118 -1.038526509 0.346610535
H 5.294681633 -1.927732817 0.894580431
C 4.261296774 -0.035522679 1.003141912
H 4.104979583 -0.105213295 2.079247050
C 1.981636493 3.451848828 0.104556320
C 1.870622444 4.756885860 0.609476440
H 2.195135261 4.983106740 1.619479727
C 1.343503489 5.772136441 -0.189245359
H 1.265222956 6.779861453 0.207393603
C 0.922544690 5.497701244 -1.491095619
H 0.514733067 6.291702381 -2.109317077

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C 1.024576788 4.199993845 -1.998239308
H 0.697695217 3.982694182 -3.010595804
C 1.543281763 3.179301594 -1.204731761
H 1.616014685 2.173534973 -1.607468074
O -0.595152054 2.253538151 2.149130142
O -0.980386549 1.058408137 4.029246218
C -1.057563273 3.436960163 2.834863436
H -2.086893380 3.305900372 3.176128889
H -0.986869861 4.238455066 2.100427238
H -0.417332969 3.645297526 3.696102185

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21B-TS

=====

C -0.696811262 0.227366114 0.437428350
C -0.045150363 -0.288298875 2.296642363
Rh 1.465300605 0.194299605 1.061159955
C 1.021072261 -2.120262963 1.181630661
C 0.778616386 -1.681961891 -0.105647540
C -0.484312516 -0.925415805 -0.528999065
C -0.104134697 -0.557947146 -1.977810248
C 1.502587546 -2.095842244 -1.373452364
O 0.666472345 -1.658676496 -2.441786007
H -1.652274308 0.195400574 0.955877848
H -0.570048651 1.234941350 0.038982288
H 1.781605301 -2.877943879 1.356768021
H 2.499730289 -1.631978461 -1.431978482
H 1.624062967 -3.182979486 -1.450373801
H -0.963288440 -0.441860318 -2.641870917
H 0.488699272 0.373687347 -1.988477199
H -1.333189088 -1.621425855 -0.536207500
C 0.266282321 -1.631790603 2.342291364
C 0.045960688 -2.465738389 3.551446248
C -0.770383275 0.528381007 3.316834022
H -0.267794929 0.431593920 4.283720902
H -0.812810496 1.579923600 3.023873995
H -1.787261122 0.151430232 3.470120778
P 2.171029740 2.340161403 1.383188035
C 3.015805085 2.893387376 2.888235220
C 4.223112694 3.608011819 2.809532558
H 4.666083999 3.829303254 1.842427653
C 4.854798268 4.030223147 3.977800503
H 5.789288031 4.579666763 3.916422643
C 4.288228678 3.745466612 5.223927013
H 4.784001164 4.075959009 6.131481516
C 3.089961044 3.032594933 5.304016207
H 2.653107148 2.807183804 6.271983942
C 2.453746610 2.601579350 4.139660675
H 1.527995666 2.038196033 4.202046671
C 3.406228004 1.604512207 0.259846994
C 3.568027654 1.926030985 -1.104531512
H 3.111553264 2.824582187 -1.506514536
C 4.321233273 1.098236649 -1.925458758
H 4.457842380 1.359648584 -2.970663818
C 4.907973812 -0.074360948 -1.418624648
H 5.490241971 -0.712155377 -2.076670905
C 4.764616139 -0.404611251 -0.077227529
H 5.243399413 -1.291202783 0.327006646
C 4.015155663 0.427080381 0.774453050
H 4.021023870 0.238324573 1.846835688
C 1.372818349 3.768455476 0.602586087
C 1.377412583 5.031027824 1.214931328

H 1.894153494 5.180614418 2.157290763
C 0.716821624 6.100135957 0.609134282
H 0.724793611 7.074886644 1.086976057
C 0.050823361 5.920949596 -0.604119404
H -0.461064088 6.756875268 -1.071137946
C 0.040213242 4.665570180 -1.217756019
H -0.475778343 4.523612140 -2.162550701
C 0.690481192 3.591186495 -0.615976431
H 0.683274615 2.619860442 -1.101185608
O -0.579597127 -2.099663259 4.528238713
O 0.632978872 -3.672107699 3.432062701
C 0.478226648 -4.550496205 4.568999395
H 0.997407539 -5.469453973 4.300073173
H 0.921479596 -4.099421013 5.460122394
H -0.580885680 -4.742449173 4.755989491

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23A-TS

=====

C -0.194387178 -0.028394008 0.070470186
C 0.086515421 -0.016852101 2.094489241
Rh 1.713165760 0.046949293 0.819096358
P 2.416395363 2.139312613 0.844604388
C -0.282674475 -1.291982810 -0.358425963
C 0.538176185 -2.352059170 0.368269966
C 0.345346594 -3.587407422 -0.557858860
C -1.018008754 -1.987735729 -1.479048776
O -0.164356830 -3.086184062 -1.787873908
C 3.970957965 1.298779176 0.398943889
C 5.027855849 1.110395349 1.314082060
H 5.004126376 1.605958793 2.279188090
C 6.108495388 0.306267419 0.967377035
H 6.929285933 0.179067861 1.666322349
C 6.144167663 -0.333933414 -0.277542031
H 6.992757890 -0.959203004 -0.538106573
C 5.100710003 -0.165789768 -1.187563604
H 5.134782522 -0.652675420 -2.157257832
C 4.014604304 0.649747489 -0.861305907
H 3.232271963 0.827911423 -1.594037565
C 1.967349940 3.308554485 -0.463188464
C 2.951158976 3.873846517 -1.291017657
H 3.995913812 3.607539776 -1.163423845
C 2.583274394 4.783711747 -2.281886571
H 3.345433078 5.219605446 -2.920870788
C 1.242201235 5.133189001 -2.449908435
H 0.960036375 5.841268989 -3.223130672
C 0.261600253 4.574911513 -1.625102057
H -0.780828472 4.848890195 -1.755187562
C 0.619169327 3.663202854 -0.634350319
H -0.148040973 3.235855035 0.004576124
C 2.615031014 3.052960809 2.393049880
C 2.651377384 4.456326217 2.408266120
H 2.534858190 5.018781360 1.487319563
C 2.839300806 5.129547602 3.615620348
H 2.867531620 6.214850410 3.625639323
C 2.987814251 4.413519582 4.805252027
H 3.129852799 4.943195322 5.742303496
C 2.945166657 3.015505089 4.793778331
H 3.048998871 2.457840373 5.719335829
C 2.754244895 2.333885507 3.594394388
H 2.698937827 1.248286861 3.587137292
H -0.762970218 0.834793275 -0.258400331

H -2.012234361 -2.332657761 -1.144253905
H -1.142536730 -1.378023205 -2.376672791
H 1.266537759 -4.132942220 -0.772004609
H -0.373224020 -4.279127198 -0.088829343
H 1.629889404 -2.096821477 0.397405144
C -0.136520468 -1.264458877 2.603360363
C 0.053348484 -2.547582645 1.817012671
C -0.432567709 1.266598836 2.689844935
C -0.723240410 -1.405990395 3.968672081
H -0.912883617 -3.069143135 1.812014150
H 0.742458013 -3.223858913 2.335165767
H 0.180117192 1.578850197 3.537799909
H -0.427276654 2.070595852 1.951172141
H -1.450325397 1.140677201 3.066884589
O -1.043648257 -2.692671419 4.230208329
O -0.876315099 -0.506329991 4.775231977
C -1.593717764 -2.937641964 5.540397774
H -1.785691593 -4.009322711 5.580534340
H -0.880991538 -2.641275997 6.313962105
H -2.518773854 -2.372593297 5.677014078

23B-TS

C -0.137816331 -0.028189601 0.021014276
C -0.063284927 0.028486806 2.034464589
Rh 1.700759558 0.015720227 0.931872548
P 2.385654605 2.113031725 0.900852805
C -0.176392445 -1.296903605 -0.401264816
C 0.451063051 -2.364687285 0.488987373
C 0.354897728 -3.625398683 -0.416253216
C -0.725018768 -1.998590627 -1.621241658
O 0.110831078 -3.148730930 -1.733390152
C 3.974058499 1.272192358 0.605552878
C 5.008619354 1.203044917 1.561882110
H 4.953033671 1.801543116 2.465046291
C 6.107876330 0.383473573 1.334474994
H 6.912968532 0.350907072 2.062212937
C 6.184173242 -0.395721194 0.172206406
H 7.047392338 -1.033263613 0.006836538
C 5.165600745 -0.345782946 -0.777133950
H 5.232581569 -0.935538443 -1.685939099
C 4.061649280 0.489343349 -0.574736383
H 3.310016522 0.588579837 -1.353466500
C 2.027945916 3.223529516 -0.483243379
C 3.073369032 3.698324506 -1.293768035
H 4.098744182 3.396446332 -1.104772812
C 2.791666733 4.570028493 -2.344667884
H 3.600339085 4.939130292 -2.968164093
C 1.476204218 4.968005073 -2.590722513
H 1.260855357 5.646555353 -3.410740605
C 0.437856723 4.498691999 -1.782524067
H -0.583936400 4.813124644 -1.972063810
C 0.704173660 3.627214864 -0.727712277
H -0.098245532 3.274642786 -0.089235135
C 2.473864754 3.081547010 2.425897659
C 2.416065135 4.483951247 2.399695648
H 2.278115363 5.008807073 1.460096839
C 2.536445014 5.202122615 3.589059756
H 2.492312698 6.286635443 3.568884774
C 2.716805418 4.530117013 4.800392096
H 2.813759738 5.094805309 5.722940772

C 2.764905282 3.133566849 4.830134888
H 2.892344054 2.611099104 5.773249311
C 2.633319592 2.406779047 3.649269492
H 2.641602463 1.320976454 3.673134412
H -0.625216950 0.853663569 -0.374375347
H -1.781552051 -2.285714908 -1.476121476
H -0.644325813 -1.417586238 -2.542628938
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H -0.477974515 -4.258636152 -0.068106008
H 1.531782907 -2.168353532 0.717394992
C -0.545034595 -1.142272035 2.537882892
C -0.302967668 -2.457653479 1.828887725
C -0.444652080 1.388423861 2.513460678
C -1.470000326 -1.260805123 3.723829196
H -1.285041690 -2.924746392 1.660926568
H 0.236078098 -3.138672438 2.501002405
H -1.042624203 -1.948875260 4.463656815
H -2.424126084 -1.699744233 3.403180974
H -1.663150920 -0.311073099 4.216088916
O -0.376189226 1.526505956 3.846751947
O -0.744184485 2.309358530 1.770489750
C -0.724958648 2.838029809 4.353247539
H -1.756139383 3.082836649 4.089481690
H -0.052412085 3.590759689 3.937629909
H -0.606053653 2.768547029 5.433439312

22

C 0.067344073 -0.012906702 0.044778950
C 0.027496114 -0.019349106 1.578193726
Rh 2.065409657 -0.029276315 2.181782171
C 1.342039311 -2.073485384 1.757035264
C 1.882418810 -1.739376125 0.529291264
C 1.110690209 -0.988445001 -0.527226617
C 2.279577854 -0.424171737 -1.348881841
C 3.160989987 -2.203453460 -0.122264499
O 3.252149794 -1.472025324 -1.347662139
H -0.934253762 -0.252687626 -0.331120804
H 0.272306769 1.004929359 -0.295753875
H 1.770105536 -2.855300534 2.380651526
H 4.030223487 -2.000493016 0.520904098
H 3.148395201 -3.278494580 -0.349724748
H 2.027265221 -0.200628268 -2.388610225
H 2.674368248 0.488620469 -0.869531257
H 0.617562869 -1.754553033 -1.143499341
C 0.309263556 -1.218259459 2.335140408
C -0.328027671 -1.643391382 3.630644235
C -0.768342629 1.089373981 2.224818954
P 2.499977050 1.872872000 3.378097242
H -0.694482713 -0.794715353 4.201674615
H -1.176588291 -2.302483935 3.403162973
H 0.381341468 -2.214639083 4.236598967
C 2.595864252 1.856284661 5.179764478
C 3.799800964 2.115817430 5.855214828
H 4.709045143 2.324324315 5.298002102
C 3.823947797 2.096987971 7.249175290
H 4.753258169 2.294614277 7.775330223
C 2.655492381 1.824687072 7.965455747
H 2.679169213 1.810751868 9.051327978
C 1.458500416 1.567800928 7.292016241
H 0.553072211 1.355285444 7.852830193

C 1.421399797 1.577375244 5.898516282
H 0.494916823 1.374667807 5.367575518
C 4.056518890 1.247579003 2.654818561
C 4.555377656 1.735933662 1.421883152
H 4.172718759 2.669426082 1.020646414
C 5.534884841 1.025164763 0.737379528
H 5.921545527 1.410642216 -0.201265390
C 6.028393420 -0.183322492 1.249861125
H 6.796902826 -0.725480091 0.707300872
C 5.541351921 -0.684194366 2.454507396
H 5.934262923 -1.611329303 2.861654848
C 4.545078309 0.009439821 3.157323601
H 4.219061657 -0.349760807 4.129926733
C 2.150494235 3.546594964 2.785441529
C 2.366146760 4.672416505 3.594783909
H 2.739226993 4.554216435 4.608023475
C 2.091718507 5.944352563 3.095089281
H 2.259376099 6.816199975 3.720464766
C 1.601431055 6.098008007 1.795602457
H 1.387666468 7.091655619 1.412383374
C 1.376910234 4.978072758 0.990711239
H 0.985944217 5.097719946 -0.015544711
C 1.643033966 3.702170764 1.484612429
H 1.445849028 2.827631365 0.871832077
O -1.256139023 1.932322756 1.300073399
O -0.931002449 1.260362386 3.420734127
C -1.970702353 3.079328816 1.813344870
H -2.803421654 2.757598473 2.442309892
H -2.330570908 3.612036086 0.933643481
H -1.293406088 3.708352670 2.396349747

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24

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C -0.012244356 -0.034467050 0.040565421
C -0.013847711 -0.045694020 1.569398642
Rh 2.093842615 0.009579353 2.061093682
C 1.424982002 -2.057459379 1.661947450
C 1.878599976 -1.698535631 0.407696049
C 1.028440136 -0.965639354 -0.601057910
C 2.130076876 -0.354940398 -1.479111832
C 3.127498996 -2.126197354 -0.318808115
O 3.150753305 -1.355679084 -1.524745364
H -1.024222664 -0.296885055 -0.296757016
H 0.144735598 1.001259281 -0.284399463
H 1.908822671 -2.823911918 2.258808092
H 4.026443363 -1.932345143 0.283209443
H 3.114212789 -3.193867377 -0.578541383
H 1.816911701 -0.147178348 -2.505452585
H 2.505911211 0.575562844 -1.021650005
H 0.526816064 -1.742143582 -1.196844159
C 0.403055111 -1.221005318 2.287425940
C -0.038641110 -1.557585176 3.685811009
C -0.968644145 0.962239078 2.163686549
H -0.894204118 1.019298333 3.245500658
H -0.781829699 1.950288390 1.734105093
H -1.998539231 0.683555315 1.902229519
P 2.541915854 1.906314827 3.258273966
C 2.902693298 1.835692915 5.026252071
C 4.091619032 2.368078422 5.553660031
H 4.827946129 2.823651625 4.897363777
C 4.325775245 2.303704070 6.925719466

H 5.243759398 2.712835632 7.336673076
C 3.380960061 1.712503519 7.769476405
H 3.567355469 1.665577153 8.838353764
C 2.203311864 1.177646572 7.244074891
H 1.474245680 0.713846226 7.901584095
C 1.958867285 1.230944754 5.871630833
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C 4.021255570 1.373768554 2.315002926
C 4.288136159 1.845222557 1.005036559
H 3.782574690 2.733765646 0.640867799
C 5.208873584 1.184543327 0.196812521
H 5.411169977 1.559499941 -0.801547109
C 5.873950536 0.042051087 0.660563073
H 6.591707927 -0.462229949 0.021565304
C 5.617498787 -0.441792166 1.942705768
H 6.141172661 -1.318434248 2.312084039
C 4.684684931 0.199659368 2.768071690
H 4.527240592 -0.153155477 3.783432869
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C 2.195747070 4.676286907 3.639671092
H 2.631784208 4.544488939 4.624675785
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H 1.906841103 6.790997492 3.891165397
C 1.214043859 6.119387286 1.963208770
H 0.892970428 7.107576640 1.648017393
C 1.046079257 5.026917160 1.108724187
H 0.594262706 5.163055341 0.130803511
C 1.446869211 3.757391121 1.518084284
H 1.304170186 2.902692818 0.862279090
O -0.433995146 -0.767109154 4.520520634
O 0.074915025 -2.875312596 3.905028066
C -0.289498059 -3.323530827 5.231885527
H -0.139732234 -4.402092383 5.224066246
H 0.349042025 -2.845657600 5.978978037
H -1.332788244 -3.075954060 5.439240640

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25

=====
Rh 0.545618397 1.040419355 -0.407019467
P -1.383807151 2.335991741 0.106776766
P -0.319145517 0.341646547 -2.526900450
C 2.688374684 0.334574590 -0.982015199
C 2.054854737 -0.760631543 -0.444328826
C 1.582072996 2.145355585 1.237582585
C 1.233886905 1.073084543 1.745617101
C 1.086389240 -0.155286708 2.557525932
O 1.215587080 -1.340593371 1.793723208
C 2.354395183 -1.325164874 0.934352593
H 1.842946525 -0.122153148 3.359044208
H 0.099803874 -0.193853945 3.029094762
H 2.656244141 -2.371244542 0.816764365
H 3.190202210 -0.788674169 1.402865849
H 1.513047894 -1.445984102 -1.092345344
H 2.000748679 3.122489652 1.099041821
H 3.394896856 0.902920911 -0.384260377
H 2.722946300 0.520068439 -2.048429718
C 0.902694541 -0.300959518 -3.757932603
C -1.496640022 -1.073119620 -2.375214502
C -1.223624496 1.554701211 -3.588938835
C -1.550298528 2.819970435 1.879655273
C -1.458695658 3.971546402 -0.748326203
C -3.052101745 1.600261067 -0.198100432
H -1.487760424 3.841270293 -1.831531733
H -2.345288346 4.530590429 -0.433302747

H -0.566786282 4.552169732 -0.499363358
H -1.606074324 1.928695730 2.509308896
H -0.694103994 3.414478000 2.200555141
H -2.464279241 3.405712534 2.015697544
H -3.216220092 1.394865224 -1.256927733
H -3.141876403 0.661589119 0.355544461
H -3.832228847 2.286228068 0.145631406
H -2.115190801 1.938563814 -3.091272854
H -0.566694952 2.395938147 -3.825816150
H -1.529922890 1.075510642 -4.523923897
H 1.560966893 0.505974315 -4.090830908
H 1.514113053 -1.102087656 -3.337592295
H 0.370095108 -0.693717710 -4.629116390
H -2.350671146 -0.795065788 -1.755269400
H -1.856222951 -1.386064514 -3.360293652
H -0.994130149 -1.917621788 -1.896421265

26

Rh 0.887941042 1.248168281 -0.584106147
P -0.617498700 2.558562998 0.676876495
P -0.826063814 0.222087892 -1.899105131
C 2.583067752 0.514214413 -2.090743698
C 2.276978372 -0.388417473 -1.311222065
C 2.568706502 2.456477511 0.213266644
C 2.486360723 1.524580116 1.021088818
C 2.672973802 0.569323230 2.123031914
H 3.034172718 -0.393122913 1.724071682
H 3.462395396 0.962908246 2.785700046
H 2.896532294 3.370883458 -0.240634400
C -0.294208303 -0.387493417 -3.559560068
C -1.465804964 -1.313113898 -1.094309483
C -2.376464425 1.118769915 -2.361442892
C 0.097771606 3.426815731 2.135551722
C -1.427332672 3.944524536 -0.238583029
C -2.015726540 1.647221643 1.467299715
C 3.101227306 1.433765890 -3.103037619
H 2.248139068 -1.342149856 -0.824437744
O 1.454627278 0.402524162 2.827458477
C 1.624626215 -0.373678612 4.026246594
C 0.279747268 -0.617352859 4.637880047
H 2.109540068 -1.329959458 3.768295133
H 2.283775599 0.158327937 4.728172888
H -0.424692441 -1.179115231 4.025309959
H -0.017916862 0.458230283 -4.195405861
H 0.570716611 -1.044711437 -3.463964015
H -1.112577766 -0.932909273 -4.039456340
H -1.909910979 -1.076528391 -0.124821585
H -2.218999958 -1.796075903 -1.724906202
H -0.641510599 -2.011562858 -0.929563904
H -2.936131424 1.435835866 -1.479497427
H -2.128765637 2.003471106 -2.954588492
H -3.019103563 0.467440593 -2.962020644
H -2.629589620 1.127694515 0.728915772
H -1.599146463 0.910988352 2.159872965
H -2.653264136 2.339017572 2.027082488
H -2.005392381 3.574933139 -1.086641415
H -2.091651624 4.505777250 0.426231985
H -0.656865384 4.620821177 -0.619064427
H 0.531004037 2.686956919 2.812225713
H 0.879785566 4.123058975 1.826334597
H -0.691490400 3.981289301 2.652492471
H 2.298277187 1.830762943 -3.731526913
H 3.618061172 2.278946737 -2.637515938
H 3.816737128 0.909950764 -3.747209107
C -0.063355787 -0.218876742 5.862884182
H 0.623734538 0.334841537 6.498402934
H -1.038568560 -0.444550243 6.283656466

26A

Rh 0.738474246 1.134145459 -0.606878672
P -0.666078920 2.593605669 0.580975074
P -0.989881435 0.343029921 -2.038996891
C 2.297467521 -0.049632857 -1.844776233
C 1.987828626 -0.844321042 -0.959426690
C 2.458301415 2.452211093 -0.134667263
C 2.493018752 1.645628226 0.801421717
C 2.950058739 0.926308074 2.003123526
H 3.664154487 0.140385348 1.704178762
H 3.502702307 1.638044207 2.638129699
H 2.677415682 3.257630539 -0.807139803
C -0.376522577 -0.416887815 -3.605816661
C -2.056905596 -0.997489842 -1.344670385
C -2.218101774 1.550500952 -2.710424613
C 0.041768458 3.188262172 2.173680974
C -1.130441950 4.167676941 -0.265155020
C -2.284182760 1.904354582 1.149216745
H 2.744615795 0.425307566 -2.692368722
C 1.772607918 -1.932899909 -0.000855933
O 1.854172493 0.368987149 2.708194328
C 2.254026486 -0.171212088 3.980362531
C 1.055152355 -0.765852458 4.651625315
H 3.030123672 -0.937696404 3.816328046
H 2.695034713 0.621493625 4.602693109
H 0.541979674 -1.551330562 4.098166583
H 0.865394442 -2.497417170 -0.241281174
H 2.620040198 -2.626892716 -0.035652509
H 1.672974384 -1.542413392 1.016340420
H 0.161984943 0.331557639 -4.193572085
H 0.306899960 -1.238864212 -3.388068554
H -1.217788062 -0.791959043 -4.196645724
H -2.570695196 -0.653521649 -0.444670365
H -2.802025987 -1.318294909 -2.079610065
H -1.437143524 -1.856695233 -1.075935339
H -2.818856155 1.998444781 -1.916805952
H -1.691293072 2.348641487 -3.240944696
H -2.891015935 1.049298924 -3.412944169
H -2.924627844 1.630317791 0.308469629
H -2.100490230 1.012192048 1.754317570
H -2.814312815 2.640931548 1.761519965
H -1.670869448 3.967297159 -1.192076326
H -1.757213281 4.785122950 0.385648888
H -0.223462557 4.725630541 -0.512492480
H 0.344267362 2.327190396 2.775010254
H 0.919509484 3.809612612 1.989060313
H -0.706568996 3.774555428 2.715860912
C 0.632165177 -0.410860491 5.864859760
H 1.130942301 0.364398681 6.441700690
H -0.219098067 -0.893545631 6.334972292

26-TS

C -0.433131020 -0.344030271 0.225679396
C -0.069105749 0.383057919 2.189530055
Rh 1.703719671 -0.261754054 1.070135404
P 2.769723117 -1.241190708 3.008475733
P 3.636862792 0.399703870 -0.159165978
C 0.470618459 0.097503500 -0.569449169
C 0.906010527 1.222677750 2.216625234
C 1.356231506 2.588829907 2.552259847
H 1.159431938 3.249931119 1.688929673
H 0.729146370 2.953200550 3.384549441
H -0.960730154 0.098984401 2.725790556
C 3.859198122 -0.478447130 -1.768618887
C 3.528337297 2.175711740 -0.638116720
C 5.329913374 0.307988991 0.569713155
C 1.567773151 -1.669418750 4.340893471

C 3.518661154 -2.879348707 2.594122335
C 4.099883943 -0.371169491 3.942452047
C -1.753018726 -0.996518143 0.416318935
H 0.574566259 0.320718771 -1.620442030
O 2.727954563 2.610052902 2.899260313
C 3.125403628 3.881330592 3.444828268
C 4.594327449 3.849585584 3.733637912
H 2.890981379 4.674691068 2.715683490
H 2.553913651 4.090146460 4.361208648
H 5.245875115 3.683008594 2.876513738
H 4.070776367 -1.536392558 -1.589282617
H 2.946865621 -0.409404021 -2.365695261
H 4.688439914 -0.044788397 -2.336241230
H 3.483770100 2.776750443 0.273386623
H 4.399751760 2.474678366 -1.229471409
H 2.619659280 2.350221112 -1.218713846
H 5.374326420 0.931771077 1.465215913
H 5.580089228 -0.721255539 0.840166931
H 6.072360790 0.667859569 -0.149597568
H 5.017195324 -0.342031815 3.351066705
H 3.788077161 0.656819800 4.141204132
H 4.308202530 -0.888197966 4.884226393
H 4.329654196 -2.753074289 1.871746558
H 3.920247664 -3.364360026 3.489485679
H 2.762116045 -3.532678119 2.150103568
H 1.111670824 -0.757063355 4.732463770
H 0.776644270 -2.306341575 3.936446175
H 2.067439235 -2.196268537 5.159590186
H -1.670782011 -1.911937267 1.009233703
H -2.478325723 -0.332739291 0.895426428
H -2.136785603 -1.265902227 -0.573869259
C 5.116771593 4.043984207 4.944758481
H 6.190054640 4.047884584 5.108957863
H 4.491411622 4.223382999 5.816191852

26A-TS

C -0.382136388 -0.380417982 0.365818148
C -0.019259970 0.429886598 2.245951587
Rh 1.670723566 -0.245371362 1.052258713
P 2.718745105 -1.301687648 2.980061204
P 3.666330549 0.419414402 -0.099639512
C 0.361446125 0.081276376 -0.576541992
C 0.962711027 1.260328265 2.243979780
C 1.431873103 2.626857708 2.549540434
H 1.227035491 3.280852953 1.683069716
H 0.824221135 3.006660959 3.389189937
H -0.912821930 0.142159427 2.7766885293
C 4.037593233 -0.517446799 -1.648039300
C 3.571144721 2.174688237 -0.653407963
C 5.296765382 0.402244706 0.764675668
C 1.471267474 -1.869845115 4.215161581
C 3.570801059 -2.876182295 2.522375583
C 3.945736127 -0.414824188 4.032781210
H -1.306011350 -0.856217643 0.652003510
C 0.335016225 0.400338616 -2.027633699
O 2.810206309 3.635904074 2.870966024
C 3.230560348 3.908912665 3.396733548
C 4.710512169 3.879053334 3.621356548
H 2.964233776 4.700337489 2.676626564
H 2.697971975 4.118545207 4.335939123
H 5.324614013 3.722136121 2.735227792
H 4.205539463 -1.572518261 -1.413728456
H 3.194745407 -0.450081646 -2.339128663
H 4.931023395 -0.118747594 -2.138624742
H 3.492475504 2.807639464 0.233669874
H 4.465341741 2.453682871 -1.219616820
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H 4.098100596 -0.946498908 4.976887429
H 4.408988059 -2.676022387 1.849736660
H 3.950865303 -3.387762531 3.412421434
H 2.868891825 -3.539837478 2.009075148
H 0.960700180 -1.006018791 4.647462339
H 0.727708252 -2.505806432 3.727440167
H 1.952730106 -2.435265427 5.018944482
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8A-TS1'

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8B-TS1'

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8A-TS1"
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C -2.384634172 -5.659282093 -0.833225492
H -1.488992143 -2.495811669 0.016983291
H 0.901763298 -5.649701405 -1.696657548
H -3.445474412 -3.998852196 0.047503251
H -1.061532843 -7.131264286 -1.684069605
H -3.246082127 -6.320563203 -0.825538621
C 1.369774115 -4.804355163 2.148581331
C 0.102611149 -5.338437471 2.429826978
C 2.297643576 -5.605536972 1.461811731
C -0.220257202 -6.639919577 2.048960611
C 1.972640357 -6.908211463 1.087272734
C 0.714299686 -7.431879312 1.382534981
H -0.634511287 -4.756642847 2.970388066
H 3.287851141 -5.231056190 1.236601366
H -1.204676817 -7.035024935 2.281625395
H 2.711546416 -7.513905183 0.570159098
H 0.463252777 -8.449013954 1.095703598
C 3.564928268 -3.238740121 3.169574591
C 4.035203032 -4.416886562 3.776952324
C 4.459967830 -2.176853952 2.979542400
C 5.368310840 -4.528243550 4.168866587
C 5.795930983 -2.292005607 3.366411420
C 6.253764277 -3.468961683 3.959865862
H 3.362160522 -5.252083873 3.939471619
H 4.113866586 -1.255509548 2.534669467
H 5.715117583 -5.445489067 4.635723491
H 6.476385246 -1.461125976 3.203136013
H 7.293641770 -3.561071247 4.259504766
C 0.879851417 -2.901174449 4.243272689
C -0.486480923 -2.576237824 4.193632063
C 1.478174977 -3.101927241 5.495440524
C -1.236459428 -2.463165670 5.362505589
C 0.725977102 -2.982885086 6.664978312
C -0.630724441 -2.664148330 6.603000000
H -0.970221792 -2.397993199 3.237778484
H 2.532222223 -3.345516778 5.566959353
H -2.289858088 -2.205764883 5.304058364
H 1.205429259 -3.140333265 7.626984117
H -1.211091981 -2.567875871 7.515540756
C -2.597236515 0.471946865 3.127442097
H -3.592575894 0.926504814 3.116174587
H -2.712912787 -0.608195880 3.258992379
H -2.036983723 0.860034276 3.982678667
C -1.814996581 2.314248301 1.539291989
H -1.314743752 2.830316409 2.364467975
H -1.275866839 2.532921047 0.614513742
H -2.832928356 2.705968243 1.453504488

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8B-TS1"

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C -0.146876346 -0.096087845 0.013215739
C 0.130056310 -0.077484589 2.338155783
C 2.614476307 0.119034363 0.088284022
C 1.332141258 0.015445055 2.744186030
Rh 1.329195312 -1.272820481 0.999891789
P 3.178591723 -2.621475130 1.884345044
P 0.705881227 -2.707503052 -0.916473573
C 0.383655884 1.013437644 -0.495706567
C 1.821479332 1.369432190 -0.216564367
C 2.165767007 2.142182499 -1.514060617
C -0.135244344 1.991651410 -1.532479218
O 0.970163084 2.855783061 -1.811790539
H 3.441400229 0.272979229 0.781131102
H 2.946687588 -0.394730444 -0.813345162
H -1.165736682 -0.429637277 -0.147816241
H -0.459671666 1.455144843 -2.437313512
H -0.968229556 2.606056789 -1.173454252
H 2.974575705 2.868000235 -1.400276516
H 2.422578607 1.433532780 -2.318801630
H 1.861634148 2.068820537 0.629196413
C 2.172885609 0.607056392 3.821590420
H 3.217723335 0.324597977 3.694957174
C -1.236250136 0.317907336 2.694758800
O -1.441982485 1.146973947 3.558462175
O -2.194789841 -0.364138312 2.048612555
C -3.552004912 -0.028556399 2.411633469
H -3.716041349 -0.204029146 3.477700877
H -3.757057412 1.020879235 2.186316336
H -4.178344912 -0.684724796 1.807928370
C 0.645402657 -1.795328257 -2.507968975
C 1.845428885 -1.402784307 -3.125564280
C -0.569079937 -1.406003885 -3.090900018
C 1.830699841 -0.655838954 -4.302924822
C -0.580850032 -0.658056407 -4.269891161
C 0.615948070 -0.281666735 -4.879474116
H 2.803081461 -1.687693410 -2.701943802
H -1.509920560 -1.685059325 -2.629612935
H 2.768280331 -0.367457647 -4.769181312
H -1.530674888 -0.369475418 -4.710646239
H 0.603365500 0.302467226 -5.794576755
C 1.526803115 -4.305897141 -1.313830935
C 1.542612668 -5.270728456 -0.295335422
C 2.087383712 -4.618737723 -2.558912870
C 2.143791088 -6.508385330 -0.503595672
C 2.686774825 -5.862600906 -2.764696777
C 2.725978877 -6.805231364 -1.737930564
H 1.074465952 -5.059920626 0.660082640
H 2.060107140 -3.903800903 -3.373177259
H 2.152282171 -7.239795660 0.299085369
H 3.120697610 -6.093279885 -3.733565436
H 3.197084575 -7.769975460 -1.901727739
C -0.997206587 -3.323225893 -0.606889663
C -1.639761662 -4.118664097 -1.571785271
C -1.623320156 -3.105442952 0.625853490
C -2.896048160 -4.658693044 -1.312723057
C -2.879816058 -3.655537108 0.886437750
C -3.518194568 -4.429181011 -0.081569531
H -1.152578338 -4.318849043 -2.521832015

H -1.148447682 -2.491841943 1.382700663
H -3.386808037 -5.266624762 -2.067089017
H -3.353968490 -3.478147430 1.847526764
H -4.495566397 -4.857837548 0.120041006
C 4.444047405 -3.320056260 0.758981484
C 5.533229009 -4.045665090 1.275293031
C 4.400013661 -3.052470475 -0.610967332
C 6.524144104 -4.526035794 0.423883531
C 5.396687043 -3.525384792 -1.464407410
C 6.456585007 -4.268934412 -0.948840967
H 5.617372429 -4.214441611 2.344730783
H 3.581991235 -2.469840710 -1.008877080
H 7.358050640 -5.089297480 0.832370107
H 5.342382263 -3.312776057 -2.528264776
H 7.235818592 -4.637641870 -1.609570382
C 2.364561433 -4.010475197 2.772374041
C 1.198448175 -3.717780401 3.503022266
C 2.825710625 -5.334818924 2.734367958
C 0.512848082 -4.727297033 4.180653732
C 2.134925797 -6.340939444 3.410559968
C 0.976820732 -6.043340308 4.133192833
H 0.826109580 -2.697903245 3.550975320
H 3.704656400 -5.592576739 2.155163835
H -0.384868592 -4.483948267 4.741797268
H 2.502664398 -7.362397060 3.368877689
H 0.440846767 -6.831088581 4.654058912
C 4.288083291 -1.874713059 3.142037102
C 4.204139091 -2.184315869 4.504611801
C 5.254361650 -0.951012791 2.705854013
C 5.056163836 -1.561606632 5.419878059
C 6.098517475 -0.329318709 3.622336102
C 5.997042851 -0.629511090 4.984157310
H 3.479615445 -2.910204327 4.858339558
H 5.360070052 -0.730647449 1.647129302
H 4.982648164 -1.809961057 6.474728097
H 6.839772280 0.384487170 3.274949013
H 6.655903719 -0.145196733 5.698760880
C 2.050820722 2.144335668 3.748054001
H 2.452659219 2.535534191 2.808424665
H 1.002964016 2.445304126 3.834643387
H 2.615219990 2.594216217 4.571313724
C 1.666499444 0.081635891 5.182567170
H 0.624487048 0.378759373 5.336324259
H 1.734642037 -1.008268809 5.239953185
H 2.275847813 0.501320738 5.989024307

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15A-TS1'

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C 0.853089406 0.548777413 -0.878371709
C 0.417681128 -0.449417720 1.768628061
C 2.511678575 0.235205491 4.532945385
C 1.222634871 0.240002598 5.067657919
H 0.418168855 0.733911030 4.535087500
C 0.957439407 -0.383585562 6.295533661
C -0.445274566 -0.411464040 6.857452065
C 2.013813875 -0.999022113 6.971866438
H 1.819409197 -1.482530087 7.927508036
C 3.321398109 -1.006519795 6.462485369
C 4.437353370 -1.675024226 7.231031748
C 3.557745858 -0.380639100 5.238826952
H 4.566032321 -0.368812686 4.832173691
C 3.831093984 2.549434084 3.702248718
C 5.201713441 2.545947634 3.973572713

H 5.820567399 1.709769475 3.666917562
C 5.795845979 3.630659035 4.627779040
C 7.285152177 3.631948799 4.878653940
C 4.979153848 4.686249900 5.057223816
H 5.432373670 5.522128698 5.584837230
C 3.594111662 4.684210507 4.844756984
C 2.706544485 5.780325738 5.384491870
C 3.034761999 3.618334791 4.133422408
H 1.967613193 3.622305371 3.920502910
C 3.918231834 -0.037111040 2.001182773
C 3.528178023 -1.411154250 2.121046347
H 2.918599444 -1.708548964 2.965612125
C 3.895494821 -2.343895146 1.191301160
H 3.578959248 -3.376793765 1.299035592
C 4.684635050 -1.976484308 0.071806671
C 5.059604935 -2.928356205 -0.910223145
H 4.709630068 -3.951512402 -0.800920005
C 5.855339342 -2.568058006 -1.973835843
H 6.143335801 -3.305705006 -2.717064036
C 6.301783421 -1.231612221 -2.097252885
H 6.929548670 -0.948672382 -2.937247826
C 5.946869025 -0.283631750 -1.163125810
H 6.284816383 0.738239383 -1.282390790
C 5.130906883 -0.622663242 -0.047923074
C 4.746731776 0.353649196 0.941911472
C 5.397350513 1.704377997 0.856932299
C 6.802031467 1.755347159 1.177692884
C 7.499066630 0.640814582 1.722667443
H 6.967187056 -0.287695208 1.896747866
C 8.836103893 0.726096556 2.042113308
H 9.344783824 -0.136179561 2.463419154
C 9.554110217 1.924777158 1.824658164
H 10.609875299 1.976080280 2.073781645
C 8.910985342 3.023185755 1.300962165
H 9.450092304 3.951579639 1.131859924
C 7.531124314 2.970450073 0.974840472
C 6.856789579 4.092892030 0.431921739
H 7.418619129 5.001022832 0.229942471
C 5.516606332 4.035481367 0.161491036
H 5.022364449 4.899854741 -0.266076983
C 4.758684800 2.854688898 0.415278613
C 2.380344058 4.579848900 0.394828300
C 1.196871712 5.013967367 -0.224079783
H 0.697770933 4.373355410 -0.947298470
C 0.654001225 6.266613807 0.079241785
C -0.603092629 6.746784156 -0.606324846
C 1.321344756 7.080245585 1.002477941
H 0.914866656 8.064082310 1.230558137
C 2.499394008 6.668552131 1.634463300
C 3.245053477 7.600731954 2.560886406
C 3.008903395 5.396455899 1.345574152
H 3.902988673 5.062466855 1.858534026
C 3.141592108 2.852107437 -1.855109157
C 3.126919100 4.006587555 -2.647939003
H 2.942140614 4.976613871 -2.198406547
C 3.331074093 3.925734453 -4.028911298
C 3.282082761 5.164237706 -4.892264825
C 3.554412457 2.667715769 -4.606836701
H 3.707367090 2.598179155 -5.682052042
C 3.588036480 1.502357222 -3.834932523
C 3.770568395 0.141049296 -4.460140109
C 3.391221208 1.611043227 -2.452048236
H 3.414696788 0.710219258 -1.846508373
P 2.907283937 1.147078992 2.996557891
P 2.964058823 2.896301831 -0.022388452
Rh 1.660762202 1.145375916 0.947803062
C -0.079554093 2.299691198 1.158152690
C -1.003554081 1.567281638 2.120058242
C -0.694008441 0.104136265 2.271149902
H 0.703589824 -1.473577215 1.982946324

C -1.873963340 -0.480466874 3.009576546
H -0.854148902 1.994181567 3.127725713
C -2.521217501 1.489249695 1.903341344
H 0.263783239 3.256054549 1.550304235
H -0.498647978 2.440425202 0.162034534
H -2.155822941 -1.466257169 2.611862409
H -1.688852779 -0.598045366 4.087275004
H -3.068876526 2.402253736 2.151649297
H -2.746687483 1.206734872 0.862007349
O -2.936872923 0.467884390 2.826677956
C 0.631066427 -0.563564904 -0.293647172
C 0.480733518 1.206137431 -2.137524001
O 0.099652373 2.358520801 -2.219716973
O 0.566283708 0.360701440 -3.180189104
C 0.186341457 0.924815131 -4.456203353
H 0.287843838 0.110606050 -5.173182135
H -0.844155461 1.285752189 -4.422154313
H 0.855266573 1.751080302 -4.708917292
H 5.400959479 -1.560026357 6.726664919
H 4.531160615 -1.250734374 8.237031090
H 4.246134287 -2.747773846 7.350415425
H -0.443300550 -0.312160439 7.947409377
H -1.059888341 0.394919600 6.445620627
H -0.943986525 -1.359845022 6.620453918
H 7.631306398 4.601205179 5.247542445
H 7.557360370 2.875435036 5.624382075
H 7.836606190 3.395426380 3.962927542
H 1.935696138 6.058499228 4.658679517
H 2.194571878 5.446024019 6.294999273
H 3.276979032 6.678107503 5.636877051
H 2.841178777 -0.436149892 -4.379783155
H 4.039491601 0.210529013 -5.517868545
H 4.547161633 -0.431112967 -3.942720921
H 4.101403394 5.176161705 -5.618680082
H 2.344885147 5.206833743 -5.460354976
H 3.346775595 6.076269903 -4.292423329
H -1.245475738 7.306373191 0.081138129
H -0.359823601 7.417176191 -1.439388682
H -1.178643794 5.911686102 -1.014236516
H 3.974228129 7.059438867 3.169290823
H 3.790018491 8.357920010 1.983873725
H 2.565212716 8.134699586 3.232154038
C 0.525249537 -1.990567704 -0.518896959
C -0.524167423 -2.773624234 -0.010728443
C 1.493606140 -2.581011151 -1.353698557
C -0.604999391 -4.124637461 -0.337149381
C 1.410142281 -3.933795557 -1.668079991
C 0.363613169 -4.707863492 -1.159149182
H -1.279769525 -2.309727636 0.611951267
H 2.301528373 -1.971581218 -1.741879780
H -1.426052343 -4.723513100 0.046121217
H 2.161217078 -4.382743531 -2.312011494
H 0.298934765 -5.763689296 -1.406494324

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15B-TS1'
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C 0.592654468 -0.350342914 -0.022956496
C 0.227933481 -0.149407375 1.928437671
C 2.186556048 0.245391072 4.487011277
C 1.017430932 0.669059194 5.136663271
H 0.486477301 1.545315211 4.778294732
C 0.528837870 -0.000587353 6.259224491
C -0.719817414 0.477154258 6.964566244
C 1.234950393 -1.117852661 6.726473408
H 0.862240417 -1.654990452 7.596403689
C 2.413087087 -1.551884103 6.111026225
C 3.149722131 -2.764623350 6.630964472
C 2.888864653 -0.854427303 4.989879563

H	3.813774238	-1.179385902	4.523576422	H	5.801674028	1.321494443	-4.636721910
C	3.363104224	2.739724942	4.038090504	C	4.553943279	0.679721221	-3.010840221
C	4.388863434	2.573415991	4.975435279	C	4.510883384	-0.768753006	-3.435154033
H	4.857675418	1.601162301	5.102228233	C	3.868214915	1.096315139	-1.859908834
C	4.819336307	3.651097030	5.751192533	H	3.310760544	0.364210943	-1.283995630
C	5.963436708	3.490151475	6.721787330	P	2.738497759	1.309566011	3.101779831
C	4.190870383	4.891339317	5.576019942	P	3.006425324	2.998617199	0.042212824
H	4.521484143	5.737321570	6.175308316	Rh	1.584143870	1.293582228	1.001835924
C	3.146767776	5.074620233	4.663639836	C	-0.084460700	2.566158763	1.177713079
C	2.516289685	6.432638333	4.469039829	C	-0.930563465	2.024783881	2.309785289
C	2.729545964	3.976704532	3.902997842	C	-0.784632352	0.539111154	2.468099689
H	1.907168221	4.082364206	3.201291316	H	0.442012889	-1.177476537	2.195213531
C	4.085869515	0.471641458	2.173177019	C	-1.966828094	0.083548793	3.292714486
C	3.886368043	-0.917550362	1.896642341	H	-0.571549069	2.468698539	3.253816156
H	3.047985213	-1.442146412	2.337818819	C	-2.463140058	2.149834420	2.325716176
C	4.718181339	-1.591801934	1.040087635	H	0.304333171	3.564238435	1.367444323
H	4.544668820	-2.645593042	0.840586130	H	-0.589277886	2.554058338	0.210940970
C	5.780268525	-0.923086063	0.383056918	H	-2.462486822	-0.779943290	2.823772508
C	6.639943873	-1.610096966	-0.515443952	H	-1.697252497	-0.191928678	4.319505856
H	6.499599346	-2.679396522	-0.652223161	H	-2.842633675	3.133018935	2.615819311
C	7.620339278	-0.937411537	-1.208475177	H	-2.883579197	1.877659477	1.342753673
H	8.269043206	-1.470729069	-1.897105851	O	-2.848300888	1.217163392	3.343339528
C	7.777134206	0.458175428	-1.026162758	C	0.652759062	0.637577440	-0.846585019
H	8.539003494	0.990387052	-1.588271514	C	0.745331512	-1.818261466	-0.134716422
C	6.974969774	1.148869575	-0.147309333	O	1.401821972	-2.520096292	0.610679695
H	7.105295162	2.217840941	-0.029059888	O	0.091072902	-2.258220903	-1.219595708
C	5.957432928	0.484212130	0.594205888	C	0.211824300	-3.674098684	-1.481438143
C	5.091219324	1.179365408	1.503314313	H	-0.389742243	-3.854551281	-2.371520010
C	5.291375142	2.656925067	1.667958929	H	1.256991180	-3.940486707	-1.658717678
C	6.420233173	3.113527234	2.425188854	H	-0.165472963	-4.250998392	-0.633265102
C	7.281321215	2.217234487	3.116360188	H	4.178183948	-2.801639680	6.260147229
H	7.087885176	1.151393981	3.064448700	H	3.182722804	-2.773105772	7.725155281
C	8.352673784	2.684028297	3.845113388	H	2.651134352	-3.688973394	6.314440611
H	8.998446218	1.980522124	4.362894028	H	-0.467938555	0.982198016	7.904928923
C	8.621248283	4.072504315	3.927738914	H	-1.288968784	1.180555920	6.349436552
H	9.472211604	4.425977401	4.502344960	H	-1.378636455	-0.360692666	7.216972744
C	7.805096633	4.967086179	3.273077380	H	5.891117065	4.199619318	7.550999637
H	8.000964877	6.034880958	3.326058955	H	5.996189016	2.478869434	7.138335603
C	6.695617740	4.516332085	2.510191658	H	6.916000838	3.667072529	6.210807327
C	5.859090410	5.417654794	1.808792104	H	1.472458291	6.349688934	4.151422623
H	6.085791637	6.480515519	1.838992424	H	2.545644196	7.029337245	5.385892549
C	4.778837282	4.965987722	1.093272703	H	3.053846888	6.996737702	3.694454621
H	4.167253462	5.681265464	0.558428344	H	3.538642669	-1.218597669	-3.206991010
C	4.460265212	3.581105575	1.037238075	H	4.693069019	-0.879129845	-4.508231345
C	2.085205045	4.507444190	-0.438847196	H	5.274539238	-1.346373411	-2.902718769
C	1.607869102	4.661776660	-1.744034837	H	7.135000952	3.623654620	-4.345805471
H	1.890196218	3.956365791	-2.516145188	H	5.650148567	4.135360971	-5.146568001
C	0.753786166	5.723374650	-2.078752653	H	6.176076544	4.948566921	-3.665949645
C	0.221989874	5.841558590	-3.487653446	H	-0.341296008	6.767857184	-3.631226120
C	0.407578230	6.642658601	-1.086568423	H	1.036354408	5.822752432	-4.221050240
H	-0.242937250	7.477413991	-1.339229627	H	-0.439116362	4.998837529	-3.721140558
C	0.879739605	6.522280151	0.227833757	H	1.249069191	7.628196939	2.053911241
C	0.478000299	7.523797302	1.285687204	H	0.294413950	8.511530277	0.852355700
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H	2.075517472	5.344985844	1.558299029	C	0.100239606	1.164533014	-2.070426540
C	3.879076597	2.436980958	-1.470155999	C	0.853344039	1.627144549	-3.163044425
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H	4.653418629	4.410335311	-1.895051625	C	0.212170838	2.109264713	-4.301034196
C	5.327461383	2.979230116	-3.348560905	C	-1.939884610	1.703218522	-3.285189320
C	6.113911626	3.977738059	-4.165444231	C	-1.182561696	2.158624455	-4.366686227
C	5.270009503	1.631967679	-3.739016595	H	1.932836700	1.585324182	-3.129198819

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H 0.808669032 2.447292979 -5.143788971
H -3.025183648 1.727970084 -3.327701388
H -1.675543600 2.540446014 -5.255936904

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15A-TS1'
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C 0.755146255 0.668091600 -0.851003932
C 0.306568932 -0.468775447 1.678987895
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C 0.907982989 -0.630677424 6.204948721
C -0.497119825 -0.623707077 6.761735916
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H 1.726747138 -1.804954213 7.806858862
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C 4.338699229 -2.062351754 7.114497955
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H 4.524486962 -0.686220482 4.757944795
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H 6.655743074 -2.908830514 -2.795762727
C 6.664787458 -0.870883774 -2.048414838
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C 5.376791776 -0.454766594 -0.021613554
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C 9.544799133 2.264806773 2.205463165
H 10.581446328 2.371759388 2.509994184
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H 9.335741569 4.311184334 1.597341912
C 7.496484757 3.216114927 1.301197705
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H 7.280906617 5.264742049 0.634886216
C 5.450671444 4.187077908 0.444509782

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C -0.492301596 6.815796708 -0.818224434
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C 2.920314615 7.516401424 2.845273571
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C 3.298759933 3.967300401 -2.520155575
H 3.162641653 4.951600242 -2.083946540
C 3.531761303 3.858644078 -3.893775535
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C 3.691089955 2.581677242 -4.451226829
H 3.867015540 2.490754732 -5.521560722
C 3.630337502 1.424230428 -3.670087611
C 3.752424775 0.047805930 -4.276927413
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H 3.359451722 0.666234824 -1.681311836
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P 2.976413943 2.907704070 0.101776956
Rh 1.643423465 1.118084559 0.973331044
C -0.016937065 2.363681926 1.292000594
C -0.985993063 1.611659705 2.186462363
C -0.770080816 0.125054302 2.213316400
H 0.519361725 -1.514814308 1.876054616
C -1.988130219 -0.443621864 2.902480661
H -0.804559439 1.933755186 3.227462433
C -2.507082588 1.654587442 1.986030203
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C 0.592605392 -1.957626263 -0.624820211
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H 0.964295794 -2.523477416 0.235697639
O 0.150238129 2.582389218 -2.121654522
O 0.344188315 0.575844850 -3.142794641
C 0.025879983 1.227421725 -4.393479047
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H -0.937453798 1.738193514 -4.325695996
H 0.806905251 1.951381235 -4.639732113
H 5.303679037 -1.984245447 6.605822185
H 4.456527151 -1.652099518 8.123894398
H 4.101124333 -3.126638267 7.225156117
H -0.495660099 -0.533464521 7.852583258
H -1.086689480 0.203972256 6.354951412
H -1.022388390 -1.555286436 6.515539132
H 7.335402504 4.569544868 5.616557227
H 7.337236896 2.827571468 5.919562641
H 7.659755819 3.433597968 4.294469808
H 1.605396894 5.775023604 4.822696581

H	1.837344857	5.123645666	6.448134944	C	6.850607444	1.160792078	-0.743115569
H	2.878445811	6.427518377	5.867561023	H	7.030135740	2.208382113	-0.534778257
H	2.776208143	-0.452821301	-4.275159256	C	5.881124288	0.454055493	0.023751208
H	4.110934405	0.088397909	-5.309392356	C	5.139669588	1.078453507	1.082324410
H	4.437765559	-0.580138847	-3.697988675	C	5.395312416	2.525276917	1.367946944
H	4.398376479	5.029531567	-5.495022525	C	6.622474467	2.897248763	2.009996061
H	2.647975909	5.191258230	-5.344772412	C	7.562924292	1.932976357	2.468845471
H	3.706648291	5.999214979	-4.182996173	H	7.351017599	0.878594829	2.328791159
H	-1.218293491	7.352904720	-0.198982093	C	8.732664185	2.320668873	3.083568972
H	-0.139486583	7.517721905	-1.584900257	H	9.436341059	1.566985355	3.424989913
H	-1.011857064	6.001824129	-1.331766866	C	9.030114525	3.692649972	3.273678090
H	3.630389866	6.965527332	3.467070655	H	9.960178420	3.983541827	3.752907163
H	3.462183203	8.344753214	2.373159093	C	8.137353667	4.650928918	2.849477661
H	2.162836541	7.959631776	3.499861317	H	8.351079925	5.707145805	2.991424697
C	1.513765656	-2.251919017	-1.823685624	C	6.920101866	4.282502057	2.216627432
H	2.550719136	-1.985892202	-1.597551283	C	5.989550958	5.250311830	1.768967521
H	1.476164619	-3.320854402	-2.060784252	H	6.219540308	6.303629343	1.903409805
H	1.193949268	-1.687013786	-2.701232042	C	4.813936685	4.878272514	1.166264996
C	-0.867785650	-2.367589668	-0.894061838	H	4.134397167	5.648147847	0.824843431
H	-1.263611836	-1.814773386	-1.751583783	C	4.489677271	3.507958001	0.970020155
H	-0.924028895	-3.437558229	-1.116938488	C	2.032408116	4.606442235	-0.206858427
H	-1.500838941	-2.158494954	-0.027595172	C	1.587143681	4.960988704	-1.484771040
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15B-TS1'							
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C	0.259467629	-0.127785250	-0.062790638	C	0.302595955	6.450236573	-3.062366729
C	0.209150838	-0.215440134	1.922117612	C	0.496582601	6.905877252	-0.576704380
C	2.642792469	-0.098415374	4.292328488	H	-0.096208616	7.806256395	-0.722645241
C	1.590484360	0.229723646	5.158784949	C	0.935807496	6.582157401	0.713388492
H	0.997401881	1.120320274	4.980830635	C	0.580486969	7.452662473	1.895708091
C	1.302189045	-0.553285166	6.277569595	C	1.695378728	5.422432142	0.886852176
C	0.181447619	-0.169065680	7.216062694	H	2.054361607	5.172606998	1.881096245
C	2.093786756	-1.683620001	6.516746057	C	3.594411379	2.505112510	-1.527636575
H	1.877829352	-2.307602687	7.381956723	C	4.380713590	3.401593408	-2.267318071
C	3.162140221	-2.025867735	5.681679662	H	4.551456664	4.408136010	-1.893925900
C	3.992785235	-3.256263421	5.963716742	C	4.949008065	3.016864857	-3.484062093
C	3.435228811	-1.218043498	4.568817611	C	5.781421474	3.980379899	-4.296896457
H	4.275479786	-1.470959653	3.929804551	C	4.726543875	1.711217498	-3.942532554
C	3.598840481	2.497257949	3.899835117	H	5.167888997	1.402206706	-4.888519208
C	4.786956988	2.422171857	4.630082114	C	3.971233041	0.789660709	-3.212943995
H	5.426485563	1.547864266	4.544233120	C	3.791352330	-0.627144575	-3.702535352
C	5.171835081	3.475618692	5.466382694	C	3.413283007	1.200561158	-1.997377479
C	6.491039042	3.425456629	6.198361336	H	2.843465288	0.484808982	-1.414884618
C	4.322771491	4.582618329	5.581017216	P	2.956120422	1.092424371	2.936360722
H	4.608770397	5.399166280	6.241317842	P	2.916430538	3.032057849	0.096818884
C	3.112132995	4.667302029	4.882283986	Rh	1.517672487	1.325679917	1.043654332
C	2.215021177	5.871735201	5.042278564	C	-0.078357792	2.572217041	1.616816369
C	2.762032562	3.611681594	4.036586370	C	-0.677979412	1.928614440	2.845333387
H	1.824637601	3.645926653	3.489697549	C	-0.617495183	0.429434207	2.755361183
C	4.175563034	0.344660624	1.777758385	H	0.387356295	-1.280531618	2.004918016
C	3.881629963	-0.998484890	1.378090412	C	-1.624984085	-0.097501066	3.752833350
H	3.069119271	-1.536723411	1.851949835	H	-0.075195977	2.213024220	3.723141761
C	4.594188282	-1.608596453	0.377987426	C	-2.148546932	2.118592656	3.256984572
H	4.353950634	-2.628328834	0.090636256	H	0.316258443	3.573577527	1.776287793
C	5.623712823	-0.916793849	-0.307295734	H	-0.776062549	2.585257580	0.781482027
C	6.376584058	-1.537253966	-1.338173564	H	-2.303617682	-0.820207821	3.273813571
H	6.184711214	-2.582977539	-1.564409268	H	-1.164554413	-0.580452378	4.622451750
C	7.323765784	-0.829755141	-2.042805079	H	-2.367160813	3.061709121	3.764332851
H	7.893396828	-1.315676196	-2.829828328	H	-2.816782328	2.011869502	2.386342024
C	7.549600935	0.537082900	-1.751096889	O	-2.344270914	1.060265836	4.205257204
H	8.281354938	1.096738391	-2.326082052	C	0.413951133	0.964343522	-0.730635364
				C	0.133217994	1.632177971	-2.035504309

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 O 1.089101964 -2.364219300 0.078216359
 O -0.689839318 -1.890392304 -1.240711955
 C -0.692664526 -3.265512806 -1.688516134
 H -1.545745960 -3.348137380 -2.360751400
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 H 4.188584687 -3.368683321 7.034927258
 H 3.471779490 -4.163114628 5.632694911
 H 0.568468265 0.396823668 8.072239524
 H -0.566130283 0.455514221 6.717049540
 H -0.325116887 -1.052809392 7.616137899
 H 6.478899473 4.052751316 7.094297683
 H 6.742411677 2.403699594 6.499470123
 H 7.298175539 3.782211344 5.548103442
 H 1.271132545 5.746379522 4.503660941
 H 1.978270714 6.054199252 6.096251529
 H 2.700983056 6.778473622 4.661829543
 H 2.999189302 -1.145264208 -3.153332373
 H 3.543111840 -0.654552389 -4.768469262
 H 4.715652269 -1.197169717 -3.561030858
 H 6.719368991 3.515667363 -4.619483233
 H 5.248986256 4.293406173 -5.202893399
 H 6.028202684 4.880772684 -3.727436132
 H 0.004878687 7.499597194 -3.136778556
 H 1.063230883 6.256283131 -3.825277238
 H -0.572648322 5.838892237 -3.313301304
 H 1.392552679 7.484319807 2.627816824
 H 0.359452041 8.478145904 1.586885277
 H -0.307965054 7.067890202 2.411370310
 C -1.069452485 2.591159384 -1.905863900
 H -1.285450299 3.037018000 -2.882908520
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 H -0.858574117 3.404744366 -1.206908994
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 H 0.786652455 -0.052389154 -3.263656556
 H -0.955336736 -0.025499110 -2.949033390

Table S5. Vibrational Frequencies of Optimized Structures

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333.21 379.96 469.81 573.78 756.63 823.64
976.59 1048.83 1055.91 1105.29 1177.40 1215.15
1301.13 1421.87 1479.89 1481.68 1484.39 1494.21
1507.13 1796.81 2363.79 3036.81 3058.37 3103.98
3107.82 3134.87 3171.55
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2
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393.76 436.89 529.38 604.89 665.50 680.57
925.84 942.14 959.64 992.85 1015.44 1033.77
1039.41 1118.74 1180.36 1258.23 1295.82 1317.89
1386.29 1423.66 1467.00 1498.47 1515.07 1724.62
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3162.20 3238.14 3495.98
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PPh3
  
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26.40 27.07 42.52 53.78 54.10 67.42
188.35 205.94 207.27 249.40 261.49 262.67
407.59 407.80 412.25 417.00 431.20 432.11
507.83 508.77 520.63 631.35 631.44 631.71
693.54 706.04 706.28 712.26 712.34 713.61
762.85 763.13 763.34 865.85 866.18 868.54
934.08 934.75 935.86 982.32 982.55 983.60
1004.42 1004.63 1005.07 1013.36 1013.41 1013.65
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1645.05 1645.09 1646.89 3168.48 3168.54 3168.89
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3

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1219.87 1245.59 1247.78 1275.87 1296.85 1332.89
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1478.87 1479.76 1493.91 1508.13 1509.06 1511.99
1530.06 1644.08 1743.33 1788.45 2966.69 2977.34
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4

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Rh(PPh₃)₂

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5

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5-TS

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6

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7

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7-TS

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629.24 630.49 645.04 662.00 697.06 710.87
711.96 713.59 721.08 724.05 747.96 756.36
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8A

12.93 23.77 28.58 35.70 39.97 44.08
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8B

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1122.65 1144.60 1177.26 1178.84 1201.44 1201.66
1201.92 1202.13 1203.23 1203.24 1209.90 1217.70
1224.33 1226.88 1228.23 1229.62 1230.50 1232.95
1233.89 1253.80 1259.32 1300.96 1322.41 1324.70
1329.62 1329.85 1333.65 1334.18 1335.95 1353.26
1364.30 1366.35 1368.08 1369.77 1369.87 1372.93
1399.30 1415.32 1470.14 1472.78 1473.63 1476.03
1476.13 1477.66 1478.45 1480.26 1480.63 1490.26
1496.60 1503.93 1508.45 1526.48 1526.85 1527.69
1528.45 1528.87 1529.33 1530.11 1624.14 1625.64
1625.96 1627.12 1627.91 1629.00 1641.96 1642.83
1643.67 1644.84 1645.38 1646.91 1706.36 1832.94
2263.13 2975.32 2997.02 3015.87 3042.64 3068.95
3070.88 3095.22 3107.98 3114.91 3125.09 3137.06
3152.35 3163.00 3183.01 3184.11 3185.64 3186.74
3186.98 3187.64 3191.16 3191.71 3192.56 3192.80
3193.65 3194.19 3197.17 3202.35 3203.36 3203.80
3206.54 3206.73 3208.68 3208.75 3208.97 3212.43
3214.27 3214.82 3215.57 3216.21 3219.90 3222.86
3225.94 3255.03 3256.93

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7.29 11.07 22.01 28.30 42.26 42.79
46.08 47.85 50.64 53.42 59.38 61.33
63.05 68.10 68.83 75.90 80.12 88.18
91.92 93.61 99.96 108.53 114.43 120.82
124.96 135.61 136.96 143.87 145.36 157.48
164.20 165.98 178.81 189.74 199.97 206.29
210.09 219.07 225.83 230.77 238.12 247.99
256.12 259.31 260.04 262.32 264.33 275.91
279.58 281.91 285.07 301.59 326.65 335.68
349.14 380.22 409.63 411.97 416.94 417.33
421.06 425.31 428.39 433.33 442.20 448.56
463.21 468.36 476.30 498.61 505.57 517.72
521.62 531.12 537.57 544.80 566.50 574.22
627.65 629.40 630.23 631.74 632.57 633.03
633.31 651.14 681.15 695.46 696.38 706.68
710.70 712.03 714.28 714.77 715.25 715.96
720.97 723.39 727.33 740.04 759.95 763.13
767.65 768.70 770.22 771.41 784.10 798.71
818.03 834.78 858.67 868.36 872.10 875.51
877.46 884.98 929.05 939.77 941.17 945.78
951.56 953.43 955.17 964.90 983.65 989.05
993.35 997.47 997.85 998.16 1003.86 1007.81
1012.84 1013.58 1014.24 1015.01 1015.09 1015.72
1015.87 1016.62 1018.03 1019.50 1019.58 1020.23
1022.25 1046.88 1052.92 1053.32 1053.32 1053.92
1054.25 1054.34 1054.85 1069.15 1072.08 1085.35
1108.40 1112.31 1112.96 1114.22 1115.36 1117.31
1119.05 1119.64 1120.83 1121.04 1121.64 1123.44
1123.92 1157.54 1180.35 1188.41 1202.77 1202.81
1202.98 1203.47 1204.10 1204.15 1211.42 1217.56
1226.00 1227.70 1228.27 1230.13 1231.30 1233.14
1235.00 1253.85 1258.74 1311.09 1319.12 1324.13
1328.43 1330.31 1333.85 1335.49 1338.04 1356.44
1366.73 1366.92 1367.63 1370.24 1371.20 1372.67
1401.62 1417.26 1464.18 1471.55 1473.36 1473.86
1476.35 1477.75 1477.88 1480.80 1481.61 1491.34

1492.00 1505.55 1506.58 1527.45 1527.51 1527.89
1528.76 1529.29 1529.72 1532.79 1623.98 1625.44
1627.75 1628.86 1630.22 1630.39 1644.16 1644.35
1645.36 1645.84 1646.28 1646.76 1702.27 1830.98
2315.51 2986.39 3004.64 3046.50 3048.28 3051.73
3066.62 3085.34 3106.31 3110.23 3127.24 3129.29
3130.22 3183.25 3185.49 3185.78 3186.39 3186.99
3187.61 3188.73 3192.29 3193.04 3193.53 3193.85
3194.71 3195.63 3196.31 3202.43 3203.99 3204.11
3205.73 3209.81 3210.36 3211.72 3213.14 3213.44
3213.93 3217.56 3218.41 3223.29 3227.40 3229.42
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8C-BPR

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-47.44 17.50 24.24 29.37 33.93 36.74
41.78 46.33 50.58 51.89 56.85 58.92
61.20 65.95 67.80 71.42 74.47 79.05
83.11 87.02 89.70 95.67 98.88 104.07
113.08 114.10 119.02 122.52 131.77 145.35
150.41 159.48 177.40 195.30 200.97 202.54
207.70 211.02 217.96 221.30 226.21 232.51
245.23 253.74 255.12 257.69 258.20 260.89
264.05 277.59 278.37 298.39 307.01 331.87
335.75 360.51 411.83 413.74 415.38 415.75
418.33 423.70 429.67 436.80 438.29 453.64
460.52 469.20 484.51 494.79 504.74 516.38
524.06 526.28 534.37 539.62 562.21 575.41
618.39 627.53 628.03 628.80 630.39 630.84
632.00 642.15 677.01 694.39 695.50 709.50
710.11 711.77 712.71 715.06 715.84 718.12
718.38 719.16 725.97 740.80 764.19 764.96
767.25 767.40 771.71 772.86 778.86 797.04
826.91 835.09 870.05 872.11 873.25 874.59
878.10 886.12 930.97 948.07 951.75 952.40
954.36 957.19 962.67 966.33 991.00 991.73
993.55 995.04 995.91 996.30 1003.28 1005.40
1008.45 1013.30 1013.41 1014.16 1014.68 1014.97
1016.18 1016.54 1017.34 1017.66 1019.23 1021.45
1023.55 1038.90 1048.13 1049.59 1050.40 1051.86
1052.28 1053.26 1063.57 1073.63 1076.15 1101.33
1110.05 1111.67 1113.27 1114.54 1115.13 1116.40
1117.43 1118.07 1118.85 1119.83 1120.43 1122.71
1127.41 1157.41 1176.09 1176.15 1199.80 1201.63
1201.96 1202.52 1203.12 1203.58 1206.24 1218.04
1222.68 1224.54 1229.04 1229.19 1231.64 1232.41
1234.75 1254.40 1297.66 1311.83 1321.28 1322.87
1327.40 1329.50 1330.55 1333.75 1334.51 1350.26
1361.59 1366.99 1368.29 1369.08 1371.62 1372.50
1396.56 1418.29 1470.81 1472.40 1474.25 1475.09
1475.99 1476.83 1478.13 1479.78 1481.43 1489.89
1491.31 1500.44 1506.54 1523.88 1526.52 1526.99
1527.58 1528.30 1528.36 1532.67 1622.72 1622.79
1625.89 1627.68 1628.42 1628.91 1641.67 1641.98
1642.41 1643.37 1643.99 1645.19 1692.76 1790.64
2302.27 2993.76 3004.97 3018.02 3041.30 3068.54
3069.86 3111.16 3115.64 3122.84 3127.95 3151.95
3179.82 3183.79 3184.57 3185.09 3185.21 3188.71
3190.10 3190.45 3191.02 3192.33 3193.57 3193.90
3195.25 3196.24 3196.73 3200.53 3200.65 3201.15
3203.70 3204.27 3206.81 3207.61 3208.98 3209.24

3210.05 3211.25 3213.20 3214.84 3215.02 3215.56
3216.88 3218.39 3264.31

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8A-TS1

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-193.65 10.30 25.26 29.00 33.57 39.81
44.75 47.53 52.91 53.89 57.36 60.77
63.75 67.12 69.76 75.01 75.29 78.87
79.86 88.83 90.25 96.84 98.77 102.30
113.32 114.50 129.37 138.96 148.20 155.16
168.05 174.33 180.33 185.62 206.12 209.65
215.42 218.26 221.84 226.53 233.31 241.82
255.38 256.14 259.39 260.66 267.92 273.06
274.35 282.14 286.40 288.94 306.28 336.86
374.65 406.83 408.52 410.63 414.46 418.55
420.68 423.79 426.44 433.71 435.39 439.68
467.56 470.47 481.95 499.24 503.59 517.84
520.26 530.57 533.70 534.92 557.40 612.63
627.51 628.01 630.01 630.75 631.52 632.01
632.79 674.05 683.42 692.22 693.97 704.84
706.68 709.31 710.64 711.50 713.63 714.27
716.25 720.39 721.70 752.25 757.98 761.11
764.95 765.49 767.23 769.58 771.95 817.19
848.10 860.01 864.00 865.75 870.06 870.54
881.45 883.64 935.27 942.18 942.32 943.99
945.23 947.81 953.52 961.53 981.01 981.92
985.05 987.98 989.42 990.71 1002.34 1008.32
1011.71 1011.94 1012.39 1013.48 1013.99 1014.71
1015.37 1015.66 1016.83 1018.22 1020.66 1021.86
1023.22 1024.15 1048.36 1051.76 1052.52 1053.63
1054.19 1054.77 1055.17 1062.69 1082.21 1083.94
1107.05 1108.74 1111.41 1114.50 1115.67 1115.88
1117.40 1118.90 1119.31 1119.82 1121.18 1121.86
1124.74 1139.84 1166.51 1181.23 1200.89 1202.03
1202.25 1202.33 1203.42 1203.71 1207.85 1219.75
1221.82 1226.66 1226.76 1229.39 1230.10 1236.55
1237.16 1258.62 1263.78 1290.71 1322.58 1324.08
1327.67 1328.87 1331.57 1335.28 1336.56 1349.54
1363.84 1365.61 1366.56 1368.20 1368.61 1374.64
1396.24 1405.92 1468.11 1473.77 1474.29 1475.75
1476.02 1479.34 1479.85 1480.09 1480.63 1486.55
1497.06 1504.10 1505.87 1524.69 1526.18 1526.52
1527.60 1527.92 1528.27 1531.49 1625.30 1626.84
1627.08 1628.86 1629.47 1630.54 1642.90 1644.47
1644.96 1645.17 1646.10 1646.85 1662.32 1803.53
1994.66 2979.15 3025.18 3029.95 3040.19 3068.15
3068.74 3108.77 3114.87 3119.57 3132.64 3152.79
3154.80 3156.45 3172.50 3181.32 3183.53 3184.19
3186.60 3186.78 3187.79 3188.66 3188.87 3193.19
3194.13 3194.83 3196.56 3198.12 3198.84 3202.27
3202.69 3204.50 3205.87 3206.35 3209.62 3211.68
3212.12 3213.58 3213.96 3218.54 3223.98 3229.02
3237.26 3256.81 3273.75

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8A-TS2

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-228.41 15.47 18.01 31.24 36.05 38.38
43.21 44.78 46.74 52.02 54.64 56.77
59.98 62.50 65.77 71.66 73.41 76.45
80.57 83.48 91.93 95.90 99.00 103.23
106.14 115.19 128.53 130.16 135.58 152.31

161.37 164.36 170.65 194.79 201.94 206.93
210.47 216.33 219.71 222.69 229.92 232.43
241.81 254.40 256.17 259.12 261.76 262.32
278.10 280.88 283.48 296.92 337.61 348.19
396.93 404.93 406.65 410.81 415.72 418.59
421.61 425.51 434.96 438.41 440.06 454.97
461.33 467.32 479.28 498.45 505.11 516.09
519.78 532.32 539.52 561.22 570.95 628.47
629.80 630.34 631.07 631.62 633.16 633.82
650.24 663.60 679.39 694.40 698.09 705.50
707.79 709.12 710.44 712.86 714.23 717.92
719.94 722.54 725.15 747.64 760.32 762.82
765.55 767.81 768.98 770.37 775.32 821.12
831.06 849.18 863.58 864.94 868.13 873.73
877.51 878.46 936.13 940.35 941.40 944.42
950.29 956.59 958.43 980.30 982.89 984.36
987.02 989.84 994.55 995.82 997.30 1004.46
1008.35 1011.93 1013.60 1013.70 1013.95 1014.21
1015.29 1015.70 1016.40 1016.88 1017.81 1018.97
1020.90 1042.86 1051.07 1051.43 1051.84 1053.58
1053.97 1054.04 1054.49 1059.03 1077.53 1082.17
1107.94 1109.35 1111.85 1113.38 1115.04 1117.21
1117.77 1118.18 1119.54 1119.88 1122.10 1123.36
1123.73 1138.64 1177.03 1177.97 1199.43 1200.09
1201.88 1202.59 1202.88 1203.34 1206.28 1213.24
1219.97 1223.07 1225.16 1227.58 1229.24 1230.26
1234.87 1249.11 1261.82 1290.40 1325.32 1326.17
1327.24 1329.75 1335.96 1337.12 1337.61 1353.76
1362.01 1363.57 1368.61 1369.77 1370.80 1374.45
1395.90 1402.39 1470.41 1473.77 1474.61 1475.50
1476.48 1476.97 1478.87 1480.52 1480.83 1481.74
1495.52 1504.29 1511.98 1524.66 1526.62 1527.60
1528.09 1528.37 1529.76 1530.74 1625.79 1626.41
1627.58 1627.84 1629.83 1630.60 1643.38 1644.30
1644.79 1645.29 1645.65 1647.39 1665.16 1779.99
1882.69 2972.83 3010.63 3039.82 3041.36 3052.36
3061.45 3065.91 3113.67 3121.83 3127.20 3150.79
3154.98 3169.18 3178.71 3182.36 3182.92 3183.37
3185.23 3186.95 3187.65 3188.46 3191.07 3191.84
3192.20 3192.76 3196.63 3198.97 3199.73 3202.33
3202.79 3205.08 3209.32 3209.61 3210.62 3212.20
3213.74 3215.81 3225.14 3225.90 3227.59 3230.73
3230.74 3234.28 3245.15

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8B-TS1

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-128.87 2.31 8.95 29.29 35.74 35.86
40.24 46.63 48.29 50.60 52.50 54.94
55.58 59.43 61.39 68.36 70.96 73.99
79.40 81.28 91.41 96.22 100.84 110.46
116.68 119.72 132.48 136.17 143.14 146.28
155.86 167.14 177.61 192.34 196.77 202.32
210.17 224.63 228.39 233.58 236.69 239.78
250.30 252.45 254.69 258.86 261.98 272.31
277.27 281.37 282.65 296.98 307.80 353.43
380.91 407.35 409.63 410.48 412.26 420.69
422.18 426.37 427.75 434.60 438.98 441.74
463.58 466.74 502.21 508.72 513.84 516.47
518.99 529.94 535.56 537.57 566.93 609.48
626.54 627.26 628.77 630.28 630.94 631.46
632.60 661.58 677.14 695.31 697.44 706.90

708.22	711.60	712.30	712.58	714.02	715.63
717.08	721.45	721.82	744.17	761.59	763.42
764.84	765.68	767.69	767.85	770.43	816.07
848.58	863.80	865.81	867.44	870.07	873.98
875.20	876.80	940.62	943.52	943.99	945.84
946.09	949.90	953.01	956.52	982.08	985.15
986.60	988.04	988.87	991.90	994.42	1008.38
1009.61	1012.45	1012.54	1013.54	1014.50	1014.94
1016.18	1016.66	1017.18	1017.52	1017.97	1019.70
1021.74	1033.38	1048.01	1050.99	1051.35	1051.82
1052.48	1053.02	1053.36	1058.12	1080.58	1083.47
1111.27	1112.77	1114.10	1114.33	1114.95	1116.60
1117.34	1118.49	1118.67	1119.52	1120.15	1121.54
1122.68	1141.35	1159.53	1177.72	1200.44	1200.84
1201.82	1203.05	1203.18	1203.25	1208.47	1215.16
1221.70	1223.12	1225.94	1226.60	1228.92	1230.12
1231.48	1255.11	1286.42	1293.96	1324.81	1325.75
1327.18	1329.19	1331.71	1336.89	1338.71	1349.11
1364.39	1365.07	1366.61	1367.63	1368.69	1371.11
1396.41	1409.01	1471.92	1473.48	1475.08	1475.35
1476.97	1477.82	1479.99	1480.92	1481.11	1485.20
1495.05	1505.97	1506.85	1525.40	1525.68	1526.61
1526.78	1527.12	1527.61	1528.61	1625.22	1626.23
1627.22	1628.70	1630.97	1631.13	1642.91	1643.71
1644.54	1645.70	1647.14	1647.60	1668.77	1799.64
1954.68	2989.26	3011.51	3032.20	3053.26	3067.08
3079.46	3105.16	3121.20	3131.94	3136.12	3149.97
3170.56	3176.47	3180.72	3181.58	3183.50	3184.25
3185.55	3186.22	3187.40	3189.23	3189.85	3190.89
3192.64	3192.96	3196.09	3198.29	3199.18	3199.56
3201.77	3206.58	3208.34	3209.56	3209.69	3210.21
3212.16	3214.54	3215.52	3217.39	3219.51	3220.78
3221.53	3224.77	3248.66			

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8B-TS2

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-212.69	7.23	12.85	16.95	24.85	34.83
38.33	43.35	47.94	50.42	51.95	55.19
60.37	64.06	66.58	67.82	70.15	78.58
79.72	81.63	86.21	93.37	97.46	103.06
104.93	115.40	121.91	125.35	130.24	139.29
148.08	169.10	189.60	196.96	202.42	205.47
214.70	217.32	223.35	229.01	230.61	243.52
253.48	254.39	256.60	259.09	260.66	262.20
277.10	280.23	285.99	297.85	330.86	346.03
364.47	404.97	406.68	410.13	412.80	415.22
419.77	421.53	422.41	434.38	436.85	443.85
458.07	466.80	488.56	499.19	510.73	514.40
518.05	525.78	532.33	539.72	568.87	626.17
628.60	629.01	630.00	631.20	632.46	633.15
658.33	678.85	693.94	697.25	705.38	707.93
708.53	709.65	712.13	713.10	715.26	717.10
724.88	726.46	736.39	757.65	761.48	763.98
765.96	768.71	769.35	769.59	772.83	820.31
837.01	849.24	865.42	866.53	870.41	872.59
874.84	883.53	933.19	942.34	942.66	950.68
951.86	955.03	956.84	978.23	983.91	985.29
985.85	990.66	991.59	994.77	996.13	1001.32
1009.49	1011.04	1011.66	1012.91	1013.50	1014.08
1015.51	1016.23	1016.47	1016.83	1016.98	1019.92
1020.21	1038.92	1049.88	1051.17	1052.03	1052.45

1052.71	1052.91	1053.95	1058.96	1076.61	1081.56
1107.26	1110.19	1111.36	1113.88	1114.76	1115.31
1115.71	1116.44	1119.00	1119.96	1120.83	1122.44
1126.62	1132.26	1169.27	1174.99	1200.20	1200.56
1201.30	1202.05	1202.36	1202.69	1205.43	1210.82
1220.41	1223.11	1224.76	1227.51	1228.41	1232.54
1233.80	1252.69	1272.49	1291.93	1323.41	1325.72
1326.67	1328.62	1334.81	1336.22	1336.58	1355.50
1362.77	1363.63	1368.38	1369.35	1373.12	1374.18
1396.21	1410.06	1468.05	1471.80	1473.26	1474.03
1475.11	1476.18	1479.16	1480.05	1480.44	1491.00
1494.05	1504.31	1512.60	1525.53	1525.94	1526.20
1528.09	1528.50	1529.78	1530.26	1623.89	1625.42
1626.32	1626.81	1629.46	1630.06	1641.78	1643.93
1644.04	1644.67	1646.14	1646.86	1665.08	1789.80
1917.87	2969.33	3013.98	3033.43	3042.20	3054.57
3065.24	3068.86	3115.98	3116.96	3126.40	3151.37
3151.84	3169.55	3182.82	3183.19	3184.82	3185.37
3186.58	3187.08	3188.18	3188.43	3190.62	3190.85
3192.83	3194.44	3194.89	3199.09	3200.38	3201.12
3203.09	3204.51	3205.77	3208.35	3210.93	3211.62
3212.28	3212.66	3216.07	3226.54	3227.78	3228.07
3235.01	3244.96	3254.20			

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21.87	27.80	30.11	38.04	41.89	48.31
49.11	51.95	58.12	60.42	64.43	67.49
70.27	73.34	73.60	79.09	82.75	86.24
91.01	93.39	94.62	98.83	103.83	106.13
118.08	123.50	130.64	150.04	154.47	172.35
179.11	191.61	196.25	197.85	202.23	204.76
209.26	219.27	227.16	230.02	238.96	250.58
253.86	257.71	261.31	263.56	278.18	278.68
282.95	312.23	317.65	343.16	368.52	404.32
408.93	411.12	412.08	415.65	416.65	423.61
428.08	432.72	437.18	443.02	451.57	459.61
472.56	493.28	500.08	506.72	514.74	522.28
528.88	537.73	541.71	576.76	616.04	630.03
630.70	630.98	631.93	632.50	633.36	647.98
695.73	698.84	705.80	707.96	708.49	709.34
710.01	711.27	712.32	714.96	717.16	719.47
722.95	744.56	756.33	759.64	762.07	763.83
765.82	767.23	768.47	792.25	798.33	858.19
862.88	865.01	868.42	868.93	871.62	901.46
915.13	934.51	938.99	942.16	946.19	948.10
948.38	952.80	957.09	962.63	982.51	983.89
987.31	988.70	989.37	990.34	1007.27	1007.72
1011.49	1012.20	1013.58	1014.23	1014.73	1015.34
1016.30	1016.70	1017.59	1017.90	1018.20	1018.77
1027.31	1049.87	1051.66	1052.42	1052.50	1053.02
1053.37	1053.51	1068.84	1080.07	1104.89	1110.93
1111.82	1113.29	1114.26	1115.35	1116.34	1117.48
1117.70	1118.57	1120.05	1121.04	1122.24	1123.13
1155.10	1179.80	1181.01	1199.79	1200.71	1201.06
1201.35	1201.78	1202.79	1216.82	1219.81	1222.89
1224.44	1225.31	1227.63	1230.20	1231.32	1236.81
1270.86	1283.13	1289.14	1315.76	1324.35	1324.80
1327.69	1328.50	1334.85	1335.12	1338.83	1355.28
1361.26	1363.45	1363.91	1365.99	1368.46	1370.37
1400.37	1417.53	1473.11	1474.69	1474.90	1475.22

1478.21 1479.86 1480.72 1483.22 1487.76 1491.87
1498.66 1501.48 1502.97 1524.67 1525.16 1525.52
1525.94 1526.95 1527.79 1529.46 1620.48 1624.66
1625.74 1626.09 1626.57 1627.98 1628.83 1642.06
1643.01 1643.82 1644.15 1644.51 1645.95 1680.52
1763.17 2944.02 2982.89 3039.70 3046.50 3065.00
3078.53 3098.02 3118.88 3129.16 3131.35 3144.32
3144.50 3172.08 3172.60 3182.31 3185.69 3186.66
3187.73 3189.17 3189.63 3190.63 3191.20 3195.62
3196.15 3197.09 3198.19 3199.19 3202.08 3203.02
3204.66 3208.30 3209.49 3209.78 3211.20 3212.93
3213.79 3215.41 3216.95 3217.76 3219.81 3224.85
3232.42 3233.01 3262.07

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9B

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11.87 17.85 21.17 28.65 34.55 35.78
41.36 43.98 48.68 49.89 53.29 55.47
58.09 66.98 68.26 73.98 83.85 84.02
87.22 91.57 97.89 105.47 114.12 115.02
122.76 129.30 132.21 137.32 153.50 154.82
161.07 180.64 184.45 198.66 203.03 214.19
215.29 218.29 232.88 239.82 242.18 257.02
259.22 260.81 263.91 264.95 274.43 286.11
298.51 314.11 323.16 350.20 371.77 399.85
405.25 408.88 416.38 417.35 418.56 423.29
424.74 431.70 435.97 447.57 458.10 471.53
475.75 482.76 502.22 509.47 515.09 522.12
530.03 535.12 547.72 607.80 615.99 626.70
628.58 630.34 630.73 631.29 632.66 634.68
681.29 692.01 695.11 702.32 705.16 709.87
712.33 715.42 715.86 719.14 721.07 723.09
723.88 726.76 755.60 761.10 765.73 768.26
769.84 770.30 771.46 783.26 795.59 849.66
856.98 867.72 870.18 871.05 878.07 878.87
932.91 946.27 947.24 948.06 950.83 957.35
958.82 962.31 971.62 978.95 982.29 990.66
992.27 994.65 998.93 1000.03 1008.69 1011.80
1012.93 1013.18 1013.34 1014.30 1015.03 1016.59
1017.01 1019.70 1020.76 1022.22 1023.10 1037.84
1042.01 1051.31 1051.89 1051.99 1053.02 1053.76
1054.06 1067.43 1081.62 1102.81 1106.06 1109.79
1110.14 1114.67 1114.97 1116.10 1117.18 1118.60
1120.58 1121.46 1125.16 1126.17 1128.69 1133.19
1163.97 1174.26 1178.05 1185.73 1201.04 1201.13
1202.19 1203.23 1203.64 1204.46 1219.00 1222.27
1226.08 1226.87 1228.71 1229.73 1235.47 1236.41
1262.58 1276.02 1292.79 1318.25 1319.78 1322.18
1322.98 1326.19 1332.71 1335.68 1348.98 1362.63
1365.82 1366.45 1367.33 1370.33 1370.74 1373.57
1410.66 1415.74 1467.33 1472.03 1472.50 1474.62
1475.55 1479.40 1479.94 1480.00 1490.58 1494.16
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1526.37 1527.04 1529.97 1530.54 1591.40 1623.20
1623.71 1624.66 1625.96 1627.95 1628.30 1641.92
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1790.29 2986.14 3024.62 3048.63 3050.97 3057.01
3063.95 3108.71 3109.69 3126.15 3143.76 3151.14
3168.23 3178.44 3181.47 3182.87 3186.69 3187.82
3189.69 3190.34 3191.17 3191.37 3192.74 3193.63
3196.24 3198.38 3198.60 3199.43 3200.00 3203.33

3206.22 3207.93 3211.02 3212.02 3212.75 3213.51
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3238.60 3241.28 3242.69

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11A

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54.32 60.12 61.31 66.13 69.06 70.38
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106.50 125.11 142.49 152.42 155.72 172.75
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254.46 257.50 261.66 268.35 270.17 272.83
276.48 289.12 315.14 325.53 353.60 376.41
406.68 407.43 408.72 410.38 415.13 416.06
418.27 422.55 431.13 444.57 457.87 464.30
467.76 501.28 508.61 511.67 512.99 517.81
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629.77 630.12 630.52 631.71 632.55 653.00
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724.35 726.70 762.40 763.16 764.98 766.37
768.09 770.37 774.40 792.50 813.29 836.95
864.63 867.01 868.76 871.80 874.03 875.21
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989.46 991.74 993.92 994.46 997.05 1012.20
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1017.97 1018.30 1018.77 1019.45 1020.91 1026.46
1042.19 1050.65 1051.00 1051.81 1052.39 1052.92
1053.58 1060.82 1087.65 1094.17 1111.86 1113.21
1113.30 1114.59 1114.97 1115.74 1116.97 1118.56
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1164.21 1178.83 1201.09 1202.04 1202.26 1202.36
1203.34 1203.42 1208.08 1214.84 1223.51 1223.82
1224.45 1226.99 1228.61 1228.86 1232.00 1242.76
1261.74 1283.93 1291.05 1322.98 1325.10 1328.89
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1497.05 1507.76 1511.94 1523.58 1524.62 1525.71
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1771.07 2962.01 2968.01 3020.22 3021.82 3062.44
3079.27 3080.14 3095.81 3102.05 3119.32 3129.16
3134.71 3138.11 3141.36 3156.91 3174.88 3184.11
3186.80 3188.50 3189.09 3189.69 3189.88 3191.63
3192.62 3196.23 3196.58 3198.61 3198.98 3199.21
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3210.14 3212.56 3213.51 3214.09 3214.36 3215.03
3216.81 3217.66 3247.07

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11B

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4.67 13.17 20.32 24.87 26.22 34.73
38.23 44.35 47.67 50.01 53.96 57.31
61.10 63.23 67.78 72.53 75.74 80.17
83.44 88.01 91.36 96.82 99.47 106.18

122.71 135.54 142.03 151.45 159.07 171.58
175.24 191.25 198.57 201.10 204.17 213.95
220.98 224.80 227.98 236.46 242.90 246.17
247.60 261.20 266.03 272.15 274.18 282.81
290.99 304.06 327.58 338.94 348.95 394.95
400.66 407.76 410.83 412.59 414.15 417.65
419.98 420.79 428.27 451.37 458.26 463.10
467.86 501.45 508.78 510.04 512.92 520.74
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711.69 713.56 714.64 717.44 720.52 721.48
722.19 762.40 763.33 765.06 765.75 766.34
769.85 770.98 781.01 784.82 813.53 863.48
864.74 866.48 868.47 869.39 876.54 879.50
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954.98 960.10 967.70 976.60 984.79 987.28
988.06 988.78 995.12 1002.06 1009.68 1012.47
1012.70 1013.18 1013.61 1013.97 1015.05 1015.88
1016.14 1016.79 1018.13 1019.31 1022.07 1028.65
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1113.95 1114.71 1115.15 1115.46 1117.24 1118.06
1118.28 1118.93 1119.87 1120.35 1121.45 1132.75
1176.69 1200.94 1201.40 1201.80 1202.11 1202.27
1202.36 1204.80 1207.32 1213.54 1222.47 1223.05
1225.78 1226.75 1227.85 1229.24 1231.74 1255.17
1266.40 1289.31 1324.35 1324.69 1329.18 1331.66
1333.60 1334.19 1334.95 1349.18 1357.28 1364.28
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1409.87 1412.64 1472.54 1472.94 1475.71 1477.07
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1501.28 1505.39 1509.20 1524.28 1526.32 1526.63
1527.35 1527.47 1528.23 1528.46 1622.69 1624.15
1625.37 1626.52 1627.88 1628.41 1630.67 1641.77
1642.61 1644.35 1644.55 1644.69 1645.39 1680.19
1715.72 2946.50 2953.68 3013.07 3027.94 3034.53
3040.54 3071.86 3075.86 3079.15 3088.27 3110.06
3160.29 3168.50 3184.03 3185.24 3185.57 3186.29
3187.26 3188.09 3190.10 3192.45 3192.55 3194.47
3194.57 3194.93 3196.42 3200.44 3201.19 3205.32
3206.06 3207.61 3208.08 3208.33 3209.95 3211.02
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3217.53 3218.43 3227.38

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9A-TS

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-307.08 11.88 17.97 28.69 36.22 39.63
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63.47 70.84 74.12 77.75 81.92 83.69
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121.22 126.99 131.41 139.67 146.66 159.64
164.39 169.27 193.00 201.02 209.80 216.88
217.69 222.93 227.13 234.76 237.03 240.23
257.63 259.12 260.99 262.94 270.87 276.48
280.66 293.76 303.42 337.18 358.92 401.31
408.13 409.89 412.71 419.88 423.17 427.04
430.30 432.92 440.31 444.89 456.78 467.08
469.90 475.98 490.22 503.64 508.52 518.02
527.35 532.71 538.67 547.08 560.63 627.59
627.82 629.15 629.84 630.85 632.28 633.20

693.60 698.02 701.59 705.31 707.24 707.82
709.60 712.44 714.15 716.50 718.12 720.92
723.72 725.15 748.50 761.33 763.67 766.79
769.03 770.40 772.96 803.17 813.82 864.80
867.92 871.43 873.96 880.67 886.92 890.08
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956.24 962.40 970.20 985.44 985.85 991.23
994.00 996.05 1001.42 1005.66 1007.23 1010.17
1012.26 1012.78 1013.56 1014.05 1014.66 1015.47
1016.41 1016.78 1018.81 1019.18 1020.80 1026.03
1037.28 1050.29 1050.85 1053.11 1053.25 1053.71
1054.63 1055.02 1075.96 1084.60 1107.62 1108.99
1109.78 1110.94 1111.55 1116.54 1117.21 1117.64
1119.00 1119.34 1122.07 1123.09 1124.95 1133.94
1155.25 1176.58 1179.98 1199.84 1200.65 1201.18
1202.95 1203.35 1203.79 1217.30 1219.42 1220.95
1222.33 1228.17 1231.42 1233.11 1233.91 1246.52
1259.09 1293.16 1300.44 1320.58 1321.58 1323.78
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1495.27 1501.30 1502.98 1522.72 1523.84 1524.81
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1625.84 1626.94 1627.09 1629.61 1630.29 1639.35
1642.88 1643.62 1644.26 1644.87 1646.87 1647.30
1769.83 2969.72 3032.36 3035.16 3045.70 3076.49
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3187.63 3188.02 3192.76 3192.84 3194.13 3194.44
3194.51 3194.83 3200.01 3201.12 3201.49 3202.25
3202.86 3203.25 3204.53 3207.55 3210.14 3211.31
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3228.01 3229.64 3233.76

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9B-TS

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119.10 129.15 130.58 135.76 141.44 162.51
165.77 181.61 195.97 199.78 213.77 216.44
221.23 224.49 229.54 237.78 239.32 257.35
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407.75 411.01 412.07 419.42 423.49 427.71
429.96 431.71 432.59 440.75 447.14 461.16
471.99 472.40 486.36 499.13 505.24 519.40
528.17 534.84 544.26 562.32 590.77 616.08
627.26 627.34 628.95 630.12 631.50 632.66
676.09 693.75 697.63 705.98 707.90 710.17
710.70 712.36 714.99 715.79 716.89 720.35
722.92 723.72 736.91 759.60 762.10 766.82
768.96 771.50 773.76 781.08 804.44 845.58
862.25 865.12 870.44 870.81 880.24 885.32
930.29 940.64 944.40 949.14 951.06 955.42
960.33 966.47 974.82 985.32 990.22 990.71
991.24 993.80 998.91 1000.77 1004.52 1011.03
1012.02 1012.65 1013.90 1014.20 1015.05 1015.50
1017.72 1018.34 1019.30 1021.20 1026.30 1026.72

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1118.60 1119.29 1120.56 1121.71 1123.89 1138.14
1161.34 1178.16 1180.19 1185.51 1200.09 1200.31
1201.77 1201.96 1203.77 1203.90 1218.75 1220.10
1221.66 1226.90 1227.24 1228.86 1230.88 1234.69
1257.33 1284.18 1292.67 1318.65 1320.58 1322.94
1326.57 1329.67 1334.91 1335.69 1341.08 1359.49
1362.61 1366.82 1367.34 1368.29 1370.07 1371.29
1410.62 1418.60 1460.33 1467.89 1473.02 1473.99
1474.17 1476.41 1479.52 1479.73 1480.80 1483.34
1495.88 1501.38 1503.91 1522.35 1524.10 1524.67
1526.42 1526.91 1527.32 1529.86 1550.93 1617.19
1623.81 1624.58 1626.64 1626.99 1629.20 1630.09
1641.79 1642.25 1644.24 1644.94 1646.27 1646.98
1771.68 2965.98 3041.29 3042.51 3056.71 3063.90
3098.55 3107.95 3116.97 3124.71 3145.55 3161.05
3177.68 3178.35 3181.36 3184.89 3185.52 3186.08
3187.34 3187.65 3187.73 3191.79 3194.25 3194.31
3194.64 3195.04 3196.86 3200.72 3202.62 3203.07
3207.03 3207.56 3207.80 3211.09 3211.15 3213.61
3214.12 3214.40 3217.43 3218.61 3227.36 3228.17
3230.21 3239.84 3251.86

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11A-TS
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-139.15 11.07 17.48 27.26 32.95 37.53
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63.23 66.97 69.91 77.75 79.05 81.62
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118.53 122.55 127.95 134.88 148.27 159.03
165.51 177.39 179.12 188.93 196.08 206.90
217.21 220.89 224.79 230.66 241.55 242.64
248.66 254.46 258.57 263.35 265.16 279.64
280.81 283.63 302.09 325.65 356.51 383.07
404.83 405.75 413.42 417.43 421.82 424.13
429.39 431.41 434.50 439.03 445.62 462.88
470.41 488.19 503.22 504.23 520.20 522.85
531.40 537.72 561.55 617.67 624.49 628.78
630.69 630.74 631.59 632.01 632.76 638.09
682.51 696.99 698.12 699.95 705.70 708.72
712.42 712.84 714.45 715.21 715.90 720.99
722.67 728.82 760.19 762.35 767.14 767.93
770.54 771.25 772.20 783.30 820.91 836.87
862.32 864.20 868.84 872.34 877.29 887.67
908.92 937.14 938.26 942.42 946.93 951.05
960.48 963.01 969.63 971.13 983.10 986.15
990.18 992.28 995.67 999.31 1008.48 1012.22
1013.67 1014.05 1014.08 1014.73 1015.26 1015.99
1016.18 1016.95 1017.59 1020.11 1022.55 1025.81
1050.51 1050.82 1052.61 1053.03 1053.53 1054.25
1055.68 1081.03 1096.52 1102.76 1111.52 1112.06
1113.18 1113.78 1115.30 1116.95 1118.43 1119.13
1121.51 1121.67 1122.33 1123.51 1125.35 1128.24
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1202.95 1203.08 1204.08 1217.06 1223.08 1226.36
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1476.58 1477.54 1478.05 1480.64 1481.68 1482.69
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1713.65 2964.19 2970.16 3016.19 3023.85 3030.59
3070.37 3090.67 3103.20 3120.98 3123.85 3125.03
3157.77 3177.80 3182.39 3184.49 3185.09 3185.68
3185.97 3186.57 3187.69 3188.17 3191.74 3193.90
3194.31 3195.05 3195.50 3197.42 3200.41 3202.94
3203.23 3204.64 3205.90 3207.22 3209.87 3211.02
3211.45 3211.82 3213.09 3217.33 3218.52 3218.72
3220.28 3225.08 3228.60

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11B-TS
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-235.68 13.53 17.54 20.66 26.07 30.10
42.16 45.28 47.98 51.36 54.05 55.70
58.25 62.32 62.89 68.39 69.95 71.91
82.82 86.66 89.96 92.51 100.35 105.62
110.15 113.99 122.86 124.03 125.21 146.99
150.41 164.88 175.24 201.29 205.26 207.27
217.09 226.18 234.32 235.97 240.92 248.43
250.99 262.09 263.35 264.87 270.17 275.18
277.11 280.53 299.14 318.64 327.29 403.32
408.61 409.94 413.99 415.24 418.68 421.31
423.32 426.57 434.23 451.13 454.07 462.08
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534.69 545.13 553.78 580.28 620.60 627.75
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1017.47 1018.30 1018.67 1018.86 1021.56 1024.45
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15B

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15A-TS1

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15A-TS2

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15B-TS2

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1466.58 1466.97 1466.98 1468.05 1471.00 1473.29
1478.02 1484.86 1493.24 1496.61 1498.24 1499.55
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1505.72 1505.99 1507.40 1509.32 1511.91 1513.75
1517.12 1520.65 1521.21 1522.37 1524.30 1531.59
1550.98 1554.14 1603.05 1603.92 1631.35 1635.11
1636.46 1638.19 1639.06 1645.40 1645.62 1649.75
1650.60 1651.05 1672.69 1674.70 1689.37 1784.93
1909.86 2806.96 2870.95 2910.44 2970.37 2987.44
3031.68 3036.01 3038.87 3039.25 3039.85 3040.64
3040.73 3043.91 3047.38 3066.29 3093.13 3094.14
3097.38 3097.41 3101.67 3102.59 3105.64 3113.11
3114.50 3117.93 3118.65 3121.78 3122.59 3124.82
3125.24 3125.61 3125.80 3128.59 3129.02 3143.73
3147.97 3165.29 3169.70 3170.80 3173.41 3176.50
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3231.17 3234.63 3235.73

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16A

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60.85 62.50 66.54 70.86 73.74 75.99
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139.75 142.83 153.53 158.27 161.60 167.58
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192.03 194.93 198.15 198.88 199.81 206.51
214.99 220.61 225.82 229.83 230.79 239.42
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282.67 286.59 292.68 293.11 296.49 319.58
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393.76 409.05 410.76 414.74 425.95 430.18
446.26 450.10 455.56 460.48 463.14 477.09
486.51 491.89 496.14 509.78 510.86 516.08
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530.69 532.75 533.47 534.48 536.01 544.31
546.60 547.49 549.42 556.95 559.14 565.14
569.39 571.81 594.63 604.44 616.23 628.09
633.44 644.22 644.64 675.47 682.70 698.32
703.98 705.61 706.83 708.10 709.09 717.23
756.03 765.16 769.36 778.23 785.70 803.35
807.94 810.47 837.94 839.15 842.50 849.36
852.80 855.89 863.21 868.59 871.58 877.47
879.58 880.10 885.52 890.47 895.17 900.71
902.49 911.62 914.50 927.81 929.79 934.61
937.91 940.87 943.42 944.17 949.86 956.68
957.34 960.67 962.23 962.96 964.74 969.15
972.42 987.18 989.87 999.27 1005.03 1006.52
1007.46 1010.28 1011.00 1012.52 1015.88 1021.28
1022.77 1023.85 1025.32 1038.53 1044.78 1045.70

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1267.82 1279.03 1284.67 1287.42 1290.97 1292.14
1292.68 1293.30 1298.50 1316.50 1321.32 1322.89
1324.04 1325.81 1334.94 1346.58 1351.10 1359.46
1362.61 1363.36 1364.33 1367.73 1386.46 1407.67
1407.87 1410.41 1421.70 1425.87 1425.91 1427.10
1427.82 1428.85 1429.22 1430.39 1430.75 1431.48
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3062.73 3070.32 3086.82 3100.00 3100.77 3101.55
3102.60 3103.07 3103.24 3105.41 3110.69 3117.49
3119.03 3123.05 3123.41 3124.65 3126.07 3128.14
3128.40 3128.52 3129.37 3131.58 3131.90 3135.71
3156.97 3157.65 3167.12 3168.29 3169.71 3170.51
3175.54 3180.78 3181.24 3181.83 3183.44 3185.12
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3233.82 3238.53 3254.16

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16B

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171.57 174.70 178.46 187.29 191.72 193.49
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286.82 291.86 293.15 298.06 304.11 308.29
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569.71 576.47 592.11 604.21 610.03 611.83
632.82 647.17 664.05 668.81 684.32 702.48
706.84 708.62 711.31 716.29 722.24 723.65
764.83 768.85 769.54 773.27 784.15 804.17
806.74 832.82 834.31 837.99 840.86 843.94
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875.02 883.02 889.38 889.97 891.12 896.05
903.79 904.29 919.25 930.64 932.30 935.52
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963.79 964.33 965.46 969.01 970.24 975.96
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1011.22 1013.72 1014.47 1014.63 1021.46 1022.95
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1070.84 1073.75 1076.93 1100.35 1129.79 1131.69
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1168.55 1172.99 1176.34 1178.61 1183.43 1189.06
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1290.33 1292.48 1298.87 1319.63 1320.27 1327.20
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3099.91 3101.51 3102.03 3105.26 3110.37 3114.97
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3129.31 3129.64 3131.34 3140.94 3144.07 3165.10
3167.93 3170.49 3170.79 3171.67 3171.96 3172.58
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937.50 940.42 941.96 947.23 951.50 957.66
960.28 965.48 966.54 971.02 972.07 975.09
985.42 997.53 999.59 1001.71 1004.70 1006.68
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3174.50 3175.95 3176.62 3180.90 3182.09 3183.59
3185.49 3186.06 3191.11 3193.62 3199.25 3202.25
3203.88 3206.39 3208.47 3209.23 3212.86 3219.71
3222.49 3226.64 3233.87

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12.27 14.34 18.00 21.86 25.37 28.38
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152.73 156.08 158.97 161.30 166.43 170.44
171.40 175.91 177.78 181.12 186.16 191.91
193.14 198.28 203.50 204.37 210.82 218.20
223.81 225.91 230.90 231.66 237.59 237.92
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310.64 328.03 336.39 341.94 357.06 390.97
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485.18 489.19 490.45 500.97 508.57 517.59
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526.27 529.80 535.86 537.02 543.09 544.22
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631.88 659.16 686.99 688.28 690.01 701.88
705.39 706.01 706.21 708.56 713.63 746.34
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872.64 876.78 878.11 878.97 881.10 892.74
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3221.29 3225.57 3233.69

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16A-TS

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16B-TS
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161.19 164.17 168.46 171.49 172.71 176.02
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1006.75 1013.20 1013.57 1014.10 1023.10 1023.69
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18A-TS

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1009.36 1011.76 1013.92 1015.31 1020.31 1024.57
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18B-TS

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532.95 533.14 535.09 538.11 542.48 546.12
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554.09 557.05 558.94 559.74 561.99 566.14
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456.45 461.06 468.54 510.76 518.38 539.08
542.17 557.71 582.01 617.41 628.13 628.71
629.61 657.42 677.39 697.76 708.66 710.21
712.49 721.80 726.01 739.24 764.36 765.85
770.41 776.09 810.12 812.48 831.70 865.54
868.49 872.31 926.35 936.90 946.23 949.31
952.97 986.53 990.40 991.85 994.66 1007.54
1012.79 1013.33 1014.17 1016.58 1020.58 1023.26
1023.65 1044.36 1051.31 1052.38 1052.46 1052.53
1062.46 1075.70 1083.18 1114.57 1116.27 1116.35
1117.85 1119.02 1121.67 1123.93 1151.41 1173.80
1176.45 1204.11 1204.94 1205.39 1208.68 1212.52
1224.60 1228.48 1230.82 1232.34 1234.49 1255.00
1303.19 1324.61 1326.52 1329.77 1336.79 1349.80
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1473.75 1474.21 1475.77 1476.52 1478.65 1480.76

1493.06 1500.62 1506.79 1524.86 1525.79 1527.91
1529.88 1623.81 1626.14 1628.51 1640.08 1643.06
1643.38 1687.57 1856.41 2264.45 2981.61 2998.84
3023.82 3034.82 3068.48 3070.96 3083.24 3110.62
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3209.56 3209.98 3212.00 3214.00 3215.74 3216.39
3218.48 3220.02 3220.51

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20B

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47.84 53.26 55.74 58.57 71.13 76.53
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218.06 226.06 232.91 243.48 251.88 255.96
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339.16 380.01 407.41 410.73 417.08 437.51
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540.03 560.52 580.35 616.30 627.15 627.87
628.77 655.52 676.95 695.91 708.22 708.64
711.66 719.50 723.23 739.50 765.81 767.21
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20A-TS1

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214.31 228.99 235.05 241.89 250.40 255.15
268.34 280.17 284.40 292.62 318.51 342.42
363.73 407.68 407.88 417.48 431.10 444.44
447.59 460.62 486.39 505.60 518.73 534.92
543.58 576.17 606.10 629.55 629.95 631.16
637.58 663.36 679.28 697.44 708.72 711.02
713.70 722.15 723.61 748.49 763.22 765.01
770.14 771.61 799.38 834.66 865.81 867.59
874.02 905.50 942.45 944.80 944.93 948.35
949.97 975.91 986.86 989.35 992.23 1003.94
1012.18 1012.25 1012.92 1013.92 1018.35 1020.01
1021.10 1022.57 1051.71 1052.51 1052.55 1053.45

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20A-TS2

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150.39 158.79 165.81 194.62 200.43 205.94
211.90 223.12 231.20 246.74 251.27 259.83
267.02 275.95 278.55 295.47 335.20 356.94
406.48 410.20 411.41 415.79 440.78 449.15
459.30 470.65 488.48 508.04 521.17 535.02
557.54 600.25 615.77 626.82 629.64 629.80
668.29 684.13 688.31 696.98 708.86 710.20
711.26 720.00 725.33 761.27 765.30 766.09
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868.83 873.56 942.03 944.84 949.95 954.26
973.26 988.88 990.11 992.56 993.75 997.26
1007.84 1008.67 1012.90 1013.79 1020.97 1021.69
1022.30 1037.68 1046.24 1048.85 1051.61 1052.46
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1287.52 1328.43 1331.41 1332.07 1335.70 1345.60
1366.62 1366.83 1369.63 1391.35 1403.32 1465.35
1469.24 1475.66 1477.04 1478.69 1479.56 1480.11
1493.80 1502.58 1504.56 1524.53 1525.24 1525.39
1527.32 1625.88 1627.64 1628.42 1642.07 1642.32
1643.44 1643.64 1791.33 1826.89 2984.57 3003.51
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20B-TS1

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206.07 220.54 227.07 229.45 249.56 255.00
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443.20 464.08 501.87 517.83 533.28 535.84
569.27 574.40 601.15 618.83 626.70 629.61

630.89 645.11 679.25 694.22 707.85 711.13
712.04 719.68 723.51 758.33 762.08 764.37
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20B-TS2

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271.25 274.58 292.75 311.04 323.66 347.50
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453.73 462.73 481.41 509.48 517.85 531.90
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668.02 687.09 697.67 707.99 708.50 709.94
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769.78 790.72 806.90 816.28 860.53 865.35
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1006.85 1011.24 1013.78 1014.82 1017.89 1020.93
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21A

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 155.72 171.04 184.04 194.58 200.73 211.32
 216.74 223.50 249.87 257.13 261.83 276.14
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 1011.14 1013.36 1014.70 1020.83 1023.95 1024.49
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21B

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23A

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 404.43 404.55 420.32 430.92 440.81 447.29
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 685.27 687.82 699.85 704.52 707.10 714.29
 721.34 727.63 753.49 762.10 765.80 768.25
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23B

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21A-TS

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21B-TS

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221.72 232.88 251.35 257.28 263.79 274.02
278.10 299.18 318.04 328.51 360.92 384.57
406.30 407.97 414.65 422.78 430.58 448.91
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679.39 687.16 706.03 708.77 711.07 728.70
730.84 732.26 738.10 758.99 765.01 765.99
785.30 803.86 846.34 859.34 864.58 873.86
929.80 937.92 945.33 953.45 954.70 971.76
987.77 988.04 988.35 996.09 998.73 1004.92
1012.13 1012.93 1022.19 1023.21 1026.06 1028.37

1036.66 1047.50 1049.38 1052.90 1070.42 1084.30
1095.30 1098.39 1111.78 1114.52 1118.40 1120.38
1120.63 1127.04 1134.56 1160.80 1177.78 1186.71
1194.61 1203.87 1205.19 1205.90 1219.54 1219.61
1220.16 1225.30 1230.40 1251.32 1290.05 1296.09
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1472.31 1475.34 1476.96 1479.20 1481.41 1487.21
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1524.84 1529.36 1596.75 1602.44 1625.76 1627.02
1634.89 1641.74 1642.40 1790.63 2966.17 3001.06
3040.49 3050.75 3068.74 3070.65 3117.10 3121.06
3128.01 3142.28 3150.89 3161.76 3173.97 3184.84
3185.92 3186.97 3188.25 3194.59 3196.11 3196.97
3202.89 3204.19 3204.46 3211.70 3211.94 3212.59
3218.33 3219.18 3219.52

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23A-TS

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987.07 988.56 993.15 996.42 1008.01 1011.94
1012.52 1019.81 1021.95 1023.38 1024.93 1028.49
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1204.67 1205.35 1206.78 1208.24 1218.13 1219.60
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3218.31 3219.25 3220.62

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23B-TS

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564.85 611.76 624.40 627.75 628.67 663.35
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731.98 732.89 762.33 768.35 769.83 773.53
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1204.72 1205.84 1206.94 1211.47 1213.99 1219.34
1223.46 1225.18 1229.17 1265.84 1273.31 1294.96
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1502.51 1505.92 1507.15 1515.44 1522.64 1522.81
1525.84 1604.60 1611.17 1624.94 1625.46 1635.06
1641.09 1642.73 1650.75 1760.57 2743.36 2965.65
2987.43 3015.36 3033.46 3059.11 3074.10 3082.97
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50.50 59.63 62.96 69.58 75.93 83.53
103.15 118.80 126.42 132.00 151.86 157.44
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409.70 414.25 423.75 433.22 448.50 455.79
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1096.80 1107.07 1111.02 1115.15 1116.66 1118.18
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1525.63 1529.83 1593.74 1602.87 1626.14 1626.82
1629.92 1641.92 1642.37 1775.08 2969.49 3009.47
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1016.71 1027.66 1032.94 1035.58 1061.87 1119.52
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1474.33 1474.66 1476.75 1478.79 1480.95 1481.79
1484.46 1487.16 1496.07 1500.51 1503.72 1524.57
1730.21 2071.53 2104.01 2973.21 2982.48 3002.94
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1486.71 1492.79 1496.75 1500.04 1505.38 1525.01
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145.23 149.37 157.66 168.02 177.72 188.25
206.98 208.69 211.94 219.27 221.52 228.58
230.99 236.51 253.60 254.75 258.26 259.85
267.30 267.86 275.07 277.05 281.60 303.31
327.51 336.87 365.72 392.18 406.74 408.56
410.44 414.72 418.64 421.63 423.53 426.15
433.52 435.12 438.59 467.59 470.22 498.70
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535.06 549.62 560.61 584.09 618.39 625.78
627.41 629.25 629.64 630.52 631.04 632.38
632.71 674.19 683.05 690.86 694.30 702.55
705.23 706.71 708.35 710.47 710.89 713.73
714.54 717.74 719.68 720.94 749.81 758.29
761.41 765.38 766.47 767.68 768.98 771.47
777.74 798.23 820.55 859.69 861.24 863.18
867.56 869.87 872.67 880.89 881.20 904.26
937.37 940.18 940.71 943.47 944.96 948.36
956.90 961.08 981.26 983.17 983.76 988.22
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15B-TS1'

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