

Supporting Information

Structural analogues of Hoveyda-Grubbs catalysts bearing 1-benzofuran moiety or isopropoxy-1-benzofuran derivatives as olefin metathesis catalysts

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Energy Values Tables

Table S1. Total energy values (E) and free energy values (G; as defined in the manuscript) for the initiation reaction following either the interchange or dissociative mechanism for **3-13**. "S" stands for pre-catalyst, "TS" for transition state, "P" for product of the reaction (activated catalyst) and "Pa" for activated catalysts with the olefin model (1-cisbutane) associated to the Ru center.

complex	structure	M06 gas-phase, LACVP++ E (Hartrees)	solvation E in DCM (hartrees)	zero-point E correction (kcal/mol)	entropy (cal/mol)	thermal correction to enthalpy (kcal/mol)	G (Hartrees)
3	S trans	-2360.878273	-0.015569	343.278	225.998	21.083	-2360.420521
	S cis	-2360.873759	-0.024206	343.389	228.559	21.490	-2360.425034
	TS	-2360.860934	-0.014719	342.810	230.493	21.321	-2360.404833
	P	-2360.872730	-0.015628	343.128	229.314	21.244	-2360.416594
	Pa	-2518.044508	-0.012019	412.198	248.103	25.011	-2517.477613
4	S trans	-2553.985438	-0.013999	398.806	246.532	24.280	-2553.442284
	S cis	-2553.972962	-0.021917	399.181	241.064	23.982	-2553.435007
	TS	-2553.948997	-0.015014	398.159	252.992	24.583	-2553.410473
	P	-2553.965761	-0.014831	398.767	247.630	24.305	-2553.423982
	Pa	-2711.133958	-0.011137	467.580	272.126	28.322	-2710.484056
5	S trans	-2553.987355	-0.014265	398.790	245.408	24.235	-2553.444030
	S cis	-2553.974271	-0.021964	399.191	247.335	24.524	-2553.438460
	TS	-2553.958670	-0.014628	398.357	243.397	23.912	-2553.415958
	P	-2553.968238	-0.015193	398.746	245.574	24.239	-2553.425983
	Pa	-2711.135555	-0.010940	473.875	284.947	29.486	-2710.479658
6	S trans	-2553.988218	-0.014264	398.794	245.480	24.212	-2553.444956
	S cis	-2553.975267	-0.022379	399.089	241.846	24.001	-2553.438261
	TS	-2553.962987	-0.014865	398.002	245.803	24.027	-2553.422037
	P	-2553.963545	-0.015299	398.677	257.368	24.981	-2553.425924
	Pa	-2711.134798	-0.012682	467.496	279.548	28.908	-2710.489166
7	S trans	-2553.988171	-0.014277	398.761	247.017	24.272	-2553.445610
	S cis	-2553.975834	-0.022484	399.277	245.338	24.413	-2553.439634
	TS	-2553.960343	-0.015371	397.952	252.556	24.555	-2553.422344
	P	-2553.966067	-0.015152	398.633	254.450	24.833	-2553.427220
	Pa	-2711.132222	-0.013007	467.541	280.929	28.920	-2710.487480
8	S trans	-2553.990238	-0.014399	398.788	243.939	24.182	-2553.446437
	S cis	-2553.977631	-0.021942	399.421	243.459	24.359	-2553.439854
	TS	-2553.963495	-0.014001	398.476	249.937	24.434	-2553.422240
	P	-2553.963164	-0.016375	398.733	249.309	24.389	-2553.423646
	Pa	-2711.129284	-0.010388	467.626	272.220	28.282	-2710.478669
9	S trans	-2553.988049	-0.014071	398.953	244.008	24.190	-2553.443677
	S cis	-2553.975342	-0.021968	399.382	247.031	24.487	-2553.439146
	TS	-2553.949738	-0.013351	398.257	245.575	24.050	-2553.406722
	P	-2553.970757	-0.015779	398.978	244.114	24.139	-2553.428185
	Pa	-2711.122159	-0.013093	467.052	279.255	28.701	-2710.477836
10	S trans	-2553.981765	-0.013874	398.781	254.310	24.918	-2553.441202
	S cis	-2553.971519	-0.020716	399.193	249.818	24.643	-2553.435447
	TS	-2553.959848	-0.013917	398.377	246.273	24.036	-2553.417561
	P	-2553.970043	-0.016404	398.673	249.848	24.411	-2553.430871
	Pa	-2711.135579	-0.011711	467.449	273.861	28.356	-2710.487230

11	S trans	-2553.989010	-0.013426	398.750	255.359	24.981	-2553.448447
	S cis	-2553.978214	-0.019461	399.087	250.496	24.706	-2553.441277
	TS	-2553.969201	-0.013021	398.438	245.936	24.049	-2553.425740
	P	-2553.974428	-0.017104	398.660	250.597	24.495	-2553.436199
	Pa	-2711.144797	-0.009761	467.851	278.172	28.783	-2710.495224
12	S trans	-2553.986474	-0.014350	399.093	246.781	24.276	-2553.443337
	S cis	-2553.970612	-0.024369	399.496	243.733	24.388	-2553.435226
	TS	-2553.960595	-0.014112	398.098	247.902	24.115	-2553.419595
	P	-2553.969053	-0.013452	398.631	251.620	24.484	-2553.427721
	Pa	-2711.146239	-0.009435	467.639	271.515	28.273	-2710.494328
13	S trans	-2553.981163	-0.014503	398.971	245.535	24.258	-2553.437811
	S cis	-2553.965048	-0.021561	399.297	247.023	24.526	-2553.428514
	TS	-2553.953978	-0.015005	398.063	248.572	24.119	-2553.414239
	P	-2553.960147	-0.014903	398.656	249.999	24.449	-2553.419513
	Pa	-2711.135795	-0.010337	467.690	269.451	28.237	-2710.483783

Precursors of complexes 3-13

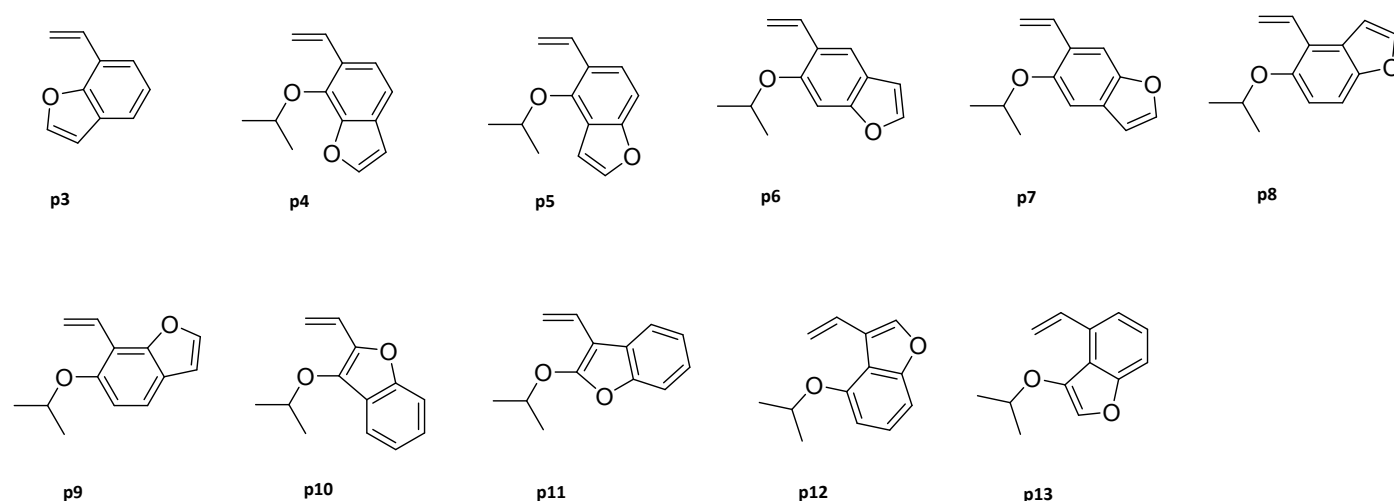


Fig. S1. Possible precursors for complexes 3-13.

Geometries in xyz format

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70
2 - S
Ru1 13.72247 4.38788 8.10592
C12 14.61814 3.25818 10.02179
C13 13.62240 5.50051 5.99007
C4 12.12427 3.55845 8.10094
C5 15.66555 6.76819 8.92381
C6 16.36873 5.74931 11.14125
H7 16.70627 6.54737 11.81818
H8 16.91546 4.83807 11.40485
H9 15.30919 5.55421 11.32881
C10 10.88701 5.96443 9.62993
N11 14.32229 6.89455 9.39769
N12 12.17722 6.56416 9.60109
C13 13.88988 8.02293 10.22353
H14 14.27985 8.96472 9.81916
H15 14.26867 7.90563 11.25052
C16 18.23978 6.42867 7.90740
C17 10.56725 5.13243 10.71006
C18 12.37161 7.91558 10.14264
H19 11.87420 8.00976 11.11507
H20 11.93082 8.65967 9.46161
C21 13.31524 6.03129 9.11021
C22 9.98758 6.21589 8.58837
C23 15.99394 7.33813 7.68027
C24 17.27722 7.13323 7.18524
H25 17.53385 7.54102 6.20642
C26 16.63640 6.14427 9.72048
C27 8.38513 4.75580 9.70046
C28 8.73781 5.59991 8.64742

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H29 8.02584 5.77205 7.83891
 C30 10.38701 7.05180 7.40961
 H31 10.65202 8.07718 7.69929
 H32 9.57119 7.11485 6.68263
 H33 11.26539 6.62696 6.90020
 C34 17.91163 5.97096 9.18070
 H35 18.66874 5.46088 9.77907
 C36 9.30687 4.54007 10.72518
 H37 9.04178 3.87966 11.55210
 C38 15.04497 8.23179 6.93802
 H39 13.99613 8.03009 7.17544
 H40 15.15912 8.11185 5.85643
 H41 15.26101 9.28231 7.18241
 C42 11.57911 4.83698 11.77586
 H43 12.39916 4.21775 11.38118
 H44 11.12127 4.30008 12.61251
 H45 12.04325 5.75060 12.17106
 C46 7.05542 4.06111 9.71649
 H47 6.31048 4.59993 9.12148
 H48 6.66843 3.95729 10.73629
 H49 7.13590 3.04896 9.29890
 C50 19.59295 6.18387 7.31272
 H51 19.52345 5.45058 6.49799
 H52 20.29810 5.79353 8.05459
 H53 20.01735 7.10042 6.88624
 H54 11.14472 3.98420 8.33428
 H55 12.13639 2.49192 7.81790
 O56 14.57007 2.60893 6.76182
 C57 14.82708 1.98266 4.60826
 C58 13.94633 2.21683 5.59856
 H59 14.58665 1.66014 3.60466
 H60 12.86766 2.17773 5.64683
 C61 15.91659 2.64752 6.47930
 C62 16.13034 2.26310 5.15132
 C63 17.43874 2.22823 4.66195
 C64 18.47122 2.57626 5.52056
 C65 18.21808 2.95150 6.84714
 C66 16.92630 2.99789 7.35777
 H67 17.63944 1.93493 3.63399
 H68 19.49827 2.55365 5.16142
 H69 19.05042 3.20958 7.49979
 H70 16.71153 3.27762 8.38668
 68

3 - S trans

Ru1 14.12752 4.48925 8.17808
 C12 14.94474 3.39134 10.13155
 C13 14.15830 5.52497 6.03105
 C4 12.60276 3.48355 7.96144
 C5 15.69014 7.04119 9.10578
 C6 16.27103 6.06399 11.37517
 H7 16.47456 6.88956 12.07250
 H8 16.86633 5.20292 11.69437
 H9 15.21959 5.77774 11.46850
 C10 11.00018 5.69839 9.44843
 N11 14.30557 7.04249 9.45596
 N12 12.21122 6.44039 9.53015
 C13 13.68688 8.09269 10.26223
 H14 13.99076 9.08342 9.90369
 H15 13.99731 7.99565 11.31475
 C16 18.35058 6.87366 8.30328
 C17 10.68418 4.83024 10.50132
 C18 12.20274 7.80850 10.06310
 H19 11.62013 7.85186 10.99083
 H20 11.73774 8.49239 9.33602
 C21 13.43791 6.05493 9.11271
 C22 10.17962 5.83914 8.32410
 C23 16.07674 7.63424 7.89215
 C24 17.40840 7.52123 7.50564
 H25 17.71679 7.94780 6.55014
 C26 16.63137 6.47910 9.98094
 C27 8.66585 4.19760 9.29813
 C28 9.01161 5.07879 8.27377
 H29 8.36377 5.16393 7.40026
 C30 10.59256 6.70704 7.17343
 H31 10.73932 7.75283 7.47335
 H32 9.83581 6.69237 6.38290
 H33 11.54427 6.36349 6.73956
 C34 17.95310 6.39078 9.54767
 H35 18.69045 5.92869 10.20553
 C36 9.50844 4.09021 10.40504
 H37 9.24963 3.40001 11.20935
 C38 15.12229 8.44083 7.06349

H39 14.08301 8.12127 7.18675
 H40 15.36217 8.35740 5.99915
 H41 15.19392 9.50274 7.34085
 C42 11.62682 4.64949 11.65266
 H43 12.54501 4.13384 11.33092
 H44 11.16517 4.05594 12.44791
 H45 11.94344 5.60895 12.08311
 C46 7.43134 3.35031 9.20046
 H47 6.69964 3.78035 8.50861
 H48 6.94850 3.22997 10.17674
 H49 7.67196 2.34271 8.83643
 C50 19.76097 6.69985 7.82432
 H51 19.85081 5.80669 7.19232
 H52 20.46000 6.57947 8.65883
 H53 20.08968 7.55375 7.22132
 H54 11.60130 3.76799 8.29295
 O55 15.08054 2.53968 6.99154
 C56 15.66681 0.63435 5.94711
 C57 16.10578 1.81679 6.43498
 H58 16.27515 -0.11557 5.45988
 H59 17.07435 2.29210 6.47145
 C60 13.96669 1.78769 6.84937
 C61 14.24835 0.58747 6.20918
 C62 13.17955 -0.29327 5.99802
 C63 11.91083 0.07857 6.43570
 C64 11.67554 1.29935 7.07648
 C65 12.72022 2.20525 7.30598
 H66 13.33077 -1.24973 5.50397
 H67 11.07733 -0.60136 6.27511
 H68 10.67278 1.56363 7.40980
 68

3 - S cis

Ru1 14.22133 4.51643 8.31262
 C12 14.55871 3.42605 10.37061
 C13 16.07487 3.45406 7.28491
 C4 12.63858 3.61359 8.08281
 C5 15.69264 7.10199 9.16073
 C6 16.64660 5.99789 11.23325
 H7 16.84210 6.78172 11.97868
 H8 17.37006 5.19335 11.39915
 H9 15.65331 5.57692 11.41477
 C10 11.02762 5.83103 9.49710
 N11 14.36977 7.03971 9.70411
 N12 12.28408 6.40314 9.86563
 C13 13.81971 7.97064 10.69096
 H14 14.08531 9.00526 10.44227
 H15 14.22046 7.74281 11.68945
 C16 18.20133 7.11539 7.95008
 C17 10.46162 4.84183 10.30822
 C18 12.32194 7.68585 10.58714
 H19 11.83095 7.59018 11.56220
 H20 11.78594 8.45745 10.01358
 C21 13.48413 6.09171 9.32936
 C22 10.37795 6.29583 8.34216
 C23 15.85377 7.73675 7.91501
 C24 17.11119 7.72598 7.32555
 H25 17.24849 8.20494 6.35460
 C26 16.77955 6.54958 9.84792
 C27 8.56823 4.73171 8.77778
 C28 9.15146 5.73566 8.00512
 H29 8.65069 6.06860 7.09409
 C30 11.00360 7.32081 7.44402
 H31 11.19736 8.27528 7.95173
 H32 10.35904 7.52632 6.58301
 H33 11.96662 6.96637 7.05576
 C34 18.02208 6.56245 9.21265
 H35 18.87180 6.10577 9.72064
 C36 9.23257 4.30285 9.92320
 H37 8.78735 3.51934 10.53765
 C38 14.70061 8.42795 7.24969
 H39 13.92853 7.71929 6.92752
 H40 15.03556 8.97997 6.36477
 H41 14.20676 9.14286 7.92186
 C42 11.16595 4.35619 11.53677
 H43 12.16234 3.95814 11.29729
 H44 10.58724 3.57003 12.03140
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H51 19.58042 6.14281 6.63029
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 H53 19.69469 7.90652 6.60764
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 C56 12.97509 5.80570 4.05259
 C57 13.95538 5.95122 4.97358
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 H59 14.90344 6.47177 4.98814
 C60 12.48325 4.61846 5.89119
 C61 11.98655 4.92512 4.63420
 C62 10.76339 4.33733 4.27898
 C63 10.15223 3.47846 5.18829
 C64 10.71138 3.18521 6.44033
 C65 11.91836 3.77165 6.83668
 H66 10.30502 4.53219 3.31296
 H67 9.20852 3.01096 4.91471
 H68 10.20298 2.50563 7.12274
 68
 3 - TS
 Ru1 14.08574 4.29164 8.43534
 C12 14.66553 3.59641 10.61765
 C13 14.70685 4.90037 6.23839
 C4 12.53547 3.43781 8.03235
 C5 15.72531 7.10201 8.95244
 C6 16.67380 6.24232 11.15130
 H7 16.92936 7.06292 11.83639
 H8 17.35755 5.41357 11.36518
 H9 15.66543 5.89035 11.38068
 C10 11.03415 5.75676 9.41736
 N11 14.38707 6.98709 9.44974
 N12 12.29801 6.36932 9.67066
 C13 13.81579 8.00767 10.33268
 H14 14.10669 9.01004 9.99825
 H15 14.18756 7.86451 11.35838
 C16 18.29830 7.34844 7.90767
 C17 10.47171 4.92717 10.39411
 C18 12.32372 7.73358 10.21422
 H19 11.79378 7.77079 11.17280
 H20 11.81908 8.42507 9.52098
 C21 13.50204 5.99710 9.17186
 C22 10.38782 6.00900 8.19910
 C23 15.90378 7.71812 7.70074
 C24 17.19356 7.82305 7.19774
 H25 17.34278 8.28289 6.21994
 C26 16.81576 6.69987 9.73128
 C27 8.56401 4.56733 8.92148
 C28 9.15098 5.40796 7.97635
 H29 8.64033 5.58615 7.02886
 C30 11.04882 6.80760 7.11572
 H31 11.44622 7.76498 7.47365
 H32 10.34718 7.01919 6.30305
 H33 11.90014 6.25483 6.69025
 C34 18.09162 6.81423 9.17414
 H35 18.94845 6.48241 9.76258
 C36 9.23476 4.34390 10.12255
 H37 8.78916 3.68387 10.86789
 C38 14.73997 8.25503 6.92468
 H39 14.16720 7.43483 6.47402
 H40 15.08315 8.90832 6.11610
 H41 14.05370 8.83236 7.55852
 C42 11.20546 4.62822 11.66496
 H43 12.15725 4.11888 11.45785
 H44 10.60574 3.98813 12.31940
 H45 11.45435 5.54161 12.22037
 C46 7.25877 3.88773 8.63061
 H47 6.62402 4.49763 7.97844
 H48 6.70112 3.67384 9.54862
 H49 7.42128 2.92990 8.11934
 C50 19.67110 7.42187 7.31069
 H51 19.82715 6.60721 6.59213
 H52 20.44977 7.33912 8.07615
 H53 19.82299 8.36198 6.76777
 H54 11.54641 3.90591 8.00184
 O55 13.58157 0.92214 9.38062
 C56 13.97152 -1.10018 8.46342
 C57 14.03527 -0.34564 9.58337
 H58 14.26834 -2.13520 8.36478
 H59 14.37544 -0.55143 10.58820
 C60 13.22490 0.99323 8.07602
 C61 13.42831 -0.24391 7.44415
 C62 13.08134 -0.38822 6.09849

C63 12.52754 0.70287 5.44034
 C64 12.32535 1.92022 6.09285
 C65 12.68334 2.10932 7.43594
 H66 13.23438 -1.33211 5.58064
 H67 12.24951 0.61477 4.39262
 H68 11.91613 2.76932 5.54704
 68
 3 - P
 Ru1 14.07060 4.49307 8.10349
 C12 15.15002 3.42145 9.91609
 C13 13.98678 5.39958 5.91697
 C4 12.56621 3.45151 8.04852
 C5 15.69384 7.12610 8.90015
 C6 16.43793 6.20622 11.14589
 H7 16.57488 7.04372 11.84526
 H8 17.13018 5.41173 11.44201
 H9 15.42489 5.81187 11.26774
 C10 11.06555 5.66415 9.58498
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 N12 12.25414 6.44362 9.53732
 C13 13.74414 8.12319 10.16049
 H14 14.02172 9.11186 9.77646
 H15 14.10788 8.03968 11.19708
 C16 18.33145 7.22147 8.01506
 C17 10.87505 4.81751 10.68154
 C18 12.25639 7.82346 10.03797
 H19 11.71718 7.88193 10.99059
 H20 11.75203 8.48635 9.31752
 C21 13.46288 6.06821 9.05683
 C22 10.15538 5.72976 8.52201
 C23 15.97787 7.72709 7.66287
 C24 17.30189 7.74621 7.23580
 H25 17.53616 8.19215 6.26817
 C26 16.71220 6.65899 9.74349
 C27 8.82384 4.02699 9.64148
 C28 9.03782 4.90186 8.57469
 H29 8.33156 4.91272 7.74314
 C30 10.43586 6.58673 7.32411
 H31 10.54506 7.64655 7.58901
 H32 9.62659 6.51006 6.59139
 H33 11.37035 6.28141 6.82979
 C34 18.02194 6.70467 9.27076
 H35 18.82323 6.32891 9.90846
 C36 9.74146 4.00567 10.68856
 H37 9.59150 3.31408 11.51845
 C38 14.92151 8.41774 6.85278
 H39 13.92122 8.00791 7.02221
 H40 15.13016 8.32828 5.78227
 H41 14.90238 9.48922 7.09906
 C42 11.91303 4.71186 11.75809
 H43 12.81857 4.21154 11.38125
 H44 11.53847 4.13382 12.60850
 H45 12.22947 5.69620 12.12811
 C46 7.64114 3.10531 9.63213
 H47 6.69583 3.65658 9.70975
 H48 7.68067 2.39340 10.46392
 H49 7.60188 2.53331 8.69621
 C50 19.74224 7.21687 7.50739
 H51 19.93290 6.33009 6.88950
 H52 20.46664 7.20361 8.32879
 H53 19.94713 8.09452 6.88398
 H54 11.65701 3.67072 8.60965
 O55 10.57475 1.36244 8.48423
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 H58 10.07039 -1.70153 7.37859
 H59 9.02005 0.14074 9.09755
 C60 11.60519 1.22130 7.61328
 C61 11.57473 -0.04453 7.01915
 C62 12.56840 -0.38022 6.09389
 C63 13.54675 0.56158 5.79892
 C64 13.55620 1.81774 6.40627
 C65 12.58230 2.19139 7.34867
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 H67 14.31991 0.32221 5.07315
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 H7 16.14011 7.74695 11.95895
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 H9 15.36022 6.19828 11.53598
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 N11 14.09269 7.01729 9.45889
 N12 12.33794 5.81387 9.93097
 C13 13.27481 7.93287 10.25490
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 H15 13.73852 8.09814 11.23931
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 H33 11.47878 5.61745 7.31015
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 H35 18.62124 7.13814 10.14320
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 C38 14.51234 8.22317 6.84542
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 H43 13.39039 3.82515 11.82134
 H44 12.14625 3.38488 13.01260
 H45 12.41247 5.08219 12.56873
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 H47 7.41540 2.07941 10.30994
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 C81 16.03543 1.24205 7.92955
 H82 15.11245 0.66731 8.06891
 H83 16.74699 0.59287 7.40050
 H84 16.44348 1.46814 8.91990
 H85 14.99592 2.44634 6.38405
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 H8 16.89961 5.35321 11.75665
 H9 15.22312 5.82648 11.50820
 C10 11.00288 5.58842 9.45399
 N11 14.25621 7.04309 9.48785
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 C63 11.74062 1.29909 7.03567
 C64 12.85538 2.13562 7.27664
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 C10 11.03740 5.68525 9.39473
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 C21 13.51281 5.97475 9.28405
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 H53 19.66657 9.04234 7.36892
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 H76 15.40957 3.38129 5.05943
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 H8 17.70661 5.52970 11.12030

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 C13 13.83158 7.85320 10.48325
 H14 14.10434 8.88139 10.22216
 H15 14.18521 7.64854 11.50616
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 C18 12.35246 7.55159 10.31592
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 H20 11.84713 8.25799 9.63745
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 C22 10.34504 5.61593 8.52702
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 C28 9.19011 4.83553 8.45786
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 C30 10.72783 6.52117 7.39473
 H31 10.98044 7.53324 7.73360
 H32 9.91418 6.60461 6.66758
 H33 11.61339 6.13457 6.86858
 C34 18.11714 7.14466 8.99333
 H35 19.04824 6.86767 9.48974
 C36 9.72338 3.79138 10.55096
 H37 9.48389 3.07105 11.33631
 C38 14.45952 8.36711 7.11746
 H39 13.79894 7.52478 6.88262
 H40 14.66383 8.89506 6.18072
 H41 13.91065 9.05624 7.77570
 C42 11.80465 4.39661 11.83554
 H43 12.76408 3.95926 11.52124
 H44 11.36029 3.75067 12.60031
 H45 12.04247 5.36010 12.30542
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 H47 7.14241 3.17864 8.38565
 H48 6.93148 3.27343 10.14119
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 H52 20.30732 8.03771 7.77626
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 H75 10.40568 -0.29042 10.28038
 H76 10.68762 1.36968 9.68845
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 H78 12.16463 1.71406 11.69754
 H79 12.10597 0.01390 12.23432
 H80 13.66944 0.79149 11.85865
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 C56 14.22337 -1.65070 5.81920
 C57 14.36600 -2.20207 7.04574
 H58 14.39813 -2.13880 4.87022
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 C60 13.73208 -0.15632 7.42837
 C61 13.80232 -0.29451 6.03802
 C62 13.49828 0.79857 5.21119
 C63 13.13626 1.98667 5.81010
 C64 13.04604 2.10964 7.21591
 C65 13.35958 1.03357 8.05392
 H66 13.56207 0.71569 4.12940
 H67 12.92747 2.86743 5.20615
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 C5 15.31210 7.46043 8.41833
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 H9 15.49397 6.01043 10.71240
 C10 10.97068 5.57960 9.70821

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N12	12.05640	6.47141	9.48611
C13	13.48564	8.24263	9.97476
H14	13.64307	9.26263	9.60612
H15	13.98351	8.14757	10.95343
C16	17.78265	7.84829	7.19281
C17	11.02825	4.74958	10.83464
C18	12.01992	7.83738	10.02239
H19	11.59637	7.83924	11.03339
H20	11.38764	8.47450	9.38416
C21	13.21566	6.20488	8.83700
C22	9.91044	5.53238	8.79811
C23	15.36730	8.14342	7.19208
C24	16.61233	8.30862	6.59239
H25	16.66936	8.82373	5.63236
C26	16.47554	7.05144	9.08582
C27	8.95094	3.71571	10.10731
C28	8.91083	4.58616	9.01924
H29	8.09156	4.50791	8.30343
C30	9.89586	6.41458	7.58687
H31	9.94760	7.47845	7.85338
H32	8.98249	6.26178	7.00365
H33	10.75606	6.20686	6.93361
C34	17.69736	7.24364	8.44466
H35	18.60956	6.91456	8.94429
C36	9.99934	3.83013	11.02077
H37	10.03301	3.16219	11.88421
C38	14.15395	8.77654	6.57835
H39	13.22399	8.27155	6.85692
H40	14.21503	8.75987	5.48572
H41	14.08451	9.82891	6.88964
C42	12.21607	4.78968	11.75017
H43	13.11716	4.41498	11.23916
H44	12.05037	4.16853	12.63679
H45	12.44819	5.80774	12.09047
C46	7.93388	2.62527	10.25302
H47	8.29480	1.71570	9.75218
H48	6.97568	2.89482	9.79628
H49	7.75604	2.37127	11.30445
C50	19.10431	8.00634	6.50234
H51	19.28574	7.17587	5.80814
H52	19.93389	8.02062	7.21739
H53	19.14226	8.93127	5.91572
H54	11.71092	3.55939	8.77654
O70	11.09065	1.21275	8.87703
C71	11.72468	0.40106	9.89880
H72	12.20906	-0.45321	9.40106
C73	10.61727	-0.09929	10.79271
H74	9.89539	-0.68704	10.21506
H75	11.02294	-0.72537	11.59498
H76	10.09175	0.74968	11.24964
C77	12.75898	1.23166	10.62349
H78	12.26915	2.07197	11.13286
H79	13.27973	0.62739	11.37559
H80	13.51351	1.64209	9.93916
O55	11.11010	-1.14300	7.22287
C56	12.05084	-1.38878	5.18451
C57	11.34536	-1.98236	6.17587
H58	12.35993	-1.84465	4.25361
H59	10.94195	-2.97928	6.28675
C60	11.69252	0.04207	6.88357
C61	12.29860	-0.04520	5.62552
C62	12.94503	1.08382	5.09890
C63	12.95742	2.23770	5.85168
C64	12.35028	2.31974	7.13567
C65	11.69618	1.18878	7.66842
H66	13.41198	1.05638	4.11799
H67	13.40869	3.14188	5.44309
90			
4 - Pa			
Ru1	14.47852	4.49827	8.56556
C12	14.79819	3.83543	10.91107
C13	14.54613	5.28819	6.25210
C4	13.12068	3.22140	8.55990
C5	15.27554	7.38075	9.59951
C6	15.22255	6.85168	12.08445
H7	15.11855	7.77199	12.67689
H8	15.77413	6.12439	12.68796
H9	14.22793	6.43179	11.90901
C10	10.94568	5.23793	8.87292
N11	13.86518	7.17042	9.55267
N12	11.95880	6.15747	9.27055
C13	12.88541	8.21927	9.83509
H14	12.85827	8.94641	9.00724
H15	13.14503	8.75348	10.75673
C16	18.04928	7.62751	9.67047
C17	10.40663	4.34555	9.80938
C18	11.59812	7.41256	9.94506
H19	11.32237	7.20774	10.99174
H20	10.74140	7.88215	9.44827
C21	13.29631	6.01050	9.14948
C22	10.48841	5.28667	7.54807
C23	15.94866	7.84646	8.45931
C24	17.33924	7.93863	8.51350
H25	17.87781	8.27279	7.62547
C26	15.95163	7.14841	10.80899
C27	8.98217	3.44434	8.05286
C28	9.51665	4.36935	7.15729
H29	9.18684	4.36105	6.11714
C30	11.06758	6.25972	6.56791
H31	11.09406	7.28167	6.97140
H32	10.48238	6.27575	5.64276
H33	12.10484	5.99499	6.31362
C34	17.33846	7.26685	10.81487
H35	17.87966	7.06266	11.74015
C36	9.41687	3.46748	9.37597
H37	9.02359	2.73056	10.07808
C38	15.21408	8.33367	7.24707
H39	14.23736	7.85706	7.12626
H40	15.78207	8.13018	6.33393
H41	15.06918	9.42151	7.31660
C42	10.91215	4.28889	11.21995
H43	12.00561	4.38961	11.27242
H44	10.64577	3.33004	11.67889
H45	10.47538	5.08283	11.84163
C46	7.98351	2.41797	7.60553
H47	8.21281	1.43926	8.04868
H48	7.98984	2.30289	6.51527
H49	6.96147	2.68184	7.90703
C50	19.54804	7.65658	9.68693
H51	19.95505	6.65410	9.49791
H52	19.93493	7.98253	10.65899
H53	19.94987	8.32231	8.91569
H54	12.79331	2.96736	9.57555
O55	11.34188	1.26727	9.38660
C56	11.58176	-0.00962	10.01856
H57	11.80170	-0.75045	9.23457
C58	10.31441	-0.38460	10.75027
H59	9.47809	-0.47315	10.04848
H60	10.43393	-1.33639	11.27979
H61	10.07190	0.39099	11.48822
C62	12.77529	0.16594	10.93011
H63	12.57262	0.95575	11.66483
H64	13.00106	-0.76395	11.46524
H65	13.66352	0.46730	10.36268
O66	10.03199	-0.37381	7.41130
C67	10.19503	-0.20230	5.16711
C68	9.60802	-0.84321	6.20543
H69	10.02307	-0.39134	4.11641
H70	8.87988	-1.64105	6.25238
C71	10.93222	0.61479	7.12748
C72	11.07616	0.77160	5.74721
C73	11.93575	1.76995	5.25958
C74	12.60480	2.55757	6.16954
C75	12.45917	2.40362	7.57516
C76	11.58718	1.39985	8.07046
H77	12.06336	1.92554	4.19151
H78	13.26185	3.35511	5.82732
C79	15.90607	2.56554	7.73170
C80	16.71525	3.61873	8.03766
H81	16.82528	4.38642	7.26676
C82	17.64190	3.71977	9.20447
H83	17.60750	4.72245	9.65058
H84	17.40979	2.99994	9.99262
H85	18.67362	3.55125	8.86270
C86	15.77463	1.30871	8.53193
H87	14.82661	0.80251	8.30960
H88	16.58375	0.60756	8.28405
H89	15.81219	1.51080	9.60833
H90	15.43167	2.58117	6.74907
78			
5 - S trans			
Ru1	14.13638	4.50385	8.19827
C12	14.96006	3.44596	10.19622

C13 14.10704 5.56725 6.04826
 C4 12.63533 3.47292 7.98677
 C5 15.67049 7.12393 9.13926
 C6 16.25683 6.18587 11.42219
 H7 16.38531 7.03200 12.11297
 H8 16.90288 5.37312 11.76881
 H9 15.22545 5.82865 11.49269
 C10 11.00180 5.70863 9.46378
 N11 14.28551 7.09118 9.47964
 N12 12.20055 6.47031 9.53288
 C13 13.64629 8.14390 10.26740
 H14 13.94442 9.13455 9.90322
 H15 13.94427 8.06126 11.32500
 C16 18.34959 7.07172 8.37876
 C17 10.70154 4.85276 10.53094
 C18 12.16865 7.84246 10.05296
 H19 11.57452 7.88845 10.97351
 H20 11.70508 8.51541 9.31449
 C21 13.43552 6.08729 9.13271
 C22 10.17843 5.81565 8.33755
 C23 16.05036 7.72687 7.92835
 C24 17.39187 7.67003 7.56186
 H25 17.69656 8.10905 6.61069
 C26 16.62218 6.60727 10.03115
 C27 8.69725 4.16045 9.33794
 C28 9.02808 5.02894 8.29759
 H29 8.38343 5.08087 7.41902
 C30 10.57274 6.67705 7.17593
 H31 10.68629 7.73084 7.46266
 H32 9.82066 6.62947 6.38213
 H33 11.53667 6.35570 6.75249
 C34 17.95370 6.57568 9.61913
 H35 18.70155 6.15434 10.29258
 C36 9.54175 4.08610 10.44582
 H37 9.30004 3.39865 11.25779
 C38 15.07704 8.49576 7.08593
 H39 14.04842 8.14133 7.20091
 H40 15.32954 8.41598 6.02420
 H41 15.11123 9.56090 7.35861
 C42 11.64817 4.70837 11.68429
 H43 12.57264 4.19824 11.37163
 H44 11.19521 4.12633 12.49310
 H45 11.95270 5.68119 12.09332
 C46 7.45347 3.32417 9.27381
 H47 7.14410 3.14213 8.23887
 H48 6.61556 3.81835 9.78199
 H49 7.59860 2.35381 9.76202
 C50 19.77471 6.96246 7.92552
 H51 19.92189 6.06225 7.31397
 H52 20.46512 6.89626 8.77329
 H53 20.06833 7.82034 7.31013
 H54 11.64377 3.73932 8.36359
 O55 14.97151 2.65501 7.05596
 C56 16.36937 2.33984 6.82999
 H57 16.44388 1.97405 5.79540
 C58 16.83175 1.30596 7.83456
 H59 16.27028 0.36856 7.75832
 H60 17.89338 1.08310 7.67405
 H61 16.69846 1.70568 8.84683
 C62 17.12374 3.64511 6.94753
 H63 17.08131 4.02597 7.97782
 H64 18.17687 3.47709 6.69238
 H65 16.70948 4.40307 6.27365
 O66 13.07476 -1.26502 5.20097
 C67 15.05352 -0.21149 5.41738
 C68 14.40966 -1.28862 4.92133
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 H70 14.75000 -2.14518 4.35732
 C71 12.84736 -0.12906 5.90322
 C72 14.04750 0.58772 6.07964
 C73 13.96670 1.79426 6.79069
 C74 12.71463 2.22282 7.27970
 C75 11.55454 1.44676 7.06389
 C76 11.59711 0.25547 6.37138
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 H78 10.61305 1.82287 7.46276
 78
 5 - S cis
 Ru1 14.14079 4.55401 8.22476
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 C13 16.02150 3.33587 7.37300
 C4 12.56535 3.68080 7.95015

C5 15.65928 7.17553 9.26795
 C6 16.73117 5.72945 11.06987
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 H8 16.72725 4.67006 10.78330
 H9 15.82101 5.88384 11.65623
 C10 10.98662 5.83552 9.54555
 N11 14.35361 6.97220 9.81789
 N12 12.25826 6.36550 9.91808
 C13 13.81288 7.83412 10.87321
 H14 14.06916 8.88377 10.68097
 H15 14.24098 7.55440 11.84634
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 C17 10.41014 4.82010 10.32113
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 C24 17.01903 8.26499 7.61298
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 H31 11.17411 8.36578 8.19610
 H32 10.27663 7.75876 6.79482
 H33 11.88841 7.12652 7.16236
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 C36 9.16517 4.33016 9.93336
 H37 8.71258 3.52506 10.51480
 C38 14.54399 8.67813 7.56795
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 C42 11.11832 4.26421 11.51724
 H43 12.10589 3.86391 11.24924
 H44 10.53059 3.46551 11.98024
 H45 11.28880 5.03610 12.27939
 C46 7.18075 4.23642 8.39861
 H47 6.74536 4.77712 7.55165
 H48 6.45112 4.24085 9.21691
 H49 7.30919 3.18892 8.09432
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 H51 19.60979 7.19376 6.61439
 H52 20.31989 7.64653 8.16662
 H53 19.60918 8.88703 7.11383
 H54 12.22928 2.90627 8.65460
 O55 13.44203 5.39331 6.05439
 C56 14.30648 5.43226 4.85743
 H57 13.77867 6.06005 4.12826
 C58 14.49901 4.04153 4.29705
 H59 13.54941 3.58800 3.99232
 H60 15.14024 4.10134 3.41031
 H61 14.98725 3.40053 5.03972
 C62 15.59343 6.10984 5.24588
 H63 16.11919 5.53759 6.01972
 H64 16.24039 6.16820 4.36282
 H65 15.41543 7.12833 5.60375
 O66 9.40305 5.01910 3.63027
 C67 11.32278 6.19717 3.72396
 C68 10.14890 6.01742 3.07913
 H69 12.06261 6.94758 3.48287
 H70 9.70184 6.51272 2.22894
 C71 10.11679 4.54276 4.68268
 C72 11.34102 5.22820 4.79281
 C73 12.19438 4.85707 5.84055
 C74 11.75711 3.90862 6.77332
 C75 10.52041 3.24979 6.59862
 C76 9.68396 3.54055 5.53923
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 H78 10.23045 2.50865 7.34142
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 5 - TS
 Ru1 14.07581 4.26011 8.73959
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 C13 14.38649 4.60996 6.40925
 C4 12.55423 3.26179 8.65860
 C5 15.65475 7.02074 9.15274
 C6 15.83674 6.80894 11.67604

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 H8 16.39836 6.14548 12.34137
 H9 14.79950 6.46169 11.67762
 C10 10.89312 5.83897 9.12743
 N11 14.23315 7.08905 9.26622
 N12 12.12332 6.55065 9.16085
 C13 13.55125 8.33719 9.61056
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 H15 13.68837 8.55963 10.68052
 C16 18.42138 6.84510 8.89449
 C17 10.37440 5.36308 10.33856
 C18 12.10545 8.01589 9.25981
 H19 11.38682 8.33694 10.02308
 H20 11.79813 8.45227 8.29664
 C21 13.37851 6.05184 9.08817
 C22 10.23800 5.64693 7.90660
 C23 16.23889 7.24400 7.89561
 C24 17.62266 7.13086 7.78975
 H25 18.08880 7.28047 6.81471
 C26 16.43486 6.82023 10.30160
 C27 8.48179 4.45660 9.10656
 C28 9.02829 4.95274 7.92315
 H29 8.50758 4.77886 6.97970
 C30 10.85240 6.10798 6.61954
 H31 10.93412 7.20211 6.57066
 H32 10.25037 5.78465 5.76404
 H33 11.86695 5.70194 6.49228
 C34 17.81444 6.71941 10.14263
 H35 18.43287 6.54399 11.02408
 C36 9.16663 4.67026 10.30317
 H37 8.75547 4.27398 11.23268
 C38 15.44032 7.68952 6.70642
 H39 14.37109 7.48109 6.80907
 H40 15.77802 7.18479 5.79618
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 C42 11.14531 5.52401 11.61453
 H43 12.06045 4.91114 11.60363
 H44 10.54393 5.22079 12.47716
 H45 11.47047 6.56092 11.77388
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 H48 6.33768 4.39250 9.30384
 H49 7.15749 2.93455 9.86602
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 H54 11.63293 3.51920 9.19622
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 H59 12.77196 0.05641 10.07669
 H60 14.00597 -0.47418 11.23446
 H61 13.72738 1.26838 10.97833
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 H63 16.17494 1.62603 10.38495
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 C68 13.08931 -1.76689 5.53938
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 C72 13.15264 0.05370 6.81983
 C73 13.36971 1.14825 7.67005
 C74 12.45608 2.20766 7.65772
 C75 11.30028 2.14602 6.84576
 C76 11.06958 1.08872 5.98799
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 H78 10.58274 2.96343 6.91475
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 5 - P
 Ru1 13.94582 4.49101 8.21109
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 C13 13.96016 5.50355 6.05666
 C4 12.42418 3.47622 8.08024
 C5 15.66439 7.00892 9.15652
 C6 16.17106 6.02715 11.44169
 H7 16.32162 6.85448 12.15042
 H8 16.77662 5.18232 11.78436

H9 15.12432 5.71388 11.49033
 C10 10.92700 5.81640 9.51162
 N11 14.27516 7.04334 9.48346
 N12 12.15223 6.53768 9.52298
 C13 13.68192 8.13333 10.25778
 H14 14.05070 9.10215 9.90107
 H15 13.94931 8.03121 11.32205
 C16 18.35477 6.87710 8.45415
 C17 10.60800 5.05049 10.63881
 C18 12.19511 7.92360 10.00630
 H19 11.57781 8.03333 10.90545
 H20 11.80032 8.60273 9.23436
 C21 13.37070 6.08952 9.14193
 C22 10.08913 5.88798 8.39345
 C23 16.08528 7.59636 7.95218
 C24 17.43238 7.50117 7.61616
 H25 17.77108 7.93222 6.67296
 C26 16.57868 6.45442 10.06396
 C27 8.57134 4.34567 9.51164
 C28 8.91484 5.13901 8.41727
 H29 8.25892 5.15756 7.54588
 C30 10.48322 6.68472 7.18696
 H31 10.63966 7.74460 7.42749
 H32 9.71053 6.62998 6.41388
 H33 11.42458 6.31376 6.75517
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 H35 18.63564 5.93596 10.36726
 C36 9.41607 4.32845 10.62121
 H37 9.15052 3.72200 11.48971
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 H39 14.10944 8.07446 7.18664
 H40 15.41903 8.28518 6.02824
 H41 15.22045 9.45599 7.34161
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 H43 12.48667 4.43596 11.49660
 H44 11.11695 4.40613 12.62729
 H45 11.86456 5.94593 12.16396
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 H47 7.57497 2.53576 8.95352
 H48 6.53451 3.96257 8.90872
 H49 6.98154 3.23531 10.46648
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 H51 19.93177 5.84095 7.42366
 H52 20.45353 6.65023 8.90416
 H53 20.11786 7.59560 7.43928
 H54 11.49810 3.67006 8.62578
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 H57 11.22157 -0.38544 9.58496
 C58 9.42739 0.45626 10.42129
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 C62 11.76538 1.33000 10.76144
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 H65 12.74807 1.49224 10.30071
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 H69 10.24268 -1.59714 7.65125
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 C72 11.78530 -0.05397 7.02984
 C73 11.63488 1.17332 7.68820
 C74 12.50900 2.22820 7.35597
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 H20 11.40931 8.19653 8.49714
 C21 13.40239 6.08045 8.92735
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 C23 15.93945 7.89336 7.67571
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 C28 9.28380 4.23420 8.03247
 H29 8.77168 3.97944 7.10278
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 H32 10.23503 5.33439 5.85815
 H33 11.82005 5.74611 6.53518
 C34 17.74152 7.07387 9.64703
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 C36 9.56634 3.94049 10.39653
 H37 9.27223 3.45811 11.33062
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 H39 13.99321 8.05655 6.73793
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 H49 7.31129 2.49148 10.16208
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 H53 19.96158 8.07170 7.26772
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 H59 9.92249 0.94518 11.36166
 H60 11.20943 -0.05814 12.07765
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 O66 10.50071 -0.24580 4.86757
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 C68 9.73671 -0.93725 5.76769
 H69 9.40202 -0.85732 7.91583
 H70 9.12711 -1.72267 5.34416
 C71 11.18020 0.68632 5.57915
 C72 10.85914 0.58557 6.93856
 C73 11.44859 1.48006 7.83897
 C74 12.35781 2.45112 7.34760
 C75 12.62184 2.50763 5.95366
 C76 12.04578 1.63698 5.05195
 H77 12.24562 1.68916 3.98627
 H78 13.28931 3.29323 5.60520
 C79 15.86874 2.62150 7.24853
 C80 16.69145 3.56943 7.77243
 H81 16.83165 4.47944 7.17792
 C82 17.60496 3.39848 8.94145
 H83 17.64986 4.31046 9.54834
 H84 17.30704 2.57571 9.59631
 H85 18.62261 3.20035 8.57329
 C86 15.68400 1.24069 7.78499
 H87 14.70039 0.84430 7.50468
 H88 16.43862 0.56152 7.36427
 H89 15.76963 1.20883 8.87653
 H90 15.41427 2.84356 6.28264
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Ru1 14.23217 4.42841 8.27453
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 H8 16.77256 5.22530 11.97275
 H9 15.11775 5.72316 11.64324
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 H51 19.97038 5.93153 7.65109
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 H53 20.15383 7.68582 7.67637
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 C56 16.60230 2.33546 7.01217
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 H63 17.23804 4.05596 8.15198
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 C71 13.34739 -0.21185 5.87771
 C72 12.03677 0.12469 6.25317
 C73 11.83204 1.31527 6.94631
 C74 12.93063 2.12887 7.24258
 C75 14.23962 1.73538 6.83543
 C76 14.47278 0.55628 6.14695
 H77 10.83985 1.63312 7.26535
 H78 15.45636 0.23219 5.82576
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 H9 15.48920 5.39719 12.04432
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 H47 7.27219 4.70166 6.49409
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 H52 20.51491 7.09327 9.35416
 H53 20.03398 8.46519 8.33469
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 H57 14.74113 6.12934 4.45610
 C58 15.32113 4.04425 4.49730
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 H64 17.12009 6.00922 5.14689
 H65 16.11959 6.89247 6.31294
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 C74 12.04269 4.01602 6.52978
 C75 12.78624 4.88681 5.69292
 C76 12.28036 5.35153 4.48870
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 H78 12.81908 6.02834 3.83450
 78
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 H9 14.49882 6.57005 11.75515
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 N12 12.10936 6.61441 8.95856
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 C17 10.23568 5.46737 9.97317
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 H20 11.89912 8.50506 8.03467
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 H35 18.14572 6.15152 11.41719
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 H53 20.34624 6.51537 8.48532
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 C58 16.23003 -0.07288 9.43735
 H59 15.53234 -0.89211 9.23122
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 H63 16.76086 2.62708 9.81271
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 C71 12.67984 -0.12285 6.14881
 C72 11.62471 0.78581 5.98359
 C73 11.59896 1.92860 6.78394
 C74 12.66713 2.17422 7.64632
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 H9 15.72687 5.43580 11.30445
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 N11 14.45153 6.83767 9.57802
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 H20 11.93579 8.29311 9.76664
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 C24 17.24632 7.93589 7.43062
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 C26 16.87446 6.48298 9.79239
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 C28 9.13669 5.27548 8.24862
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 C30 10.95536 6.75029 7.33021
 H31 11.34267 7.70260 7.71452
 H32 10.20381 6.97788 6.56790
 H33 11.79833 6.24558 6.83410
 C34 18.14932 6.67139 9.25402
 H35 19.00825 6.26636 9.79117
 C36 9.34975 4.17264 10.36817
 H37 8.94441 3.50518 11.13101
 C38 14.79184 8.42392 7.24416
 H39 14.14835 7.67725 6.76297
 H40 15.13479 9.11936 6.47162
 H41 14.17263 8.98884 7.95452
 C42 11.44180 4.39869 11.76079
 H43 12.31626 3.80577 11.45043
 H44 10.86872 3.81294 12.48723
 H45 11.83502 5.28595 12.27268
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 H47 7.33176 3.05979 8.13264
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 H52 20.50306 7.38012 8.24837
 H53 19.86281 8.53731 7.06493
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 H57 11.30205 -0.67808 9.88702
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 H59 9.33503 -0.25104 8.34278
 H60 8.78283 -0.72785 9.96254
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 H63 10.15760 1.68142 11.44555
 H64 10.22947 0.00248 12.03548
 H65 11.73336 0.91203 11.72829
 O66 12.91968 -1.62137 5.63497
 C67 14.07593 -0.02662 4.52895
 C68 13.71835 -1.32787 4.55653
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 C71 12.77074 -0.46230 6.31729
 C72 13.46480 0.57539 5.68528
 C73 13.40898 1.85196 6.24521
 C74 12.66001 2.05274 7.40929
 C75 11.99137 0.95312 8.03671
 C76 12.02740 -0.31928 7.48201
 H77 13.89345 2.70652 5.77344
 H78 11.52445 -1.17704 7.91473
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 C6 15.86015 7.20554 11.46957
 H7 15.72706 8.21435 11.88744
 H8 16.51972 6.65195 12.14538

H9 14.89438 6.69188 11.46945
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 N11 14.24278 7.21069 9.07876
 N12 12.27467 6.27925 9.06067
 C13 13.33854 8.32844 9.35613
 H14 13.26002 8.98081 8.47087
 H15 13.70919 8.92831 10.19546
 C16 18.42577 7.53923 8.68819
 C17 10.69618 4.54721 9.77014
 C18 12.03753 7.59810 9.66358
 H19 11.86888 7.48589 10.74658
 H20 11.15250 8.07082 9.22239
 C21 13.58556 6.05345 8.83045
 C22 10.63812 5.43835 7.48774
 C23 16.20939 7.64603 7.68502
 C24 17.59979 7.70160 7.57970
 H25 18.04398 7.89048 6.60124
 C26 16.45569 7.29154 10.09697
 C27 9.07741 3.69830 8.15711
 C28 9.58636 4.57881 7.19940
 H29 9.16466 4.57378 6.19217
 C30 11.20458 6.34399 6.43697
 H31 11.32391 7.37454 6.79884
 H32 10.55794 6.36929 5.55382
 H33 12.20215 6.00065 6.12092
 C34 17.83617 7.36710 9.94065
 H35 18.47069 7.28398 10.82438
 C36 9.63278 3.70636 9.43164
 H37 9.24451 3.02144 10.18712
 C38 15.36240 7.98616 6.49608
 H39 14.35809 7.55918 6.55494
 H40 15.81252 7.61157 5.57163
 H41 15.27504 9.07885 6.40897
 C42 11.27991 4.51035 11.15168
 H43 12.33865 4.79829 11.16820
 H44 11.21462 3.49589 11.56579
 H45 10.73175 5.17529 11.83299
 C46 7.97700 2.75041 7.78569
 H47 8.30272 2.07330 6.98311
 H48 7.09384 3.28460 7.41390
 H49 7.66581 2.13465 8.63671
 C50 19.91814 7.53144 8.54633
 H51 20.29262 6.50242 8.46314
 H52 20.40825 7.98262 9.41653
 H53 20.24399 8.07060 7.65046
 H54 13.05820 2.97586 9.64610
 O55 12.06728 1.00765 9.66896
 C56 11.49284 -0.06084 10.42291
 H57 11.47643 -0.96737 9.79546
 C58 10.09040 0.30106 10.87305
 H59 9.43443 0.53617 10.02708
 H60 9.64205 -0.52474 11.43672
 H61 10.13071 1.18092 11.52844
 C62 12.43496 -0.26568 11.58757
 H63 12.52130 0.66626 12.15993
 H64 12.06568 -1.05495 12.25116
 H65 13.43479 -0.53827 11.23543
 O66 9.79957 0.06976 5.51643
 C67 10.74844 1.75192 4.34062
 C68 9.87577 0.72365 4.30668
 H69 10.99132 2.42027 3.52554
 H70 9.24066 0.32063 3.53103
 C71 10.65537 0.71362 6.34393
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 C73 12.18282 2.56557 6.38422
 C74 12.41821 2.31465 7.74194
 C75 11.74686 1.20729 8.37648
 C76 10.86347 0.39278 7.67723
 H77 12.70221 3.40029 5.91729
 H78 10.34240 -0.44562 8.12598
 C79 15.84635 2.25768 7.78406
 C80 16.72404 3.30311 7.80319
 H81 16.80397 3.88764 6.88292
 C82 17.75240 3.58289 8.85108
 H83 17.78803 4.65348 9.09501
 H84 17.56977 3.03864 9.78068
 H85 18.74538 3.30712 8.46707
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 H87 14.76346 0.69520 8.78893
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7 - S trans
Ru1 14.19053 4.49049 8.19460
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H7 16.37923 7.04285 12.13210
H8 16.91746 5.39075 11.78524
H9 15.23467 5.82612 11.50905
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H15 13.91837 8.02796 11.34210
C16 18.34430 7.11136 8.39768
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C18 12.14660 7.77309 10.07080
H19 11.55355 7.79774 10.99283
H20 11.66573 8.44078 9.33880
C21 13.45197 6.05317 9.13858
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C24 17.38019 7.70082 7.58268
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H57 16.52607 1.95498 5.79148
C58 16.94425 1.34075 7.83605
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H60 18.00182 1.11347 7.65877
H61 16.83015 1.76146 8.84213
C62 17.20533 3.66383 6.89658
H63 17.16645 4.06874 7.91830
H64 18.25799 3.50004 6.63734
H65 16.77796 4.40261 6.20994
O66 10.88479 -0.68025 6.03852
C67 12.84255 -1.44752 5.21451
C68 11.51293 -1.67095 5.35413
H69 13.55153 -2.08982 4.70988
H70 10.87581 -2.48018 5.02461
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C72 13.10063 -0.19696 5.86678
C73 14.24328 0.58833 6.08300
C74 14.07993 1.77223 6.77949
C75 12.80931 2.19241 7.27041
C76 11.67494 1.40086 7.05298
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78
7 - S cis

Ru1 14.25808 4.65607 8.08652
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H8 17.14002 4.95865 10.44893
H9 16.02009 5.94749 11.35586
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7 - TS
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 H20 11.99720 8.44873 8.02512
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 H37 8.51385 4.49534 10.80379
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 H39 14.61062 7.19560 6.79050
 H40 16.06432 6.76197 5.90236
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 H44 10.16683 5.42902 12.20405
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 H53 20.39681 6.38471 8.27898
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 H57 15.87954 0.59144 7.38030
 C58 15.96384 -0.45680 9.28837
 H59 15.20975 -1.21349 9.04425
 H60 16.95598 -0.89266 9.12829
 H61 15.86263 -0.20762 10.35166
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 H63 16.61840 2.19023 9.89055
 H64 17.81772 1.51990 8.75622
 H65 16.67219 2.76997 8.20064
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 C68 10.68302 -0.49160 4.64023
 H69 12.29370 -1.93389 4.85799
 H70 10.00059 -0.84698 3.88161
 C71 11.32515 0.96129 6.13015
 C72 12.27484 -0.06616 6.13790
 C73 13.36144 -0.00106 7.02275
 C74 13.46449 1.11103 7.84642
 C75 12.49663 2.15285 7.79998
 C76 11.37794 2.04932 6.97351
 H77 14.10058 -0.79697 7.05805
 H78 10.59963 2.80887 6.99025
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 H9 15.49258 5.91998 10.82115
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 N11 14.06681 7.23716 9.15155
 N12 12.06249 6.52335 9.64015
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 H20 11.47242 8.55152 9.53973
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 H44 11.93923 4.19330 12.77318
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 H47 7.83332 2.12236 9.86019
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 H49 7.55390 2.69016 11.51203
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 H51 19.27042 6.68751 5.92551
 H52 19.94835 7.71399 7.19060
 H53 19.14715 8.44307 5.78381
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 C58 10.15364 0.23286 10.80597
 H59 9.34514 -0.27658 10.27057
 H60 10.44138 -0.37386 11.67161
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 H63 12.10446 2.14705 11.00193
 H64 12.86099 0.59471 11.43325
 H65 13.30350 1.41324 9.92160
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 C72 12.45112 -0.04778 5.77355
 C73 11.69168 -0.00924 6.94822
 C74 11.61170 1.18079 7.65383
 C75 12.27804 2.36188 7.20479
 C76 13.01739 2.32578 6.00630
 H77 11.15239 -0.88370 7.30583
 H78 13.47380 3.22609 5.59695
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 C6 16.34598 7.06726 11.13625

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 H8 17.17629 6.53266 11.61129
 H9 15.43970 6.48253 11.31779
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 N12 12.27140 6.21281 9.28645
 C13 13.36687 8.22283 9.72565
 H14 13.51446 9.18959 9.22965
 H15 13.61751 8.33674 10.79134
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 H31 11.22029 7.05866 6.63162
 H32 10.95211 5.65002 5.59445
 H33 12.44829 5.78952 6.53114
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 H35 18.74092 7.30722 9.93363
 C36 9.48784 3.81763 9.75979
 H37 9.00556 3.27006 10.57098
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 H45 11.02673 5.75989 11.84260
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 H49 7.35070 2.42098 9.05842
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 H51 19.93860 6.99035 6.90398
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 H53 19.73995 8.73208 6.71990
 H54 13.05282 2.74171 9.72919
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 H57 11.06164 -1.02177 9.33650
 C58 9.85826 0.32794 10.53118
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 H63 12.28258 0.16446 11.87488
 H64 11.55509 -1.45881 11.77457
 H65 13.01597 -1.07165 10.83514
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 H70 9.83043 1.75522 2.90119
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 C72 10.64724 1.09391 6.02471
 C73 10.77457 0.62177 7.33797
 C74 11.69292 1.24520 8.17330
 C75 12.48698 2.36285 7.72623
 C76 12.38124 2.77985 6.39161
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 H78 12.99762 3.60025 6.03122
 C79 15.89600 2.15837 8.33988
 C80 16.78635 3.18244 8.50643
 H81 17.03746 3.75947 7.61246
 C82 17.65330 3.40399 9.70405
 H83 17.81696 4.47523 9.87676
 H84 17.23132 2.97648 10.61682
 H85 18.63993 2.95191 9.52482
 C86 15.60674 1.09626 9.35608
 H87 14.66026 0.58653 9.14303
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 8 - S trans
 Ru1 14.13790 4.51435 8.18940
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 C5 15.68572 7.11830 9.15625
 C6 16.29402 6.13937 11.41757
 H7 16.44390 6.97034 12.12233
 H8 16.93487 5.31212 11.73879
 H9 15.25954 5.79359 11.49686
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 N11 14.30337 7.08138 9.50847
 N12 12.21748 6.46652 9.57434
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 H14 13.97244 9.11891 9.96588
 H15 13.98890 8.02560 11.37186
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 C17 10.71867 4.84737 10.57165
 C18 12.19565 7.82918 10.12030
 H19 11.61432 7.85959 11.04963
 H20 11.72318 8.51632 9.40081
 C21 13.44615 6.08652 9.15372
 C22 10.17722 5.84272 8.39677
 C23 16.05680 7.74642 7.95558
 C24 17.39483 7.69495 7.57630
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 C30 10.56915 6.71055 7.23913
 H31 10.69597 7.76029 7.53515
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 H33 11.52646 6.38476 6.80413
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 H35 18.72575 6.12252 10.26409
 C36 9.54411 4.10282 10.49849
 H37 9.30324 3.41146 11.30723
 C38 15.07896 8.53583 7.13770
 H39 14.04844 8.19087 7.26386
 H40 15.31453 8.46692 6.07138
 H41 15.12895 9.59697 7.42317
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 H47 7.06293 3.26762 8.33183
 H48 6.60995 3.88597 9.92335
 H49 7.56329 2.40620 9.80133
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 H51 19.91652 6.08500 7.27123
 H52 20.47722 6.88639 8.74221
 H53 20.07015 7.84220 7.30230
 H54 11.63678 3.75724 8.31308
 O55 14.99204 2.69954 7.03050
 C56 16.38500 2.37540 6.80350
 H57 16.45880 1.98953 5.77447
 C58 16.84900 1.35119 7.81785
 H59 16.27680 0.41916 7.75948
 H60 17.90631 1.11564 7.65034
 H61 16.72719 1.76330 8.82649
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 H63 17.10374 4.07488 7.92603
 H64 18.19752 3.50538 6.64780
 H65 16.73111 4.42915 6.21830
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 H70 8.70445 -0.06997 6.67844
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 C72 11.63199 1.41168 6.96051
 C73 12.73583 2.24989 7.23066
 C74 13.99312 1.82866 6.74853
 C75 14.15929 0.63918 6.03144
 C76 13.06457 -0.17949 5.76985
 H77 13.17406 -1.10630 5.21423
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C5 15.81789 6.72468 9.92560
C6 16.24084 4.81142 11.55483
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H8 16.14966 3.82965 11.07343
H9 15.25514 5.03118 11.97374
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N12 12.27128 6.49701 9.73270
C13 13.77618 7.50432 11.20149
H14 14.27432 8.47756 11.28466
H15 13.85450 6.99495 12.17326
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C17 10.09919 5.39836 9.57401
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C22 10.79682 6.99049 7.85244
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C24 17.66188 7.82176 8.83914
H25 18.04018 8.59946 8.17325
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C28 9.58211 6.79001 7.20438
H29 9.38956 7.31514 6.26691
C30 11.82073 7.91708 7.26822
H31 12.07775 8.73794 7.95185
H32 11.45326 8.36143 6.33722
H33 12.75392 7.38509 7.03870
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H35 18.74419 5.25583 10.76039
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H39 14.64007 8.18486 7.76957
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H47 7.46905 5.74999 5.89583
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H49 6.86922 4.75173 7.23428
C50 20.01658 6.98115 9.08393
H51 20.22243 6.48249 8.12793
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H53 20.36075 8.01744 8.98809
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H57 14.96669 6.53727 4.54976
C58 15.49894 4.44093 4.40562
H59 14.64487 4.16116 3.78037
H60 16.35999 4.60564 3.74790
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C68 8.80775 3.25565 5.14038
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C72 10.80925 4.01607 5.73372
C73 12.05349 4.37524 6.29120
C74 12.88800 5.20125 5.52387
C75 12.48962 5.70995 4.28203
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8 - TS

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H15 13.85048 8.11321 11.19154
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C18 12.21343 7.94265 9.74964
H19 11.52346 8.12105 10.58210
H20 11.88433 8.55914 8.89715
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C23 16.16615 7.52400 7.92696
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H32 10.76058 6.80286 5.71349
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H64 16.97276 0.30768 10.49964
H65 17.15564 1.26792 9.01138
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C72 11.61038 1.85218 6.49102
C73 12.67600 2.12586 7.38379
C74 13.59249 1.07468 7.59517
C75 13.45208 -0.17411 6.96709
C76 12.41053 -0.42875 6.08858
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 H33 10.65235 5.75767 7.19273
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 H37 10.08999 3.52701 12.56908
 C38 14.26234 8.56759 6.47814
 H39 13.36168 8.50514 7.09771
 H40 14.04880 7.99784 5.56753
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 H45 12.84562 5.70242 12.34108
 C46 7.65585 3.43822 11.33694
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 H51 19.55769 7.01835 6.09815
 H52 20.01270 8.26129 7.26339
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 H57 10.05954 -0.56016 8.95600
 C58 8.69090 1.03876 8.45384
 H59 8.86220 0.96902 7.37367
 H60 7.76741 0.49858 8.69271
 H61 8.55951 2.09948 8.70602
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 H63 9.62544 1.59764 11.05149
 H64 8.74955 0.04417 11.02832
 H65 10.51609 0.07857 11.25228
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 C67 14.69427 2.52563 5.87971
 C68 15.10627 1.75760 4.84200
 H69 15.16733 3.45743 6.18276
 H70 15.91089 1.87484 4.12997
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 C72 13.57805 1.84081 6.45800
 C73 12.69958 2.09978 7.54103
 C74 11.74457 1.08960 7.83391
 C75 11.60364 -0.04198 7.01300
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 H77 12.33515 -1.13184 5.29313
 H78 10.83618 -0.77899 7.22309
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 8 - Pa
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 C12 15.23920 3.80636 10.04641
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 C4 12.94297 3.49758 8.19179

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 C6 16.04046 6.70767 11.25972
 H7 15.99987 7.59290 11.91137
 H8 16.74492 5.99827 11.70479
 H9 15.06072 6.22105 11.25999
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 N11 14.16582 7.33174 9.13060
 N12 12.19972 6.41000 9.28361
 C13 13.39747 8.30596 9.90771
 H14 13.55203 9.31876 9.51761
 H15 13.71771 8.28619 10.96141
 C16 18.29483 7.63672 8.34700
 C17 10.80138 4.65382 10.20417
 C18 11.97620 7.79387 9.72352
 H19 11.37722 7.81485 10.64145
 H20 11.43167 8.34906 8.94371
 C21 13.46722 6.20523 8.85476
 C22 10.31575 5.55396 7.97654
 C23 15.99060 8.05473 7.68047
 C24 17.36149 8.09835 7.42400
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 C28 9.27289 4.63698 7.86458
 H29 8.68675 4.61540 6.94391
 C30 10.60351 6.52557 6.87213
 H31 10.28189 7.54235 7.13843
 H32 10.06624 6.24284 5.96054
 H33 11.67407 6.56516 6.62859
 C34 17.83924 7.17641 9.58320
 H35 18.56188 6.85802 10.33614
 C36 9.73668 3.76991 10.05175
 H37 9.50500 3.07550 10.86125
 C38 15.04148 8.69462 6.71301
 H39 13.99628 8.45701 6.93021
 H40 15.23813 8.36433 5.68834
 H41 15.16922 9.78533 6.74666
 C42 11.65919 4.62109 11.43394
 H43 12.64982 4.18520 11.22198
 H44 11.18775 4.02282 12.22130
 H45 11.84820 5.62508 11.83601
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 H57 12.15416 -0.74187 9.80639
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 H59 9.99429 0.48124 10.38959
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 H64 13.23849 -0.55687 12.07710
 H65 14.27281 0.07783 10.76953
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 C68 10.82695 3.04327 4.15657
 H69 12.20715 4.46144 5.08862
 H70 10.55936 3.41112 3.17553
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 C72 11.60155 2.58665 6.19235
 C73 12.14817 2.50945 7.49572
 C74 11.79645 1.35862 8.26099
 C75 10.94487 0.36037 7.76545
 C76 10.39589 0.46467 6.49341
 H77 9.72440 -0.29268 6.09845
 H78 10.70625 -0.50611 8.37386
 C79 15.39468 2.68648 6.66993
 C80 16.29672 3.70670 6.72780
 H81 16.22391 4.46979 5.95015
 C82 17.50661 3.78214 7.60235
 H83 17.60758 4.77829 8.05669
 H84 17.49000 3.05106 8.41362
 H85 18.40647 3.61648 6.99240
 C86 15.45403 1.42569 7.47420

H87	14.46603	0.95812	7.55089	H77	13.28272	-1.14702	5.24944
H88	16.12203	0.70032	6.98819	H78	15.15207	0.43884	5.45047
H89	15.81824	1.60745	8.49091	78			
H90	14.66537	2.72338	5.85745	9 - S cis			
78				Ru1	14.06711	4.68174	7.94216
9 - S trans				C12	14.63100	3.47738	9.89821
Ru1	14.09862	4.60705	7.99887	C13	15.86124	3.62478	6.76278
C12	15.17590	3.59348	9.89116	C4	12.52561	3.71436	7.84205
C13	13.80514	5.69078	5.88084	C5	15.54837	7.32450	9.06822
C4	12.65969	3.47362	7.90738	C6	16.82191	5.78197	10.65056
C5	15.50974	7.28978	8.88220	H7	17.66294	6.05550	11.29841
C6	16.33431	6.37670	11.09938	H8	16.97933	4.75649	10.29651
H7	16.46392	7.23165	11.77907	H9	15.90514	5.75671	11.24447
H8	17.05574	5.60709	11.39105	C10	10.96838	5.73774	9.53050
H9	15.33593	5.95678	11.25123	N11	14.29354	7.01616	9.68395
C10	10.98996	5.55192	9.52317	N12	12.24331	6.28400	9.87163
N11	14.16068	7.16668	9.33109	C13	13.78436	7.74606	10.84833
N12	12.12946	6.40374	9.51346	H14	14.00410	8.81718	10.76232
C13	13.50923	8.16373	10.17892	H15	14.26360	7.37216	11.76492
H14	13.70390	9.17608	9.80510	C16	17.92754	7.96136	7.75663
H15	13.89373	8.09717	11.20916	C17	10.44816	4.68274	10.28848
C16	18.11245	7.37150	7.89415	C18	12.29499	7.42494	10.79837
C17	10.84970	4.64784	10.58357	H19	11.87944	7.14565	11.77290
C18	12.04375	7.75688	10.07510	H20	11.69320	8.25779	10.40170
H19	11.52632	7.73637	11.04184	C21	13.40520	6.11533	9.20230
H20	11.47204	8.41043	9.39780	C22	10.23802	6.32034	8.48296
C21	13.35609	6.11529	9.02115	C23	15.54190	8.30009	8.05294
C22	10.07673	5.60900	8.46482	C24	16.73406	8.60094	7.41006
C23	15.75412	7.91864	7.64997	H25	16.73528	9.34432	6.61095
C24	17.06088	7.93033	7.17010	C26	16.73884	6.72726	9.49434
H25	17.26089	8.38970	6.20093	C27	8.41860	4.77370	8.94218
C26	16.55954	6.81682	9.68487	C28	8.97193	5.81883	8.20235
C27	8.84404	3.78794	9.50996	H29	8.40350	6.24842	7.37520
C28	9.00717	4.71515	8.48191	C30	10.81397	7.42666	7.65103
H29	8.30338	4.71859	7.64850	H31	11.11097	8.29374	8.25607
C30	10.30359	6.52716	7.30174	H32	10.08781	7.77098	6.90721
H31	10.36222	7.57938	7.60966	H33	11.71063	7.09021	7.11311
H32	9.49217	6.43984	6.57232	C34	17.91126	7.05291	8.80573
H33	11.24897	6.29090	6.78957	H35	18.84087	6.57110	9.11164
C34	17.85035	6.84783	9.15916	C36	9.17156	4.21637	9.97163
H35	18.67252	6.45772	9.76058	H37	8.75959	3.38361	10.54336
C36	9.76583	3.77404	10.55616	C38	14.26970	8.99925	7.67524
H37	9.65665	3.04025	11.35613	H39	13.51338	8.29390	7.30640
C38	14.67583	8.64255	6.90050	H40	14.44997	9.74111	6.88986
H39	13.67791	8.24332	7.10535	H41	13.81729	9.52344	8.52819
H40	14.83528	8.57404	5.82013	C42	11.24224	4.06289	11.39658
H41	14.68765	9.70771	7.17390	H43	12.24077	3.75616	11.05557
C42	11.89171	4.56075	11.65785	H44	10.72613	3.18570	11.79888
H43	12.82685	4.13332	11.26352	H45	11.39457	4.76686	12.22579
H44	11.55149	3.92760	12.48337	C46	7.03651	4.28179	8.63251
H45	12.14806	5.54694	12.06785	H47	6.88421	4.18651	7.55055
C46	7.70993	2.80668	9.48653	H48	6.27506	4.97573	9.01066
H47	7.33573	2.65556	8.46764	H49	6.84743	3.30305	9.08617
H48	6.86485	3.14808	10.09839	C50	19.18939	8.25401	7.00262
H49	8.02299	1.83385	9.88436	H51	19.20656	7.71096	6.04903
C50	19.49547	7.33131	7.31635	H52	20.07661	7.95032	7.56753
H51	19.63213	6.43635	6.69455	H53	19.28017	9.32116	6.76863
H52	20.26092	7.30346	8.09933	H54	12.30296	2.92517	8.57052
H53	19.68978	8.19987	6.67702	O55	13.09802	5.47653	5.87674
H54	11.67892	3.66655	8.34544	C56	13.78865	5.88749	4.65054
O55	14.98071	2.82992	6.75938	H57	13.09617	6.55839	4.11822
C56	16.36338	2.60306	6.39116	C58	14.13357	4.67829	3.80936
H57	16.35784	2.19717	5.36711	H59	13.24491	4.11865	3.50032
C58	17.00872	1.64235	7.36758	H60	14.65906	5.00528	2.90490
H59	16.51201	0.66639	7.38164	H61	14.79234	4.01471	4.38202
H60	18.05932	1.48853	7.09522	C62	15.00427	6.67446	5.06304
H61	16.95706	2.06649	8.37729	H63	15.68416	6.05224	5.65817
C62	17.02646	3.96192	6.38670	H64	15.53677	7.00786	4.16478
H63	17.06337	4.37724	7.40446	H65	14.72555	7.55975	5.64015
H64	18.05618	3.86161	6.02378	O66	9.99334	2.20956	7.43321
H65	16.48529	4.66302	5.74223	C67	8.46539	2.42212	5.78478
O66	10.52375	1.42925	7.56620	C68	8.80369	1.77096	6.92051
C67	10.62022	-0.55317	6.48800	H69	7.57799	2.25537	5.18871
C68	9.84717	0.29331	7.20167	H70	8.32553	0.98234	7.48410
H69	10.32154	-1.51205	6.08626	C71	10.43072	3.17319	6.59082
H70	8.81971	0.24769	7.53375	C72	9.52742	3.36283	5.54113
C71	11.77296	1.29590	7.06482	C73	9.82492	4.33118	4.57674
C72	11.90641	0.08533	6.37908	C74	11.01067	5.04876	4.67236
C73	13.14030	-0.21634	5.79367	C75	11.90636	4.81119	5.72352
C74	14.19709	0.67868	5.90826	C76	11.62643	3.88045	6.73485
C75	14.02942	1.88085	6.60588	H77	9.14469	4.52295	3.75027
C76	12.80272	2.23075	7.20808	H78	11.24193	5.79093	3.91414

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9 - TS

Ru1 14.14558 4.23871 8.51133
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C13 14.44393 4.77247 6.22329
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C5 15.69059 7.04660 9.07741
C6 15.93663 6.67450 11.57658
H7 15.94461 7.65094 12.08276
H8 16.53679 5.98527 12.17899
H9 14.91289 6.28923 11.57256
C10 10.96309 5.70662 9.04941
N11 14.27030 7.04572 9.22506
N12 12.17417 6.44826 9.13733
C13 13.55873 8.24515 9.66971
H14 13.92959 9.12772 9.13515
H15 13.72108 8.40024 10.74785
C16 18.45585 7.02219 8.75771
C17 10.47123 5.10850 10.21671
C18 12.11400 7.90110 9.33910
H19 11.40956 8.14377 10.14332
H20 11.76321 8.39314 8.41874
C21 13.44162 5.99629 8.99789
C22 10.30527 5.60150 7.82035
C23 16.23614 7.38050 7.82757
C24 17.62086 7.34083 7.68917
H25 18.05876 7.57589 6.71795
C26 16.50350 6.80965 10.19535
C27 8.60721 4.24074 8.91592
C28 9.12666 4.85790 7.77982
H29 8.61372 4.73633 6.82423
C30 10.88590 6.20999 6.58065
H31 10.98397 7.30041 6.66390
H32 10.25163 6.00230 5.71257
H33 11.88549 5.80356 6.37168
C34 17.88280 6.78659 10.00536
H35 18.52708 6.58181 10.86155
C36 9.28957 4.37797 10.12639
H37 8.89984 3.88632 11.01894
C38 15.39102 7.87049 6.68888
H39 14.34885 7.54538 6.76067
H40 15.77542 7.50612 5.73110
H41 15.41075 8.96972 6.65882
C42 11.25051 5.18091 11.49619
H43 12.19322 4.61756 11.41807
H44 10.67584 4.76480 12.32951
H45 11.52693 6.21171 11.75527
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H48 6.46654 4.06793 9.10921
H49 7.35139 2.60338 9.54177
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H52 20.48020 7.13118 9.49869
H53 20.29023 7.65099 7.81162
H54 11.71755 3.42152 8.96186
O55 14.09022 0.86264 8.93219
C56 14.84449 -0.28915 9.32094
H57 15.31947 -0.71874 8.42321
C58 13.93508 -1.30733 9.98215
H59 13.12374 -1.62804 9.31953
H60 14.50460 -2.19492 10.28126
H61 13.48746 -0.86598 10.88055
C62 15.91799 0.21483 10.25832
H63 15.45987 0.71186 11.12113
H64 16.53548 -0.61969 10.61000
H65 16.55840 0.94884 9.75980
O66 11.24437 3.17019 5.91814
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C68 10.67873 2.79560 4.72963
H69 10.69303 1.00611 3.49384
H70 10.07171 3.55323 4.25360
C71 11.96743 2.10686 6.34261
C72 11.86233 1.04624 5.43713
C73 12.52828 -0.14360 5.73706
C74 13.26433 -0.23184 6.90879
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C76 12.70906 2.07118 7.52148
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9 - P

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C13 13.54493 8.28966 9.72784
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C18 12.09941 7.85950 9.95007
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H20 11.40529 8.33567 9.24035
C21 13.30819 6.02921 9.11155
C22 9.97962 5.41481 9.26202
C23 15.39869 7.50577 7.01250
C24 16.62175 7.45586 6.35214
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C26 16.54897 6.91101 9.09291
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C28 8.94073 4.58974 9.69310
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H52 19.95571 7.15879 6.91229
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O55 10.41107 1.18746 8.54202
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H59 10.65241 2.46304 6.16755
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H64 7.28568 1.18044 7.38733
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C73 13.20272 -0.77623 7.17054
C74 11.95064 -0.41731 7.65136
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H78 11.14600 -1.14964 7.66959

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9 - Pa

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 H8 16.98990 5.94884 11.54608
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 C18 11.98247 7.82447 9.97596
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 C24 16.98301 7.63140 7.04498
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 C28 8.71403 4.86035 9.18988
 H29 7.92618 4.80562 8.43599
 C30 10.10674 6.14750 7.53363
 H31 10.38305 7.20805 7.59158
 H32 9.20395 6.06841 6.91975
 H33 10.93048 5.64614 7.00505
 C34 17.77764 6.93478 9.19400
 H35 18.60324 6.68119 9.86106
 C36 9.53797 4.30655 11.37416
 H37 9.40462 3.81539 12.33941
 C38 14.57614 8.11839 6.59434
 H39 13.57610 7.83786 6.93800
 H40 14.68827 7.71532 5.58166
 H41 14.63088 9.21396 6.52546
 C42 11.85798 4.98420 12.10797
 H43 12.72839 4.43287 11.72058
 H44 11.55427 4.51941 13.05107
 H45 12.21081 6.00115 12.32799
 C46 7.19958 3.59469 10.73967
 H47 6.95869 2.81067 10.00847
 H48 6.37699 4.31997 10.70877
 H49 7.19962 3.13358 11.73352
 C50 19.43559 7.18400 7.31085
 H51 19.53909 6.28290 6.68822
 H52 20.18865 7.13088 8.10430
 H53 19.66705 8.04510 6.67293
 H54 11.68153 3.44315 9.33972
 O55 10.66161 1.15700 9.17552
 C56 9.50685 0.32003 9.28944
 H57 9.80240 -0.73174 9.15503
 C58 8.49647 0.72973 8.23762
 H59 8.89283 0.58869 7.22568
 H60 7.57265 0.14744 8.33114
 H61 8.25884 1.79461 8.36056
 C62 9.01257 0.51045 10.70499
 H63 8.87175 1.57917 10.90008
 H64 8.05903 -0.00815 10.85607
 H65 9.74129 0.12709 11.42587
 O66 14.69433 2.42387 7.07479
 C67 15.01329 0.61136 5.77964
 C68 15.50934 1.81392 6.14246
 H69 15.46443 -0.06929 5.07026
 H70 16.39878 2.36858 5.86624
 C71 13.65630 1.58692 7.27934
 C72 13.78796 0.43261 6.51916
 C73 12.76769 -0.51550 6.63664
 C74 11.70705 -0.27830 7.50409
 C75 11.62087 0.90196 8.26611
 C76 12.60018 1.91360 8.12668
 H77 12.79053 -1.43783 6.06159
 H78 10.93142 -1.03352 7.58512
 C79 18.13690 4.15371 5.09815
 C80 18.54027 3.68429 6.28584
 H81 19.48138 3.12929 6.30699
 C82 17.84398 3.81636 7.59869
 H83 18.47723 4.31645 8.34439
 H84 16.91210 4.39183 7.53676

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 C86 16.89346 4.92543 4.79877
 H87 17.13042 5.86968 4.28904
 H88 16.22942 4.36828 4.12231
 H89 16.30676 5.16774 5.69162
 H90 18.77850 3.94737 4.23854
 78
 10 - S trans
 Ru1 14.14498 4.54708 8.22211
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 C13 14.07787 5.61418 6.07925
 C4 12.64023 3.46916 7.99293
 C5 15.61936 7.11324 9.17725
 C6 16.25203 6.12412 11.42577
 H7 16.42009 6.95585 12.12529
 H8 16.88814 5.29049 11.73921
 H9 15.21503 5.78984 11.52134
 C10 10.98171 5.63231 9.52734
 N11 14.24087 7.07860 9.54509
 N12 12.16607 6.41520 9.61491
 C13 13.59606 8.10034 10.36625
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 H15 13.91317 8.00187 11.41687
 C16 18.27205 7.00777 8.33290
 C17 10.70251 4.73670 10.56711
 C18 12.11921 7.77271 10.17062
 H19 11.54219 7.78353 11.10302
 H20 11.62843 8.45469 9.45859
 C21 13.40086 6.06914 9.18801
 C22 10.15462 5.75543 8.40537
 C23 15.97754 7.72764 7.96494
 C24 17.30551 7.64475 7.55643
 H25 17.59073 8.08745 6.60098
 C26 16.58585 6.56071 10.03175
 C27 8.70753 4.04364 9.35878
 C28 9.01880 4.94955 8.34496
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 C30 10.53279 6.65323 7.26584
 H31 10.63928 7.69979 7.58039
 H32 9.77582 6.62031 6.47596
 H33 11.49636 6.35216 6.82662
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 H35 18.65998 6.05117 10.22063
 C36 9.55682 3.95172 10.46137
 H37 9.33281 3.23251 11.25052
 C38 14.99562 8.52668 7.16196
 H39 13.96536 8.18262 7.29408
 H40 15.22277 8.46597 6.09332
 H41 15.04931 9.58489 7.45719
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 H43 12.58781 4.08417 11.37562
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 H47 7.17846 3.02285 8.23043
 H48 6.63285 3.64713 9.79016
 H49 7.64720 2.20424 9.73177
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 H51 19.77078 5.96736 7.19577
 H52 20.39305 6.75353 8.65009
 H53 19.97834 7.71888 7.21851
 H54 11.62299 3.67547 8.33070
 O55 15.12266 2.73811 7.00897
 C56 16.50120 2.35577 6.77558
 H57 16.54453 1.96270 5.74669
 C58 16.92841 1.31370 7.78570
 H59 16.33307 0.39668 7.71014
 H60 17.98028 1.05068 7.62350
 H61 16.80968 1.71939 8.79740
 C62 17.29644 3.63671 6.87043
 H63 17.26122 4.03224 7.89580
 H64 18.34355 3.43915 6.61363
 H65 16.89609 4.39742 6.19094
 O66 11.92692 1.31672 6.99765
 C67 14.11335 1.88380 6.82468
 C68 12.87848 2.26870 7.30631
 C69 12.58088 0.34203 6.32707
 C70 13.95786 0.62366 6.17533
 C71 14.76675 -0.29932 5.49101
 C72 14.18224 -1.44815 4.99243
 C73 12.81068 -1.70099 5.16105
 C74 11.98816 -0.80934 5.83162

H75 10.92592 -0.98763 5.97055
 H76 12.38517 -2.61612 4.75599
 H77 14.79412 -2.17158 4.45921
 H78 15.82961 -0.11943 5.35137
 78
 10 - S cis
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 C13 16.13949 3.64274 6.97514
 C4 12.69873 3.93820 7.72068
 C5 15.88620 7.07601 9.47863
 C6 16.73546 5.62490 11.37473
 H7 16.85757 6.27708 12.25140
 H8 17.47380 4.82104 11.45616
 H9 15.74476 5.16286 11.41449
 C10 11.15266 6.00558 9.36121
 N11 14.54104 6.94142 9.94368
 N12 12.41739 6.44142 9.85935
 C13 13.98233 7.70702 11.06035
 H14 14.30803 8.75379 11.01311
 H15 14.32397 7.28443 12.01611
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 C17 10.50500 4.92977 9.98243
 C18 12.47981 7.52859 10.84802
 H19 11.94563 7.24394 11.76190
 H20 11.99701 8.43173 10.44438
 C21 13.62529 6.16289 9.32581
 C22 10.57943 6.68053 8.27491
 C23 16.11121 7.93338 8.38716
 C24 17.40146 8.03468 7.88121
 H25 17.58958 8.68941 7.02867
 C26 16.93802 6.40473 10.11347
 C27 8.70010 5.14043 8.36065
 C28 9.35050 6.23361 7.79467
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 H33 12.20941 7.47344 7.11221
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 C38 14.98394 8.72572 7.79342
 H39 14.28242 8.08076 7.24677
 H40 15.36295 9.47812 7.09303
 H41 14.39927 9.24892 8.56229
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 H43 12.12761 3.84324 10.90147
 H44 10.50508 3.38456 11.47107
 H45 11.24975 4.89699 12.00869
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 H47 6.98572 5.31876 7.06143
 H48 6.68908 4.36490 8.52999
 H49 7.63724 3.67905 7.21037
 C50 19.82581 7.37612 7.82765
 H51 19.91348 6.65563 7.00434
 H52 20.60584 7.13331 8.55686
 H53 20.03779 8.36917 7.41514
 H54 12.29661 3.12446 8.33559
 O55 13.66531 5.84918 5.84743
 C56 14.46687 6.04359 4.62933
 H57 13.89352 6.75031 4.00928
 C58 14.66387 4.73254 3.90272
 H59 13.71695 4.29787 3.56545
 H60 15.28696 4.90422 3.01776
 H61 15.17476 4.02001 4.56121
 C62 15.76708 6.67795 5.04839
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 H64 16.38506 6.84785 4.15953
 H65 15.60257 7.64271 5.53682
 O66 10.75853 3.87565 6.19649
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 C68 12.00569 4.33632 6.55432
 C69 10.42236 4.54823 5.06978
 C70 11.43506 5.44634 4.66862
 C71 11.22082 6.24002 3.53058
 C72 10.02676 6.10473 2.84482
 C73 9.04277 5.19494 3.26331
 C74 9.22612 4.40094 4.38581
 H75 8.47679 3.69141 4.72615
 H76 8.11872 5.11143 2.69627

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 H78 11.96869 6.95364 3.19376
 78
 10 - TS
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 C13 14.61101 4.91002 6.34454
 C4 12.64978 3.35214 8.34129
 C5 15.70490 7.01839 9.35614
 C6 15.85193 6.45170 11.82545
 H7 15.90129 7.38699 12.40178
 H8 16.39085 5.68498 12.39112
 H9 14.80775 6.13174 11.76519
 C10 10.97646 5.79474 9.03560
 N11 14.28176 7.07103 9.45245
 N12 12.18353 6.53022 9.19559
 C13 13.56919 8.26287 9.91139
 H14 13.99720 9.16521 9.45896
 H15 13.64974 8.35318 11.00663
 C16 18.47450 6.87001 9.11132
 C17 10.42927 5.18050 10.16877
 C18 12.14545 7.97491 9.45251
 H19 11.38639 8.20823 10.20833
 H20 11.88433 8.51402 8.52831
 C21 13.44744 6.05228 9.12178
 C22 10.40485 5.66398 7.76504
 C23 16.30684 7.40740 8.14725
 C24 17.69053 7.30747 8.04509
 H25 18.17033 7.58544 7.10562
 C26 16.46839 6.65365 10.47437
 C27 8.68956 4.24268 8.74984
 C28 9.25906 4.87937 7.64776
 H29 8.81642 4.73754 6.66109
 C30 11.05734 6.26744 6.55913
 H31 11.21627 7.34723 6.67392
 H32 10.44454 6.11308 6.6568
 H33 12.04526 5.81847 6.37628
 C34 17.85128 6.57045 10.32022
 H35 18.45732 6.27054 11.17639
 C36 9.28134 4.40934 10.00235
 H37 8.85379 3.90164 10.86820
 C38 15.51462 8.00171 7.02084
 H39 14.48447 7.63440 6.98784
 H40 15.97186 7.76385 6.05546
 H41 15.48974 9.09725 7.11653
 C42 11.12790 5.26057 11.49324
 H43 12.06845 4.68752 11.47315
 H44 10.50124 4.85322 12.29279
 H45 11.39560 6.29104 11.76222
 C46 7.46323 3.39338 8.59550
 H47 7.39710 2.96623 7.58906
 H48 6.54976 3.97810 8.76334
 H49 7.45638 2.56805 9.31612
 C50 19.95879 6.72835 8.95371
 H51 20.21454 5.75123 8.52486
 H52 20.47692 6.80843 9.91536
 H53 20.36557 7.49148 8.28056
 H54 11.67013 3.56678 8.77338
 O55 14.87604 1.62797 7.80931
 C56 15.62469 0.58459 8.47997
 H57 15.84139 -0.19506 7.73133
 C58 14.82444 0.01984 9.63240
 H59 13.90970 -0.47801 9.28987
 H60 15.42576 -0.71651 10.17733
 H61 14.55336 0.83197 10.31953
 C62 16.90735 1.24923 8.91914
 H63 16.68264 2.03072 9.65634
 H64 17.57720 0.51340 9.37715
 H65 17.41691 1.70707 8.06490
 O66 11.53515 1.88601 6.75139
 C67 13.66550 1.36028 7.30937
 C68 12.69691 2.34328 7.35537
 C69 11.81203 0.64781 6.28408
 C70 13.12193 0.24039 6.60587
 C71 13.56083 -1.02961 6.20120
 C72 12.68526 -1.83412 5.49533
 C73 11.38746 -1.39752 5.18138
 C74 10.93191 -0.14490 5.56315
 H75 9.93226 0.20882 5.32825
 H76 10.72490 -2.05807 4.62691
 H77 13.00619 -2.82150 5.17239
 H78 14.56711 -1.37363 6.42560

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10 - P
Ru1 13.64649 4.58168 7.97188
C12 14.81106 3.25991 9.58026
C13 13.29521 5.69717 5.91437
C4 12.08928 3.60209 8.07738
C5 15.53479 7.00606 8.76367
C6 16.41523 5.84741 10.84430
H7 16.69020 6.61889 11.57830
H8 17.06480 4.98280 11.01315
H9 15.39053 5.52262 11.04706
C10 10.92784 5.79789 9.90627
N11 14.22850 7.02849 9.33784
N12 12.15527 6.50171 9.76877
C13 13.81845 8.03969 10.31050
H14 14.11552 9.03959 9.97349
H15 14.29596 7.84581 11.28456
C16 18.05994 6.92055 7.59444
C17 10.79253 4.91159 10.98066
C18 12.30968 7.83993 10.35179
H19 11.89103 7.86517 11.36460
H20 11.77202 8.58160 9.74028
C21 13.26640 6.09756 9.10839
C22 9.90820 5.99740 8.96783
C23 15.74675 7.67440 7.54766
C24 17.01448 7.60219 6.97605
H25 17.18904 8.09860 6.02057
C26 16.58494 6.37975 9.45318
C27 8.56619 4.35717 10.16807
C28 8.73437 5.26394 9.12110
H29 7.93583 5.38520 8.38789
C30 10.11296 6.90398 7.79198
H31 10.36321 7.92814 8.09799
H32 9.21039 6.95246 7.17505
H33 10.93988 6.54979 7.15795
C34 17.83392 6.33772 8.83988
H35 18.65533 5.83713 9.35443
C36 9.59547 4.20508 11.09677
H37 9.47088 3.50647 11.92685
C38 14.68741 8.52266 6.90950
H39 13.67476 8.21207 7.18430
H40 14.75447 8.47535 5.81816
H41 14.82118 9.57309 7.20648
C42 11.93427 4.67247 11.92310
H43 12.76127 4.15298 11.41291
H44 11.62021 4.05584 12.77179
H45 12.35008 5.60861 12.31900
C46 7.32157 3.52603 10.25269
H47 7.38885 2.67110 9.56577
H48 6.43112 4.09848 9.96969
H49 7.16594 3.12735 11.26142
C50 19.40200 6.81260 6.93490
H51 19.47516 5.88702 6.35016
H52 20.21253 6.79397 7.67202
H53 19.58219 7.64623 6.24760
H54 11.21692 3.79812 8.70331
O55 10.32223 1.15896 8.54439
C56 10.59263 0.35858 9.72492
H57 10.96567 -0.62345 9.38844
C58 9.26636 0.20131 10.42542
H59 8.51608 -0.23213 9.75620
H60 9.37203 -0.44512 11.30315
H61 8.90860 1.18333 10.76091
C62 11.63123 1.03834 10.58930
H63 11.26179 2.02725 10.89364
H64 11.82012 0.44522 11.49122
H65 12.58698 1.18003 10.07035
O66 13.08969 2.07949 6.51286
C67 11.34452 1.22165 7.67591
C68 12.08468 2.35741 7.41821
C69 12.99037 0.76315 6.21591
C70 11.92208 0.16392 6.90432
C71 11.65441 -1.19779 6.70751
C72 12.47210 -1.90438 5.84449
C73 13.53732 -1.27845 5.17369
C74 13.81158 0.07097 5.34033
H75 14.62672 0.57124 4.82618
H76 14.16041 -1.86721 4.50453
H77 12.28987 -2.96297 5.67547
H78 10.81896 -1.67843 7.21205
90
10 - Pa

Ru1 14.32080 4.35580 8.49834
C12 14.69539 3.58877 10.80663
C13 14.22273 5.07912 6.18818
C4 12.78413 3.31388 8.52556
C5 15.57953 7.16319 8.95578
C6 16.14299 6.52261 11.34801
H7 16.28304 7.43764 11.94084
H8 16.77217 5.74038 11.78581
H9 15.10722 6.18771 11.45442
C10 11.01355 5.52527 9.49635
N11 14.18873 7.13625 9.27140
N12 12.16480 6.36464 9.48134
C13 13.47206 8.25236 9.88743
H14 13.69694 9.19260 9.37028
H15 13.76884 8.35594 10.94370
C16 18.26642 7.02527 8.23833
C17 10.65342 4.92176 10.70905
C18 12.02405 7.80663 9.73099
H19 11.41044 7.98450 10.62153
H20 11.52807 8.28638 8.87251
C21 13.42361 6.02711 9.13147
C22 10.27066 5.34092 8.32375
C23 15.96898 7.59477 7.67691
C24 17.31542 7.49887 7.33658
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C26 16.52303 6.77885 9.92142
C27 8.78167 3.86836 9.56779
C28 9.15611 4.50687 8.38692
H29 8.57642 4.33165 7.47904
C30 10.68999 5.97181 7.03072
H31 10.77812 7.06341 7.11313
H32 9.96331 5.75643 6.24087
H33 11.67210 5.60104 6.70040
C34 17.86019 6.70914 9.53321
H35 18.60312 6.38484 10.26453
C36 9.53165 4.09599 10.72029
H37 9.24793 3.60080 11.65121
C38 14.99108 8.20055 6.71661
H39 13.98169 7.79708 6.84123
H40 15.29097 8.00842 5.68186
H41 14.95329 9.29058 6.85791
C42 11.49847 5.09620 11.93475
H43 12.47289 4.59705 11.81019
H44 11.00458 4.66828 12.81342
H45 11.71400 6.15199 12.14704
C46 7.63625 2.90306 9.57373
H47 7.97357 1.93383 9.18130
H48 6.80928 3.24541 8.94112
H49 7.24907 2.73524 10.58520
C50 19.69324 6.83054 7.82189
H51 19.87584 5.77999 7.55709
H52 20.38940 7.08429 8.62933
H53 19.94658 7.43646 6.94553
H54 12.24717 3.24231 9.48011
O55 10.53573 1.33465 8.97449
C56 10.94067 0.23994 9.83592
H57 11.34400 -0.56220 9.19339
C58 9.68571 -0.22727 10.53408
H59 8.93853 -0.58171 9.81511
H60 9.91162 -1.03871 11.23420
H61 9.25002 0.60593 11.10099
C62 11.99872 0.72761 10.79963
H63 11.59733 1.54946 11.40825
H64 12.31011 -0.08121 11.47096
H65 12.89162 1.10360 10.28641
O66 12.64481 2.31652 6.28392
C67 11.22710 1.48356 7.83506
C68 12.20498 2.43547 7.58482
C69 11.96884 1.28712 5.73133
C70 11.07015 0.71511 6.64446
C71 10.26761 -0.36427 6.25423
C72 10.40356 -0.83557 4.96199
C73 11.31303 -0.24514 4.06461
C74 12.10936 0.83007 4.42884
H75 12.80833 1.30007 3.74352
H76 11.38992 -0.64247 3.05506
H77 9.79724 -1.67322 4.62548
H78 9.55724 -0.80560 6.95046
C79 15.49096 2.27738 7.52188
C80 16.44211 3.18892 7.86112
H81 16.62019 3.99973 7.14771
C82 17.42675 3.05865 8.97666

H83	17.63117	4.03093	9.44052	C73	11.16553	-1.24780	5.64895
H84	17.08729	2.37767	9.76080	C74	12.51645	-0.92477	5.53594
H85	18.37931	2.68343	8.57409	H75	13.23079	-1.57082	5.03399
C86	15.22378	0.99905	8.25134	H76	10.80448	-2.17997	5.22161
H87	14.20634	0.63384	8.05758	H77	9.22291	-0.67909	6.36891
H88	15.91496	0.21235	7.91771	H78	9.98766	1.47198	7.36682
H89	15.34223	1.11750	9.33444	78			
H90	14.97213	2.43434	6.57675	11 - S cis			
78				Ru1	14.25886	4.71678	8.12663
11 - S trans				C12	14.46494	3.24112	9.93672
Ru1	14.13592	4.56100	8.16014	C13	16.17553	3.82101	7.00638
C12	14.96608	3.36751	10.08085	C4	12.67620	3.91513	7.63760
C13	14.07610	5.63907	6.01741	C5	15.65947	7.04644	9.55331
C4	12.64722	3.47576	7.89635	C6	16.48471	5.61971	11.47450
C5	15.60814	7.09429	9.16973	H7	16.48519	6.28824	12.34731
C6	16.22606	6.05974	11.40124	H8	17.28067	4.88355	11.62278
H7	16.37821	6.88076	12.11693	H9	15.53503	5.07464	11.45242
H8	16.86743	5.22720	11.70688	C10	10.97554	5.72688	9.49553
H9	15.19148	5.71350	11.48002	N11	14.31034	6.89261	9.99794
C10	10.96787	5.61633	9.45499	N12	12.22374	6.25952	9.93731
N11	14.22817	7.05746	9.53114	C13	13.71220	7.62296	11.11622
N12	12.14976	6.39886	9.56959	H14	14.01286	8.67745	11.09676
C13	13.57974	8.06180	10.36980	H15	14.03643	7.18643	12.07279
H14	13.85601	9.07350	10.04824	C16	18.23914	7.27929	8.53666
H15	13.88603	7.93844	11.42116	C17	10.41649	4.64535	10.18861
C16	18.26404	6.99581	8.33473	C18	12.22489	7.40880	10.85679
C17	10.68486	4.69308	10.46955	H19	11.65225	7.17635	11.76158
C18	12.10300	7.74453	10.15280	H20	11.75394	8.27766	10.36945
H19	11.51701	7.73921	11.07974	C21	13.44297	6.04621	9.39641
H20	11.62295	8.44446	9.45080	C22	10.30973	6.33215	8.42072
C21	13.38860	6.05700	9.14596	C23	15.88713	7.87826	8.44333
C22	10.15312	5.75855	8.32635	C24	17.18391	7.98102	7.95232
C23	15.97200	7.72388	7.96722	H25	17.37634	8.61323	7.08400
C24	17.30154	7.64463	7.56319	C26	16.70924	6.39543	10.21413
H25	17.59176	8.10166	6.61603	C27	8.48425	4.75142	8.70778
C26	16.56912	6.52274	10.01798	C28	9.06940	5.82525	8.04164
C27	8.71261	4.00875	9.21942	H29	8.56038	6.25891	7.17831
C28	9.02660	4.94235	8.23146	C30	10.92177	7.47353	7.66538
H29	8.39031	5.02147	7.34882	H31	10.88618	8.41360	8.23361
C30	10.53730	6.68680	7.21369	H32	10.39095	7.64244	6.72221
H31	10.64502	7.72363	7.55816	H33	11.97569	7.28234	7.42980
H32	9.78371	6.67759	6.41996	C34	17.98856	6.51920	9.67483
H33	11.50237	6.39532	6.77093	H35	18.81113	5.98731	10.15355
C34	17.88836	6.47083	9.56975	C36	9.17295	4.17305	9.77230
H35	18.64167	6.00623	10.20778	H37	8.73216	3.32233	10.29428
C36	9.54919	3.89859	10.33045	C38	14.75741	8.62761	7.80100
H37	9.32285	3.15852	11.09942	H39	14.14157	7.96470	7.17684
C38	14.99399	8.53410	7.17041	H40	15.13774	9.43021	7.15970
H39	13.96250	8.19144	7.29651	H41	14.08517	9.07706	8.54357
H40	15.22307	8.48363	6.10169	C42	11.14475	3.99994	11.32645
H41	15.04946	9.58903	7.47688	H43	12.11273	3.59402	11.00051
C42	11.62904	4.50701	11.61885	H44	10.55197	3.18655	11.75624
H43	12.56478	4.03309	11.28319	H45	11.36177	4.71755	12.12869
H44	11.18543	3.87224	12.39238	C46	7.14477	4.22639	8.28658
H45	11.91168	5.46217	12.08130	H47	6.94626	4.44559	7.23146
C46	7.49748	3.13756	9.09446	H48	6.33724	4.67564	8.87835
H47	7.20181	3.00865	8.04738	H49	7.08043	3.14020	8.42399
H48	6.63988	3.57106	9.62447	C50	19.60708	7.31551	7.92655
H49	7.67275	2.14430	9.52370	H51	19.70275	6.52972	7.16586
C50	19.67217	6.85977	7.83705	H52	20.38903	7.14143	8.67324
H51	19.77317	5.98023	7.18695	H53	19.80707	8.27366	7.43404
H52	20.38321	6.73817	8.66127	H54	12.27850	3.06587	8.21044
H53	19.97684	7.73117	7.24656	O55	13.63838	5.91513	5.73992
H54	11.63573	3.69508	8.24582	C56	14.42681	6.08131	4.49418
O55	15.14853	2.73065	6.89900	H57	13.80791	6.71124	3.83982
C56	16.52814	2.31284	6.64638	C58	14.68282	4.73002	3.86877
H57	16.53803	1.89151	5.63130	H59	13.75556	4.23172	3.56604
C58	16.93620	1.28741	7.67841	H60	15.29646	4.86338	2.97092
H59	16.34301	0.37093	7.59720	H61	15.22463	4.09039	4.57583
H60	17.99044	1.02523	7.53400	C62	15.68925	6.79698	4.89469
H61	16.80394	1.70707	8.68295	H63	16.25585	6.18591	5.60905
C62	17.32978	3.59049	6.71068	H64	16.30666	6.96046	4.00454
H63	17.30009	4.00788	7.72757	H65	15.46980	7.77161	5.34277
H64	18.37376	3.37941	6.45326	O66	11.68472	5.55688	4.56505
H65	16.93162	4.34028	6.01830	C67	11.98517	4.32018	6.45614
O66	14.20072	0.77750	6.09261	C68	12.48763	5.27821	5.61240
C67	12.85416	2.26574	7.19106	C69	10.58606	4.72804	4.71401
C68	14.11811	1.94240	6.74019	C70	10.72423	3.93358	5.85706
C69	12.90049	0.27239	6.09833	C71	9.71627	3.02052	6.16268
C70	12.03434	1.15242	6.75896	C72	8.61483	2.94944	5.31857
C71	10.68765	0.80910	6.86035	C73	8.49964	3.77459	4.19330
C72	10.27021	-0.39334	6.30032	C74	9.49787	4.68834	3.86606

H75 9.43530 5.33273 2.99383
 H76 7.62032 3.69651 3.55849
 H77 7.81885 2.24066 5.53871
 H78 9.78907 2.38977 7.04678
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 11 - TS
 Ru1 14.24043 4.38524 8.41090
 C12 14.74933 3.50985 10.58534
 C13 14.64808 5.12994 6.19662
 C4 12.77183 3.34748 8.04418
 C5 15.69078 7.07595 9.36680
 C6 15.87851 6.36536 11.79514
 H7 15.86593 7.26523 12.42724
 H8 16.46827 5.60409 12.31568
 H9 14.85788 5.98061 11.71214
 C10 10.98781 5.73678 8.97587
 N11 14.26743 7.05463 9.47346
 N12 12.18434 6.47197 9.19481
 C13 13.52402 8.17491 10.04947
 H14 13.91709 9.12780 9.67648
 H15 13.61816 8.16752 11.14711
 C16 18.46303 7.10544 9.11337
 C17 10.46438 4.99260 10.03951
 C18 12.10446 7.88519 9.58421
 H19 11.34959 8.02195 10.36751
 H20 11.81182 8.49864 8.71745
 C21 13.46149 6.04043 9.06374
 C22 10.37863 5.77056 7.71594
 C23 16.26401 7.57598 8.18565
 C24 17.65109 7.56229 8.07685
 H25 18.11043 7.92819 7.15743
 C26 16.47818 6.68735 10.45981
 C27 8.66910 4.25902 8.56979
 C28 9.21049 5.03214 7.54201
 H29 8.72640 5.03303 6.56321
 C30 11.01883 6.48780 6.56645
 H31 11.18462 7.55169 6.77850
 H32 10.39576 6.42035 5.66873
 H33 12.00317 6.05375 6.33168
 C34 17.86251 6.69594 10.30148
 H35 18.48818 6.37969 11.13738
 C36 9.30412 4.25451 9.81091
 H37 8.89792 3.64324 10.61787
 C38 15.43674 8.20494 7.10398
 H39 14.42066 7.80222 7.05801
 H40 15.89156 8.04471 6.12166
 H41 15.37159 9.29087 7.26707
 C42 11.18880 4.92245 11.35033
 H43 12.13838 4.37477 11.24676
 H44 10.58327 4.41380 12.10689
 H45 11.44624 5.91890 11.73401
 C46 7.43632 3.44017 8.33080
 H47 7.40826 3.05957 7.30285
 H48 6.52587 4.03406 8.48180
 H49 7.38604 2.58374 9.01112
 C50 19.95253 7.06212 8.94829
 H51 20.26442 6.12857 8.46332
 H52 20.46778 7.11671 9.91330
 H53 20.31094 7.88628 8.32114
 H54 11.74695 3.60954 8.32633
 O55 14.92958 1.24630 7.94219
 C56 15.29998 0.08642 8.75110
 H57 15.35704 -0.77544 8.07078
 C58 14.24849 -0.12395 9.81767
 H59 13.27703 -0.38877 9.38385
 H60 14.55161 -0.93804 10.48538
 H61 14.13809 0.79628 10.40611
 C62 16.65692 0.42754 9.31285
 H63 16.57737 1.32325 9.94106
 H64 17.03028 -0.40309 9.92127
 H65 17.37410 0.62410 8.50974
 O66 13.47400 0.11162 6.57505
 C67 12.90312 2.25151 7.13235
 C68 13.80353 1.22006 7.27560
 C69 12.27908 0.40566 5.94756
 C70 11.87267 1.70402 6.26653
 C71 10.66998 2.17943 5.74863
 C72 9.92233 1.33098 4.93926
 C73 10.36149 0.03798 4.63263
 C74 11.56255 -0.45354 5.13990
 H75 11.92179 -1.45439 4.91853
 H76 9.75729 -0.59539 3.98788

H77 8.97913 1.68206 4.52547
 H78 10.33366 3.19020 5.97774
 78
 11 - P
 Ru1 13.84016 4.59071 7.94360
 C12 15.26048 3.48943 9.50473
 C13 13.17617 5.49929 5.84064
 C4 12.39866 3.47263 8.21886
 C5 15.48275 7.34132 8.39978
 C6 17.02799 6.30539 10.12613
 H7 17.28214 7.08000 10.86422
 H8 17.87569 5.61454 10.07223
 H9 16.17083 5.73533 10.49374
 C10 11.23246 5.61237 10.14233
 N11 14.35465 7.09676 9.24370
 N12 12.46938 6.30662 10.01930
 C13 14.06339 7.95587 10.39220
 H14 14.22432 9.00939 10.13591
 H15 14.72407 7.69879 11.23491
 C16 17.64963 7.90339 6.74060
 C17 11.09573 4.67371 11.17091
 C18 12.61078 7.61156 10.67637
 H19 12.37907 7.52959 11.74455
 H20 11.91042 8.33727 10.23099
 C21 13.46216 6.07527 9.12066
 C22 10.19329 5.88871 9.24333
 C23 15.27843 8.11105 7.24035
 C24 16.37253 8.36632 6.42212
 H25 16.22682 8.95422 5.51502
 C26 16.76410 6.93244 8.79163
 C27 8.82292 4.25184 10.41450
 C28 8.99600 5.19631 9.40321
 H29 8.17783 5.39050 8.70778
 C30 10.38506 6.83264 8.09532
 H31 10.84192 7.78107 8.40358
 H32 9.42880 7.06091 7.61432
 H33 11.05082 6.39529 7.33540
 C34 17.82835 7.20935 7.93280
 H35 18.82949 6.88364 8.21895
 C36 9.87813 4.00448 11.29021
 H37 9.75680 3.26385 12.08246
 C38 13.93069 8.67670 6.91188
 H39 13.24878 7.88814 6.56979
 H40 14.00985 9.42336 6.11526
 H41 13.46955 9.15882 7.78450
 C42 12.25631 4.34595 12.06081
 H43 13.10253 3.95724 11.47500
 H44 11.97797 3.59271 12.80476
 H45 12.62782 5.22847 12.59774
 C46 7.52974 3.50069 10.52270
 H47 7.45717 2.73448 9.73735
 H48 6.66701 4.16431 10.39558
 H49 7.42956 2.99736 11.49091
 C50 18.80307 8.16324 5.81856
 H51 18.84803 7.40821 5.02326
 H52 19.75970 8.13437 6.35120
 H53 18.71301 9.14015 5.32982
 H54 11.58320 3.68426 8.91422
 O55 10.49954 1.25307 8.84274
 C56 9.81572 0.02573 9.22297
 H57 10.53752 -0.79686 9.13918
 C58 8.64974 -0.19464 8.28655
 H59 8.98692 -0.31315 7.25231
 H60 8.09940 -1.09710 8.57422
 H61 7.96203 0.65837 8.33475
 C62 9.40484 0.22071 10.66163
 H63 8.72108 1.07370 10.74887
 H64 8.89098 -0.67401 11.02888
 H65 10.27645 0.41108 11.29549
 O66 11.64792 0.05726 7.26958
 C67 12.34209 2.20579 7.59105
 C68 11.44933 1.20467 7.94167
 C69 12.73153 0.28542 6.42905
 C70 13.19516 1.59032 6.58819
 C71 14.28879 2.00419 5.82936
 C72 14.86656 1.09093 4.95453
 C73 14.37176 -0.21052 4.82152
 C74 13.27703 -0.64218 5.56766
 H75 12.87360 -1.64706 5.48459
 H76 14.84636 -0.89722 4.12517
 H77 15.72060 1.39799 4.35571
 H78 14.67365 3.02376 5.89763

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11 - Pa
Ru1 14.38532 4.59452 8.01385
C12 15.07437 4.12147 10.35027
C13 14.08105 5.06808 5.65657
C4 13.00275 3.38833 8.37344
C5 15.31083 7.62942 8.27753
C6 16.34697 7.18348 10.55061
H7 16.37731 8.13742 11.09669
H8 17.18778 6.57556 10.90062
H9 15.43316 6.64818 10.82061
C10 11.02148 5.43085 9.00316
N11 14.00131 7.37776 8.79265
N12 12.10440 6.35286 9.13225
C13 13.22614 8.35074 9.56479
H14 13.29478 9.34934 9.11810
H15 13.60926 8.40558 10.59544
C16 17.83264 7.98224 7.14931
C17 10.64831 4.66943 10.12145
C18 11.82799 7.74921 9.49988
H19 11.28740 7.79837 10.45192
H20 11.20127 8.22330 8.72737
C21 13.36096 6.19239 8.65297
C22 10.33778 5.33178 7.78343
C23 15.41086 8.10794 6.95924
C24 16.68048 8.26821 6.41515
H25 16.77315 8.61834 5.38625
C26 16.44613 7.44230 9.07883
C27 8.92430 3.61039 8.76829
C28 9.29709 4.40831 7.68985
H29 8.78449 4.28798 6.73326
C30 10.74083 6.14398 6.59160
H31 10.78383 7.21859 6.81426
H32 10.03271 6.00018 5.76893
H33 11.73845 5.85069 6.23255
C34 17.69846 7.59845 8.48122
H35 18.59165 7.42892 9.08413
C36 9.59991 3.76615 9.98013
H37 9.32317 3.14041 10.83035
C38 14.18836 8.44403 6.16152
H39 13.69820 7.52828 5.80655
H40 14.45193 9.04786 5.28708
H41 13.45435 9.00501 6.75413
C42 11.39523 4.78363 11.41608
H43 12.47111 4.59812 11.28105
H44 11.00962 4.06533 12.14734
H45 11.30457 5.78621 11.85547
C46 7.85078 2.57271 8.62942
H47 8.28371 1.56383 8.68055
H48 7.32786 2.66065 7.67124
H49 7.10967 2.64672 9.43427
C50 19.18283 8.07638 6.50461
H51 19.42909 7.14056 5.98433
H52 19.97287 8.25816 7.24094
H53 19.21741 8.87767 5.75787
H54 12.86645 3.32065 9.46083
O55 11.70333 1.19749 9.84006
C56 13.04335 0.80066 10.29092
H57 13.75108 1.58360 9.98410
C58 13.39235 -0.52297 9.65499
H59 13.42764 -0.43999 8.56093
H60 14.37879 -0.85503 9.99712
H61 12.65163 -1.28603 9.92280
C62 12.96286 0.77069 11.79281
H63 12.21822 0.03855 12.12746
H64 13.93839 0.50014 12.20954
H65 12.69062 1.75987 12.17632
O66 10.63242 0.73429 7.92963
C67 12.14701 2.43727 7.74847
C68 11.53729 1.49113 8.57148
C69 10.59259 1.20407 6.63202
C70 11.52814 2.22704 6.44384
C71 11.59267 2.82766 5.18529
C72 10.72476 2.38294 4.19447
C73 9.79517 1.36417 4.42685
C74 9.71133 0.75019 5.67182
H75 8.99637 -0.03745 5.89369
H76 9.12888 1.04749 3.62772
H77 10.76840 2.84513 3.21052
H78 12.30462 3.62832 4.99847
C79 16.53712 3.53781 7.45052
C80 15.68999 2.47222 7.37628

H81 15.47168 1.96425 8.31846
C82 15.19415 1.81484 6.13193
H83 14.18664 1.40826 6.28100
H84 15.14942 2.50962 5.28809
H85 15.84677 0.97338 5.85988
C86 17.18295 4.25195 6.30647
H87 17.11549 5.34220 6.42554
H88 18.25253 3.99787 6.28382
H89 16.74123 3.99833 5.34030
H90 16.92007 3.78454 8.44455
78
12 - S trans
Ru1 13.90928 4.27970 8.74763
C12 14.17029 3.15929 10.86441
C13 14.33784 5.35723 6.64291
C4 12.33796 3.44713 8.29829
C5 15.39251 6.70495 10.28027
C6 14.76531 5.84755 12.59567
H7 14.70634 6.68025 13.31144
H8 15.06384 4.95302 13.15067
H9 13.76539 5.65648 12.19815
C10 10.67796 5.87811 9.19400
N11 14.00709 6.88706 9.98457
N12 11.92547 6.50894 9.46451
C13 13.32026 8.08207 10.47458
H14 13.83152 8.98727 10.12488
H15 13.32149 8.09276 11.57644
C16 18.10172 6.38753 10.88025
C17 10.06235 5.16600 10.23285
C18 11.92536 7.91374 9.89103
H19 11.12328 8.08871 10.61874
H20 11.74798 8.56920 9.02561
C21 13.16300 5.95252 9.46607
C22 10.10789 5.97773 7.92017
C23 16.35664 7.18117 9.37785
C24 17.70220 6.99732 9.69444
H25 18.45847 7.34138 8.98643
C26 15.76460 6.16697 11.52497
C27 8.25961 4.59502 8.70328
C28 8.89718 5.32183 7.69810
H29 8.44661 5.37027 6.70564
C30 10.81428 6.69963 6.81438
H31 10.95089 7.76453 7.04361
H32 10.24700 6.63279 5.88090
H33 11.81639 6.28115 6.64049
C34 17.12066 5.99947 11.79046
H35 17.41758 5.55588 12.74194
C36 8.85362 4.52999 9.96371
H37 8.37048 3.95416 10.75429
C38 15.99001 7.92726 8.13096
H39 14.97594 7.70189 7.79265
H40 16.66856 7.67005 7.30977
H41 16.07722 9.00962 8.30027
C42 10.73542 5.01540 11.56383
H43 11.62939 4.37725 11.48194
H44 10.06125 4.55816 12.29465
H45 11.07117 5.97951 11.96947
C46 6.95318 3.90506 8.44442
H47 6.81722 3.68480 7.38006
H48 6.10676 4.52910 8.75835
H49 6.88074 2.96341 9.00034
C50 19.55138 6.13141 11.16249
H51 19.84331 5.13151 10.81447
H52 19.76831 6.17416 12.23556
H53 20.19715 6.85413 10.65192
H54 11.35830 3.78396 8.64661
O55 15.28735 2.48610 7.81323
C56 16.71051 2.46688 8.09158
H57 17.21745 2.22135 7.14652
C58 17.00197 1.43683 9.16311
H59 16.68359 0.43188 8.86606
H60 18.07779 1.40873 9.37246
H61 16.46585 1.71078 10.07970
C62 17.11565 3.86201 8.50066
H63 16.65801 4.14134 9.46060
H64 18.20351 3.89662 8.63762
H65 16.83783 4.59507 7.73529
O66 11.39472 0.63638 6.20819
C67 12.29793 2.28192 7.47544
C68 11.15050 1.70548 6.99449
H69 10.11108 1.97714 7.13211
C70 12.75780 0.48374 6.17088

C71	13.36728	1.47586	6.93341
C72	14.76056	1.49282	7.05409
C73	15.47970	0.50084	6.38986
C74	14.82190	-0.47283	5.62326
C75	13.44169	-0.51278	5.49262
H76	12.92596	-1.26878	4.90950
H77	15.42543	-1.22509	5.12117
H78	16.56177	0.45804	6.45616
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12 - S cis			
Ru1	13.88200	4.19874	8.85114
C12	13.35188	3.17904	10.92028
C13	15.08573	2.18630	8.22726
C4	12.28148	3.65214	8.16015
C5	15.45159	6.86504	10.35371
C6	15.71690	5.45189	12.43420
H7	15.25829	6.10231	13.19208
H8	16.50430	4.87861	12.93223
H9	14.94651	4.74977	12.09228
C10	10.77093	6.02547	9.19861
N11	14.03068	6.74323	10.44701
N12	11.94455	6.36302	9.94071
C13	13.29045	7.63662	11.34573
H14	13.73193	8.64019	11.33796
H15	13.32837	7.24763	12.37401
C16	18.21161	7.27279	10.21031
C17	9.82138	5.16444	9.76194
C18	11.89038	7.58053	10.76224
H19	11.10411	7.49736	11.52110
H20	11.66008	8.45304	10.13011
C21	13.21679	5.93284	9.72285
C22	10.54362	6.65315	7.96163
C23	15.97719	7.70656	9.35647
C24	17.35371	7.89760	9.30338
H25	17.77095	8.53789	8.52432
C26	16.27996	6.26336	11.30922
C27	8.43247	5.45939	7.77972
C28	9.37538	6.35293	7.27079
H29	9.20567	6.81048	6.29398
C30	11.53334	7.61506	7.37699
H31	11.51791	8.58345	7.89629
H32	11.31345	7.80571	6.32139
H33	12.55640	7.23003	7.44090
C34	17.65723	6.47031	11.20283
H35	18.31430	5.98934	11.92843
C36	8.66804	4.88584	9.02571
H37	7.93233	4.19891	9.44611
C38	15.08701	8.34184	8.33221
H39	14.69166	7.58309	7.64116
H40	15.63623	9.08220	7.74164
H41	14.21921	8.84116	8.78246
C42	10.02969	4.55622	11.11294
H43	10.97543	4.00092	11.16720
H44	9.20733	3.88023	11.36615
H45	10.07592	5.32915	11.89110
C46	7.20812	5.12482	6.98106
H47	7.48151	4.76036	5.98181
H48	6.57216	6.00659	6.83334
H49	6.60314	4.35396	7.46953
C50	19.69600	7.44242	10.09223
H51	20.10677	6.75596	9.34021
H52	20.20428	7.23010	11.03850
H53	19.96181	8.45891	9.78055
H54	11.61392	3.02953	8.77291
O55	14.67915	5.17168	6.83569
C56	16.10590	5.14956	6.46294
H57	16.33112	6.16539	6.09941
C58	16.35179	4.10335	5.39677
H59	15.83661	4.31577	4.45537
H60	17.42738	4.04820	5.19310
H61	16.02005	3.13067	5.78055
C62	16.93836	4.88436	7.69499
H63	16.93957	3.82148	7.94911
H64	17.96686	5.21276	7.49808
H65	16.57592	5.45209	8.55528
O66	10.52973	4.18704	5.01756
C67	11.87941	3.91756	6.81711
C68	10.68295	3.60652	6.23065
H69	9.84706	3.01817	6.58657
C70	11.66486	4.92024	4.79238
C71	12.55215	4.76056	5.85649
C72	13.79416	5.39972	5.81485
C73	14.05509	6.24073	4.73535
C74	13.12487	6.39126	3.69858
C75	11.90808	5.72190	3.68987
H76	11.19186	5.81692	2.88016
H77	13.37713	7.04724	2.86902
H78	14.99989	6.77315	4.67267
78			
12 - TS			
Ru1	13.93545	4.27516	8.92857
C12	14.40081	3.89278	11.24874
C13	14.28431	4.36550	6.57473
C4	12.36320	3.33846	8.89146
C5	15.64238	6.85777	9.20813
C6	15.80241	6.80909	11.73793
H7	15.93177	7.85026	12.06805
H8	16.30213	6.16468	12.46783
H9	14.73691	6.56244	11.76599
C10	10.82215	6.04954	9.15620
N11	14.23551	7.08225	9.30397
N12	12.09292	6.68729	9.16681
C13	13.64264	8.39627	9.54677
H14	14.11805	9.15519	8.91405
H15	13.78273	8.68754	10.59958
C16	18.34333	6.23374	8.97231
C17	10.25520	5.69418	10.38712
C18	12.17805	8.15386	9.19609
H19	11.47930	8.56092	9.93660
H20	11.90644	8.56426	8.21129
C21	13.30981	6.10123	9.15692
C22	10.18338	5.79730	7.93816
C23	16.24389	6.89947	7.93977
C24	17.59198	6.56380	7.84643
H25	18.06707	6.56346	6.86454
C26	16.39190	6.62916	10.37229
C27	8.33449	4.81058	9.18383
C28	8.93290	5.17980	7.97889
H29	8.41796	4.96939	7.03953
C30	10.85485	6.11124	6.63607
H31	11.11273	7.17471	6.55154
H32	10.20713	5.85761	5.79082
H33	11.79435	5.54794	6.52779
C34	17.73745	6.30266	10.22569
H35	18.32796	6.09613	11.11924
C36	9.00927	5.07239	10.37656
H37	8.55915	4.77078	11.32328
C38	15.50600	7.37900	6.72545
H39	14.42503	7.22307	6.79573
H40	15.84797	6.85651	5.82721
H41	15.69120	8.45335	6.58084
C42	11.01687	5.89546	11.66281
H43	11.88587	5.22039	11.71342
H44	10.38459	5.69927	12.53406
H45	11.41351	6.91524	11.75197
C46	6.98705	4.15314	9.20361
H47	6.77373	3.64237	8.25862
H48	6.19019	4.89038	9.36412
H49	6.91374	3.41765	10.01228
C50	19.77483	5.80999	8.83594
H51	19.84381	4.72898	8.65883
H52	20.34940	6.02817	9.74262
H53	20.26402	6.30714	7.99092
H54	11.48246	3.71705	9.42476
O55	14.77853	1.09764	8.88367
C56	16.18632	0.82912	8.94405
H57	16.46795	0.26584	8.03976
C58	16.48158	0.02973	10.19641
H59	15.94280	-0.92463	10.20387
H60	17.55482	-0.17698	10.28171
H61	16.16625	0.60711	11.07413
C62	16.87629	2.17858	8.93903
H63	16.56557	2.76373	9.81629
H64	17.96479	2.05122	8.97566
H65	16.62064	2.74558	8.03429
O66	10.73985	0.95798	6.69112
C67	12.09576	2.22906	7.99670
C68	10.89562	2.13106	7.34481
H69	10.07943	2.83985	7.26635
C70	11.84495	0.20790	6.97881
C71	12.71765	0.93085	7.79242
C72	13.94629	0.34310	8.14359
C73	14.20507	-0.95484	7.71002
C74	13.27960	-1.64739	6.91419

C75 12.07658 -1.08206 6.52089
 H76 11.35759 -1.60075 5.89533
 H77 13.52231 -2.65929 6.59831
 H78 15.13594 -1.44307 7.98656
 78
 12 - P
 Ru1 13.78942 4.36853 8.38109
 C12 14.66881 3.36461 10.35325
 C13 13.79502 5.22335 6.15357
 C4 12.22212 3.44465 8.40078
 C5 15.68274 6.97423 8.94559
 C6 16.34233 6.12465 11.24605
 H7 16.55709 6.97851 11.90476
 H8 16.95831 5.28473 11.58295
 H9 15.29766 5.83198 11.38330
 C10 10.94691 5.95125 9.71421
 N11 14.31972 7.04596 9.36463
 N12 12.18646 6.62920 9.55101
 C13 13.80031 8.23051 10.05165
 H14 14.18042 9.14361 9.57991
 H15 14.12345 8.22594 11.10514
 C16 18.33328 6.86914 8.10074
 C17 10.69265 5.34382 10.95015
 C18 12.29720 8.05252 9.89678
 H19 11.73326 8.26812 10.81172
 H20 11.88151 8.66950 9.08478
 C21 13.36986 6.09889 9.16574
 C22 10.02531 5.92795 8.66345
 C23 16.02043 7.49837 7.68655
 C24 17.34843 7.41931 7.28166
 H25 17.62361 7.80747 6.29987
 C26 16.65774 6.48462 9.82539
 C27 8.53131 4.63369 10.08750
 C28 8.82237 5.25546 8.87364
 H29 8.09510 5.20890 8.06200
 C30 10.35158 6.55583 7.34229
 H31 10.54899 7.63170 7.43892
 H32 9.52451 6.43263 6.63624
 H33 11.25246 6.10812 6.89791
 C34 17.97448 6.42669 9.37110
 H35 18.74244 6.03320 10.03860
 C36 9.47433 4.68874 11.11527
 H37 9.25286 4.20942 12.07126
 C38 15.01921 8.21223 6.82718
 H39 13.99465 7.86547 6.99363
 H40 15.24089 8.06329 5.76574
 H41 15.05645 9.29396 7.02316
 C42 11.73166 5.36301 12.03177
 H43 12.59209 4.73084 11.76011
 H44 11.32381 4.99387 12.97854
 H45 12.12622 6.37268 12.20794
 C46 7.21708 3.94249 10.29737
 H47 6.78228 3.61080 9.34878
 H48 6.48968 4.61148 10.77544
 H49 7.32234 3.06539 10.94643
 C50 19.74866 6.76229 7.61815
 H51 19.89477 5.84369 7.03615
 H52 20.45875 6.73713 8.45162
 H53 20.01463 7.60237 6.96658
 H54 11.37028 3.61348 9.06539
 O55 11.12562 1.25634 10.22872
 C56 11.01114 0.77740 11.57380
 H57 11.56108 -0.17405 11.65107
 C58 9.54802 0.58283 11.91603
 H59 9.06378 -0.14159 11.25201
 H60 9.43093 0.23916 12.95002
 H61 9.02462 1.54218 11.80859
 C62 11.67533 1.82167 12.43914
 H63 11.13360 2.76965 12.33563
 H64 11.66040 1.52247 13.49307
 H65 12.71088 1.98902 12.12178
 O66 12.70023 0.76697 5.95684
 C67 12.28034 2.22541 7.63592
 C68 12.79993 2.04845 6.37620
 H69 13.21275 2.76829 5.67875
 C70 12.12333 0.05732 6.97533
 C71 11.83819 0.90592 8.03977
 C72 11.31845 0.37535 9.22664
 C73 11.06488 -0.99447 9.26910
 C74 11.34423 -1.80972 8.16084
 C75 11.88694 -1.30980 6.98606
 H76 12.12520 -1.93835 6.13428

H77 11.13137 -2.87345 8.23617
 H78 10.64879 -1.44963 10.16364
 90
 12 - Pa
 Ru1 14.32944 4.40820 8.36317
 C12 15.00935 3.83435 10.65252
 C13 13.91821 4.96944 6.01733
 C4 12.90114 3.24267 8.61432
 C5 15.56822 7.28881 8.86828
 C6 16.02178 6.89468 11.33858
 H7 15.98111 7.86811 11.84885
 H8 16.72028 6.25938 11.89231
 H9 15.04038 6.41529 11.40628
 C10 11.06005 5.49658 9.39497
 N11 14.16649 7.22353 9.13155
 N12 12.18907 6.36575 9.44583
 C13 13.43579 8.31286 9.78242
 H14 13.57008 9.24992 9.22864
 H15 13.80842 8.46150 10.80727
 C16 18.30390 7.32105 8.33221
 C17 10.74832 4.73210 10.52967
 C18 12.00324 7.79079 9.75433
 H19 11.47507 7.90988 10.70794
 H20 11.39859 8.26937 8.96935
 C21 13.43956 6.08808 9.02381
 C22 10.27534 5.45686 8.23712
 C23 16.00763 7.62458 7.57952
 C24 17.38195 7.61252 7.33283
 H25 17.73544 7.85243 6.32871
 C26 16.47637 7.07067 9.92094
 C27 8.84717 3.80956 9.32142
 C28 9.17673 4.59887 8.22188
 H29 8.57327 4.53120 7.31489
 C30 10.63220 6.26673 7.02810
 H31 10.52158 7.34516 7.20566
 H32 9.98286 6.00805 6.18522
 H33 11.67241 6.08933 6.71878
 C34 17.83483 7.08110 9.62498
 H35 18.54935 6.89158 10.42763
 C36 9.63652 3.89702 10.46808
 H37 9.38741 3.28209 11.33512
 C38 15.07198 8.05175 6.48999
 H39 14.03515 8.12124 6.83426
 H40 15.07630 7.33224 5.66419
 H41 15.38152 9.02887 6.09923
 C42 11.60978 4.78463 11.75431
 H43 12.58728 4.30875 11.57804
 H44 11.12316 4.27847 12.59563
 H45 11.82753 5.81647 12.05929
 C46 7.67809 2.87261 9.28241
 H47 7.23365 2.82371 8.28268
 H48 6.89501 3.18117 9.98599
 H49 7.98653 1.85562 9.56136
 C50 19.77154 7.24547 8.03670
 H51 20.08172 6.20260 7.88728
 H52 20.37040 7.64242 8.86437
 H53 20.03222 7.79803 7.12801
 H54 12.80739 2.91953 9.65871
 O55 11.71075 1.10552 10.40411
 C56 11.71200 0.36989 11.62938
 H57 11.59818 -0.70188 11.39496
 C58 10.58054 0.84307 12.52078
 H59 9.60522 0.75538 12.02711
 H60 10.54971 0.26250 13.44958
 H61 10.73935 1.89789 12.77986
 C62 13.07257 0.62516 12.23907
 H63 13.22725 1.70453 12.36857
 H64 13.15994 0.13337 13.21421
 H65 13.86937 0.25785 11.58389
 O66 10.62028 1.97878 6.03955
 C67 11.95865 2.56879 7.76770
 C68 11.61830 2.78309 6.45244
 H69 12.01546 3.49045 5.73371
 C70 10.27739 1.18138 7.10059
 C71 11.06770 1.49852 8.19910
 C72 10.89066 0.77089 9.38800
 C73 9.91635 -0.22644 9.41068
 C74 9.13912 -0.50100 8.27245
 C75 9.30031 0.19528 7.08471
 H76 8.71191 -0.01045 6.19629
 H77 8.39176 -1.28853 8.33278
 H78 9.74886 -0.80949 10.31203

C79	15.35062	2.24315	7.53027	H69	16.05776	0.23833	5.64522
C80	16.27795	3.24440	7.47662	C70	12.89953	0.60792	5.72329
H81	16.26589	3.86659	6.57798	C71	13.21540	1.59563	6.65637
C82	17.44961	3.42879	8.38625	C72	12.20200	2.32166	7.30919
H83	17.57718	4.48551	8.66017	C73	10.88171	1.98620	6.96832
H84	17.35916	2.85718	9.31268	C74	10.58994	1.00733	6.01468
H85	18.36718	3.11933	7.86547	C75	11.59625	0.29270	5.37012
C86	15.31473	1.12591	8.52409	H76	11.38268	-0.47913	4.63657
H87	14.29205	0.75561	8.66752	H77	9.55107	0.79244	5.77602
H88	15.92241	0.28345	8.16536	H78	10.06962	2.52518	7.45663
H89	15.69426	1.43943	9.50141	78			
H90	14.66925	2.16850	6.68042	13 - S cis			
78				Ru1	14.08274	4.19658	8.55640
13 - S trans				C12	13.91963	3.16452	10.68190
Ru1	14.07235	4.19429	8.56781	C13	15.73151	2.54250	8.00807
C12	14.50226	3.12765	10.68693	C4	12.45261	3.47502	8.12503
C13	14.35635	5.18199	6.40115	C5	15.68148	6.87029	9.76915
C4	12.45386	3.37538	8.26277	C6	16.39896	5.26235	11.60608
C5	15.70052	6.71670	9.70533	H7	17.19520	5.28562	12.35740
C6	15.86911	5.81461	12.07252	H8	16.32677	4.23950	11.21394
H7	15.91015	6.66152	12.77270	H9	15.44138	5.45511	12.09882
H8	16.42149	4.98481	12.52557	C10	10.91413	5.79939	9.42852
H9	14.82959	5.49059	11.97082	N11	14.29963	6.69419	10.09889
C10	10.89519	5.77275	9.38019	N12	12.17536	6.21521	9.95405
N11	14.28199	6.78232	9.83708	C13	13.68495	7.57180	11.10251
N12	12.16034	6.39780	9.55707	H14	14.05222	8.59872	10.98823
C13	13.64815	7.93497	10.47777	H15	13.94716	7.22548	12.11289
H14	14.11385	8.86701	10.13557	C16	18.35293	7.47260	9.22061
H15	13.76596	7.87203	11.57144	C17	10.13141	4.88899	10.15270
C16	18.47115	6.59365	9.41757	C18	12.20336	7.41736	10.79860
C17	10.36222	5.05310	10.45606	H19	11.58918	7.27047	11.69431
C18	12.20156	7.78616	10.03421	H20	11.79178	8.27548	10.24429
H19	11.47701	7.93170	10.84422	C21	13.40697	5.85792	9.51680
H20	11.93764	8.47209	9.21408	C22	10.44581	6.38479	8.24365
C21	13.39192	5.86195	9.37692	C23	15.98867	7.82189	8.77874
C22	10.23401	5.88236	8.15120	C24	17.32312	8.12108	8.53585
C23	16.29536	7.26760	8.55843	H25	17.57058	8.85811	7.76979
C24	17.67981	7.17553	8.42981	C26	16.68877	6.23734	10.50862
H25	18.15166	7.57806	7.53198	C27	8.42063	5.05199	8.42491
C26	16.47526	6.20622	10.75895	C28	9.20121	5.99173	7.75795
C27	8.44769	4.49836	9.06230	H29	8.84363	6.41507	6.81790
C28	9.00847	5.23440	8.01676	C30	11.25423	7.40538	7.50027
H29	8.48644	5.28572	7.05980	H31	11.25839	8.37676	8.01504
C30	10.86983	6.59733	6.99820	H32	10.84579	7.57026	6.49718
H31	11.08496	7.64809	7.23337	H33	12.29932	7.09453	7.38818
H32	10.21712	6.57989	6.11986	C34	18.01713	6.54044	10.19503
H33	11.82826	6.13246	6.72227	H35	18.80972	6.04011	10.75251
C34	17.85579	6.13972	10.58304	C36	8.89560	4.52360	9.62408
H35	18.46779	5.72307	11.38473	H37	8.28847	3.79546	10.16452
C36	9.13321	4.42129	10.27364	C38	14.91136	8.45174	7.94892
H37	8.71193	3.83535	11.09152	H39	14.49742	7.71392	7.24392
C38	15.50616	8.01741	7.52673	H40	15.30461	9.29034	7.36543
H39	14.43907	7.77798	7.55207	H41	14.06957	8.81921	8.54889
H40	15.85997	7.78393	6.51771	C42	10.60507	4.31864	11.45296
H41	15.62714	9.09912	7.68220	H43	11.57742	3.82049	11.34512
C42	11.14582	4.88211	11.72303	H44	9.88152	3.59801	11.84628
H43	12.03153	4.24890	11.55474	H45	10.73608	5.10314	12.21036
H44	10.53650	4.41135	12.50079	C46	7.09955	4.61048	7.86951
H45	11.51753	5.83852	12.11492	H47	6.99092	4.89899	6.81809
C46	7.13298	3.80108	8.87518	H48	6.26085	5.05048	8.42389
H47	7.07455	3.31992	7.89134	H49	6.98936	3.52066	7.93426
H48	6.29523	4.50700	8.93646	C50	19.78447	7.76234	8.88356
H49	6.97290	3.03232	9.63820	H51	20.10256	7.18062	8.00824
C50	19.95123	6.44696	9.22627	H52	20.45540	7.50242	9.70877
H51	20.19146	5.48298	8.75731	H53	19.93423	8.82025	8.63945
H52	20.48772	6.48332	10.18084	H54	12.00853	2.79127	8.86479
H53	20.35411	7.23077	8.57551	O55	14.38077	5.24380	6.37685
H54	11.56450	3.66949	8.82691	C56	15.59389	5.17862	5.53129
O55	15.29511	2.41458	7.58163	H57	15.49930	6.03095	4.83935
C56	16.72863	2.22748	7.69643	C58	15.62293	3.87264	4.77059
H57	17.09648	2.03641	6.67465	H59	14.73674	3.74422	4.14009
C58	17.00256	1.05349	8.61237	H60	16.50464	3.85477	4.11993
H59	16.53517	0.13328	8.24508	H61	15.68805	3.03835	5.47752
H60	18.08209	0.88179	8.69363	C62	16.80480	5.39767	6.39565
H61	16.59923	1.27299	9.60822	H63	16.92227	4.58653	7.12166
C62	17.31595	3.52049	8.20298	H64	17.69235	5.41365	5.75184
H63	16.96070	3.73525	9.22008	H65	16.75033	6.35337	6.92110
H64	18.40823	3.43142	8.24424	O66	11.75538	5.70530	3.98528
H65	17.05896	4.35881	7.54503	C67	13.24171	5.29886	5.63130
O66	14.02466	0.01456	5.25399	C68	12.98877	6.01083	4.49656
C67	14.63763	1.58210	6.75359	H69	13.56966	6.71352	3.91727
C68	15.07915	0.61800	5.89823	C70	11.21487	4.77708	4.81780

C71 12.08112 4.50297 5.87531
 C72 11.69649 3.62184 6.90298
 C73 10.46598 2.97403 6.73804
 C74 9.64066 3.22079 5.63462
 C75 9.98770 4.14839 4.65922
 H76 9.34527 4.37107 3.81222
 H77 8.69486 2.69003 5.55090
 H78 10.13484 2.28432 7.51335
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 Ru1 13.88093 4.21455 8.83052
 C12 14.30772 3.78479 11.14760
 C13 14.26135 4.33843 6.48511
 C4 12.31020 3.27846 8.75130
 C5 15.61695 6.74933 9.17502
 C6 15.75108 6.65242 11.70530
 H7 15.90715 7.68327 12.05569
 H8 16.22473 5.98030 12.42762
 H9 14.67880 6.43601 11.71904
 C10 10.77706 6.04730 9.06824
 N11 14.21412 7.00213 9.26026
 N12 12.06542 6.64804 9.10776
 C13 13.64493 8.32068 9.53161
 H14 14.13515 9.08489 8.91677
 H15 13.78743 8.58584 10.59092
 C16 18.30351 6.05991 8.95378
 C17 10.18817 5.67139 10.28278
 C18 12.17741 8.11207 9.17274
 H19 11.48378 8.51253 9.92158
 H20 11.91455 8.55040 8.19767
 C21 13.27080 6.04125 9.08930
 C22 10.12994 5.88237 7.83980
 C23 16.23279 6.80026 7.91400
 C24 17.57272 6.43134 7.82734
 H25 18.05723 6.43627 6.85012
 C26 16.34889 6.48088 10.34218
 C27 8.22252 4.95484 9.04095
 C28 8.84450 5.34041 7.85353
 H29 8.32385 5.19516 6.90537
 C30 10.82686 6.20213 6.55177
 H31 11.12792 7.25641 6.49251
 H32 10.17739 5.99357 5.69558
 H33 11.74334 5.60291 6.43679
 C34 17.68695 6.12182 10.20257
 H35 18.26232 5.88193 11.09776
 C36 8.91043 5.11949 10.24363
 H37 8.44110 4.80232 11.17584
 C38 15.51980 7.32172 6.70225
 H39 14.43441 7.19447 6.76029
 H40 15.85582 6.80672 5.79755
 H41 15.73541 8.39312 6.57993
 C42 10.94939 5.79346 11.56912
 H43 11.80626 5.10194 11.59172
 H44 10.30895 5.56693 12.42702
 H45 11.36282 6.80127 11.71092
 C46 6.83675 4.38145 9.03234
 H47 6.59666 3.92317 8.06706
 H48 6.08492 5.15865 9.22173
 H49 6.71560 3.61911 9.80986
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 H51 19.76472 4.51812 8.63611
 H52 20.29735 5.79204 9.73661
 H53 20.23288 6.09061 7.98706
 H54 11.42816 3.65984 9.28384
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 H57 16.45442 0.33736 7.90405
 C58 16.56820 -0.17252 10.00854
 H59 16.00522 -1.10863 9.91805
 H60 17.63817 -0.41058 10.01395
 H61 16.30794 0.29063 10.96820
 C62 16.94806 2.11658 9.01989
 H63 16.65829 2.60502 9.95995
 H64 18.03466 1.96833 9.01989
 H65 16.68699 2.78734 8.19006
 O66 13.07179 -1.05367 6.67058
 C67 14.00336 0.43405 8.08816
 C68 14.14122 -0.77763 7.48437
 H69 14.91389 -1.53183 7.52096
 C70 12.23816 0.00979 6.76614
 C71 12.74445 0.97976 7.64469
 C72 12.01551 2.17692 7.83599

C73 10.78604 2.27834 7.16576
 C74 10.32699 1.30173 6.28017
 C75 11.04895 0.13536 6.06826
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 H77 9.37914 1.45079 5.76886
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 C5 15.73719 6.98627 9.60714
 C6 15.74140 5.80149 11.85800
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 H8 16.31462 4.97558 12.28983
 H9 14.74441 5.41516 11.63027
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 H15 13.76583 7.89746 11.46071
 C16 18.52370 6.90614 9.52772
 C17 10.90024 4.55631 10.49590
 C18 12.11342 7.65218 10.03022
 H19 11.43917 7.65336 10.89503
 H20 11.69671 8.32887 9.26940
 C21 13.51847 5.97595 9.19079
 C22 10.29581 5.41197 8.28202
 C23 16.41174 7.66646 8.58267
 C24 17.80406 7.59665 8.55715
 H25 18.33875 8.10573 7.75378
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 C27 9.04953 3.56576 9.27013
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 H35 18.37635 5.80421 11.36859
 C36 9.85357 3.64318 10.40659
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 H39 14.63404 8.29166 7.51327
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 H43 12.77346 4.04816 11.41430
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 H47 7.23080 2.75368 8.43156
 H48 7.53548 2.27804 10.11515
 H49 8.47500 1.55416 8.80598
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 H52 20.46950 6.73410 10.44326
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 H54 12.00229 3.29730 8.60000
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 H57 12.47859 -0.72524 10.56527
 C58 10.37575 -0.33262 10.89418
 H59 10.01083 -0.87689 10.01566
 H60 10.28870 -0.99010 11.76664
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 C62 12.29959 0.97233 11.87012
 H63 11.63055 1.82843 12.02110
 H64 12.31815 0.38226 12.79303
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 C68 11.99789 -0.98766 8.04904
 H69 11.68206 -1.86469 8.59479
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 C71 12.61277 0.99968 7.21537
 C72 13.00037 2.32656 6.91649
 C73 13.54049 2.55475 5.64256
 C74 13.66969 1.52481 4.70372

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 H77 14.07882 1.75705 3.72355
 H78 13.82481 3.57037 5.37388
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 H8 16.69125 5.79233 11.82821
 H9 15.02538 6.02594 11.32580
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 H20 11.49736 8.14229 8.87857
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 C28 9.17916 4.43640 8.30216
 H29 8.54050 4.35067 7.42083
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 H31 10.32303 7.16750 7.18243
 H32 9.97020 5.75170 6.18636
 H33 11.62587 6.04690 6.74502
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 H35 18.56020 6.44252 10.43428
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 H37 9.51789 3.16907 11.42515
 C38 15.19541 8.21694 6.63479
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 H40 15.50905 7.95657 5.61899
 H41 15.23450 9.31214 6.72676
 C42 11.76152 4.66290 11.72375
 H43 12.72344 4.17266 11.50183
 H44 11.31248 4.16394 12.58972
 H45 12.00019 5.69535 12.01264
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 H47 6.82345 3.18140 9.06393
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 H51 20.08263 5.93932 7.81566
 H52 20.44112 7.22127 8.97398
 H53 20.13574 7.61964 7.27053
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 H57 11.72616 -0.78613 11.06064
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 H69 9.63767 -0.83365 9.81545
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 C72 11.94294 2.53437 7.45241
 C73 11.73160 2.85608 6.10332
 C74 10.74266 2.23032 5.34126
 C75 9.92669 1.23461 5.87075
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 H78 12.34335 3.64065 5.66263
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 H81 16.28927 3.91705 6.35130
 C82 17.44347 3.22897 8.09888
 H83 17.58640 4.23728 8.51243
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 C86 15.22901 1.00666 7.96710
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 H88 15.81769 0.18942 7.52735
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