

Electronic supplementary information

Chiral transition-metal complexes as Brønsted-acid catalysts for the asymmetric Friedel-Crafts hydroxyalkylation of indoles

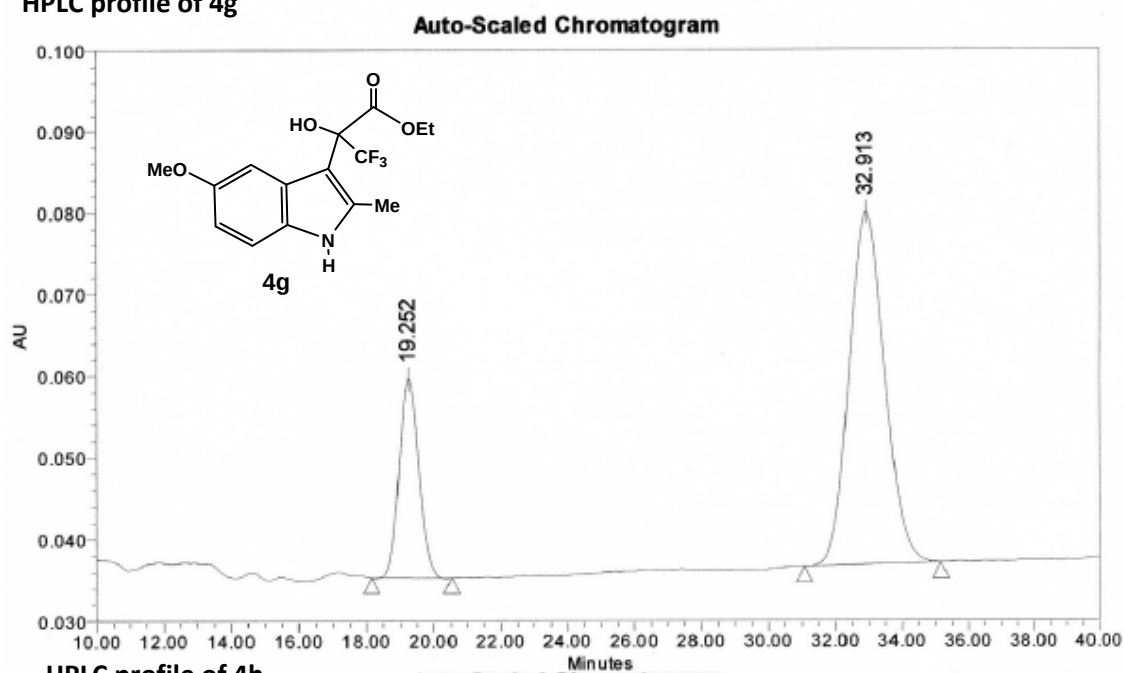
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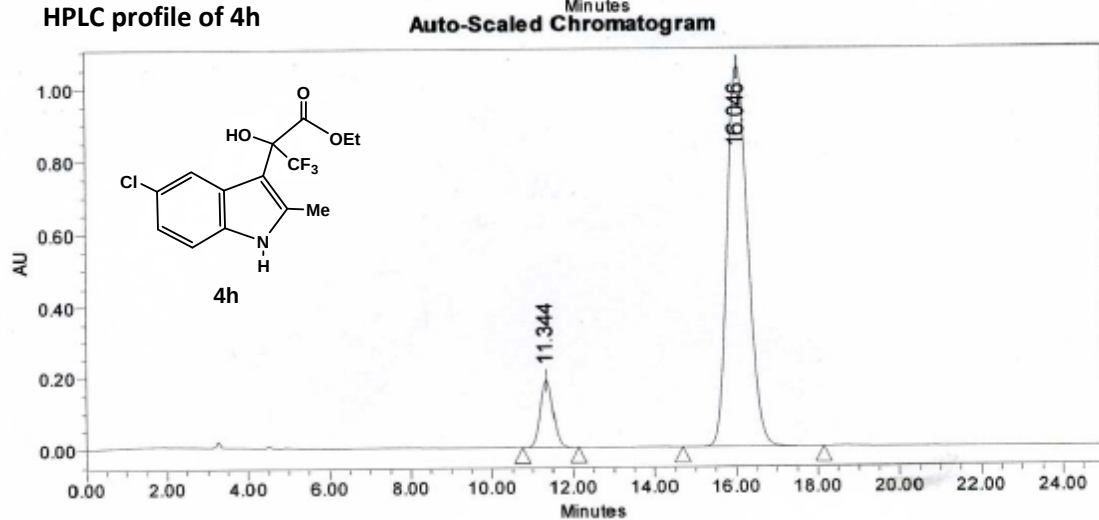
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HPLC chromatograms

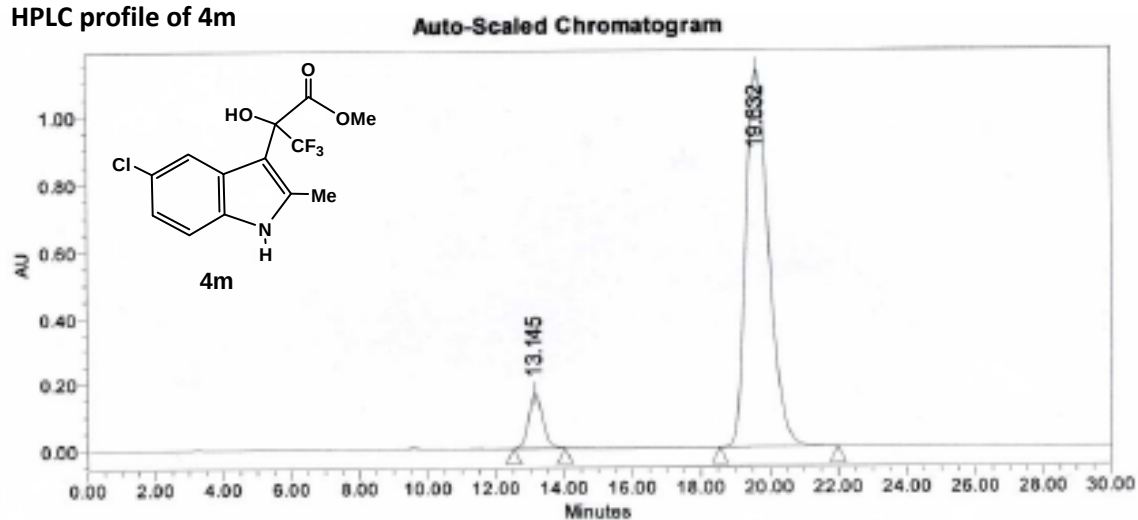
HPLC profile of 4g



HPLC profile of 4h

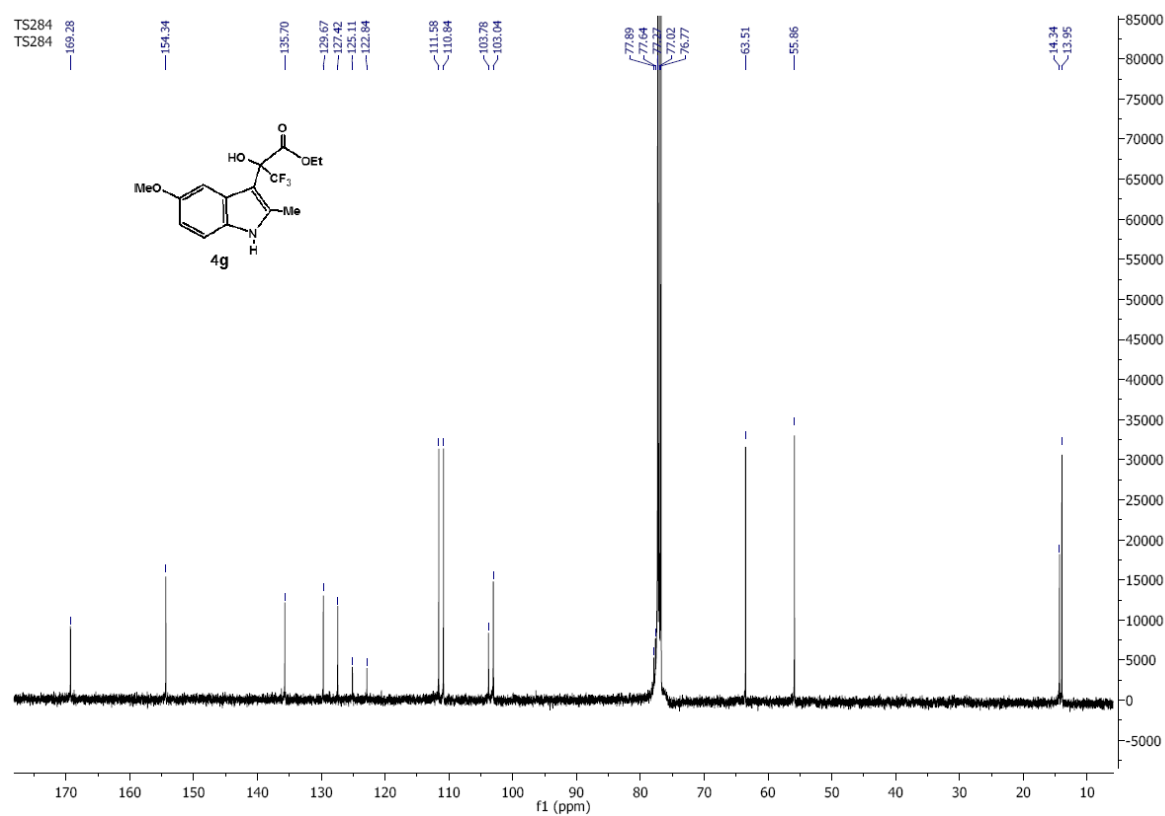


HPLC profile of 4m

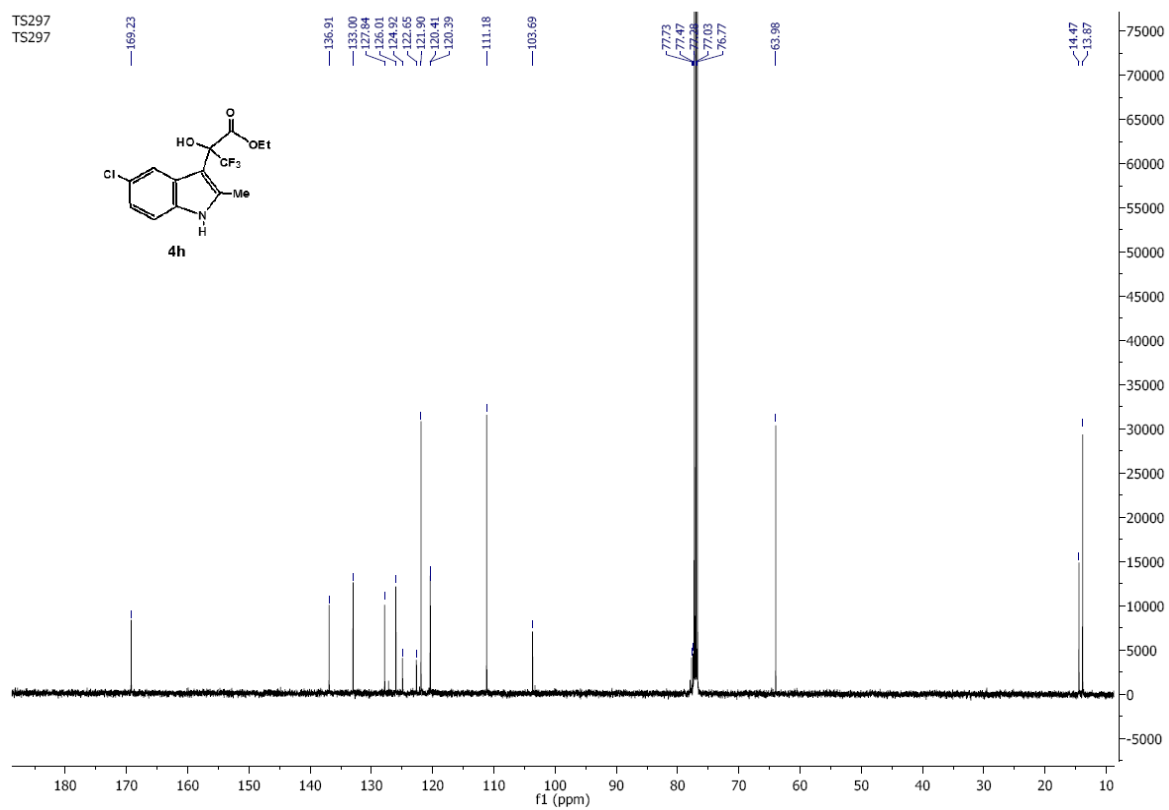


^{13}C NMR spectra

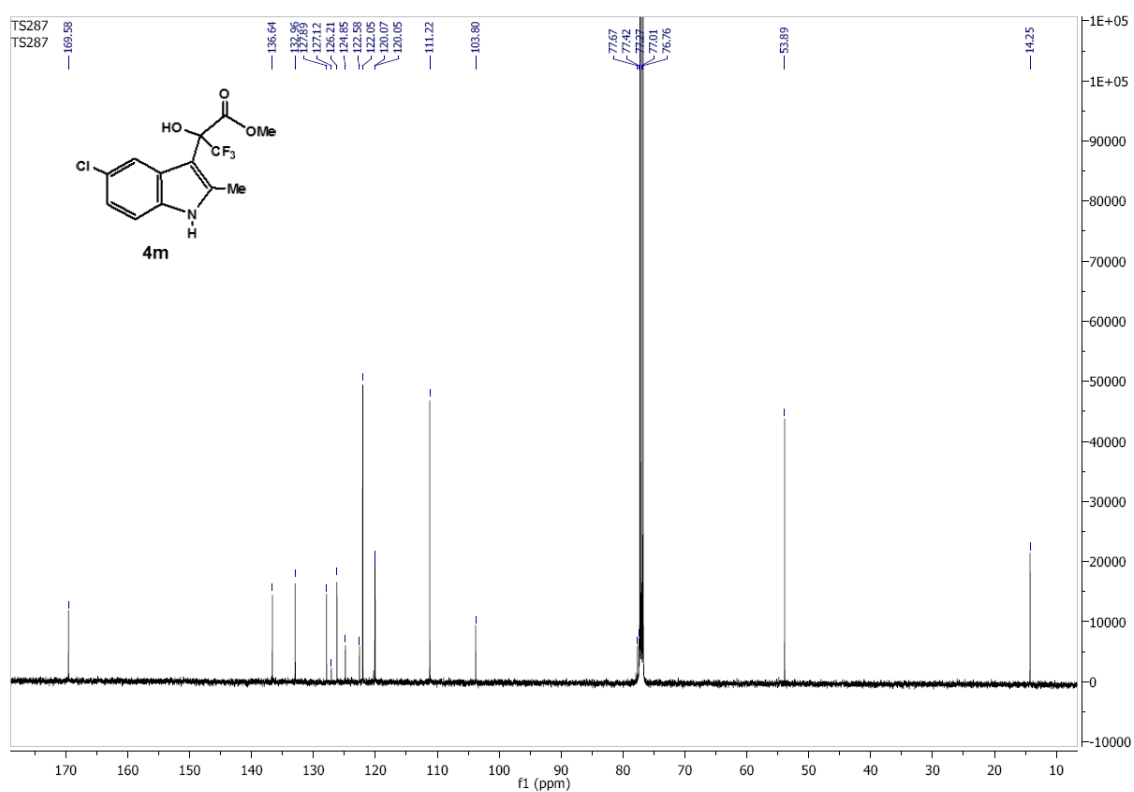
^{13}C NMR spectrum of 4g



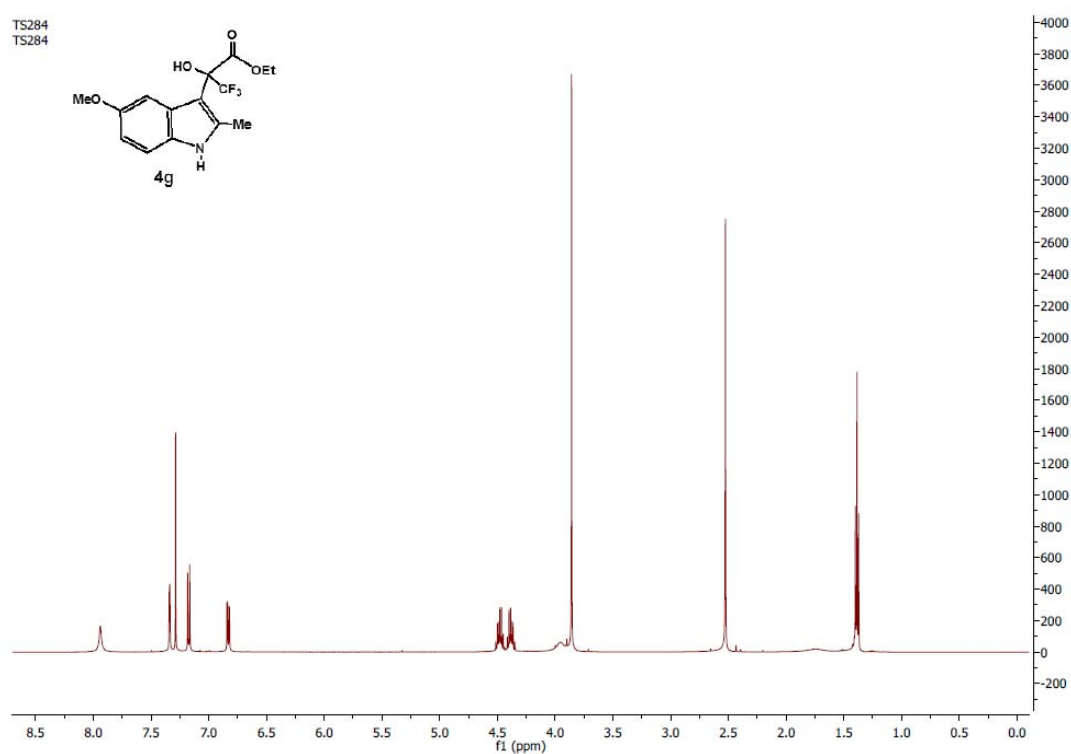
¹³C NMR spectrum of 4h



^{13}C NMR spectrum of 4m

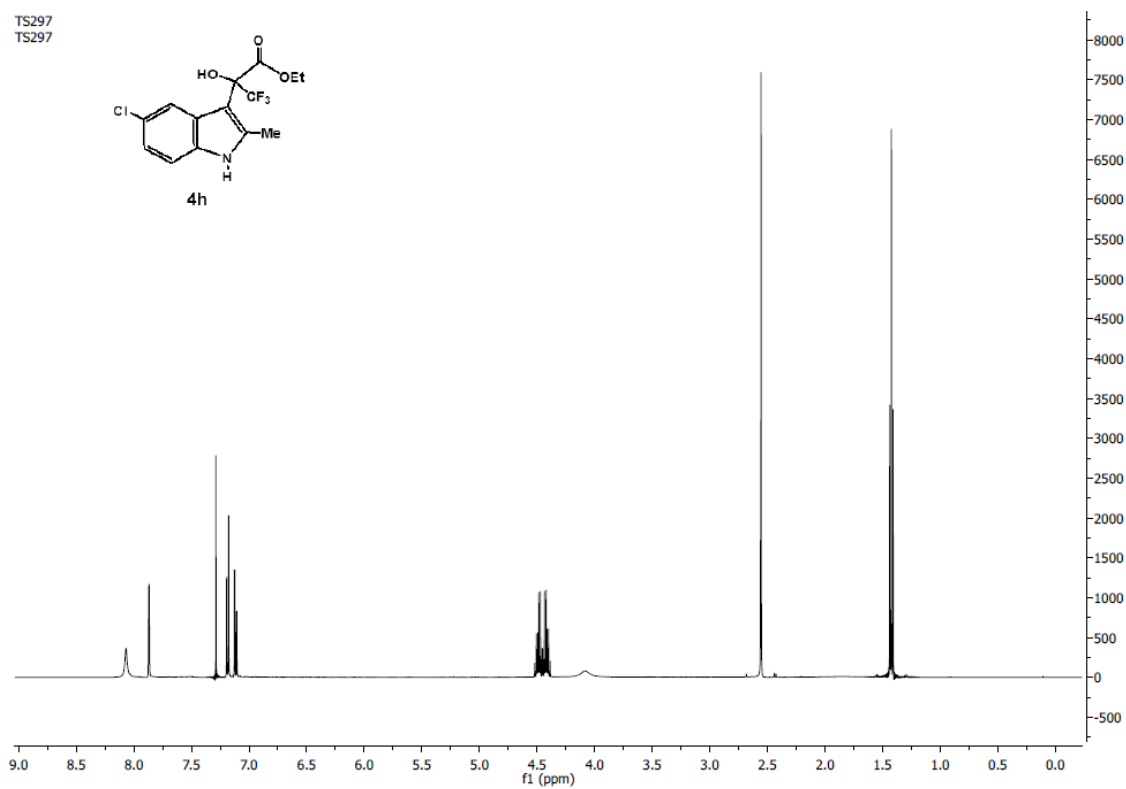


¹H NMR spectrum of 4g



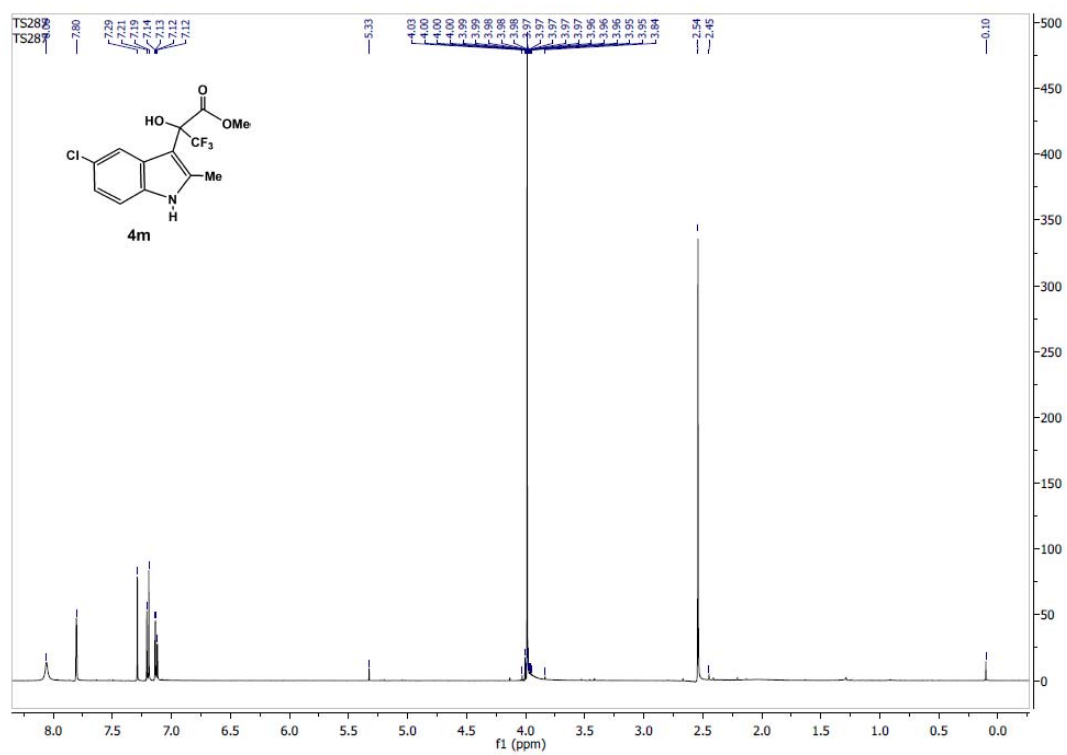
1

¹H NMR spectrum of 4h



6

¹H NMR spectrum of 4m



Cartesian coordinates (Angstroms) of the computed structures

1-t

O	-0.31862800	-0.39536600	2.27754800
H	-0.01522800	-1.22706300	2.68236300
H	-0.12109300	0.30171900	2.92778200
P	-1.39513800	1.56078700	0.06268400
P	-1.39898700	-1.49581400	-0.43388300
C	-2.89725700	0.80872200	-0.70189000
C	-3.01884200	-0.63829600	-0.23635100
H	-2.78260800	0.87352100	-1.79283600
H	-3.27729800	-0.69260300	0.83148400
H	-3.80386700	-1.17328600	-0.78512900
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C	2.48949000	0.69175500	0.39136500
C	1.51513400	0.22959900	-1.65405500
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O	1.42584300	-0.71396700	-0.07636000
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3a

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C 1.255809 -1.312430 -0.806899

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F 0.302548 -2.211696 -1.026424

O 0.585494 -1.275549 1.439770

C 2.088262 0.429596 0.795833

O 2.526015 0.382608 1.922043

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F 3.543881 -3.761931 -0.434610
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H -1.695183 -2.961998 3.400869
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H -2.720787 -4.132408 -1.535547
C -5.591170 -1.542437 -1.863164
H -4.137899 -0.061594 -1.315058
C -5.835811 -2.895922 -2.088237
H -4.989333 -4.874389 -2.151072
H -6.396073 -0.815279 -1.958141
H -6.834935 -3.230718 -2.358751
C -0.657113 -2.972564 -0.664567
C 0.211531 -3.522934 -1.609606
C -0.921269 -3.686328 0.512837
C 0.812143 -4.756819 -1.371560
H 0.438263 -3.010822 -2.542112
C -0.336832 -4.924246 0.740236
H -1.614141 -3.270061 1.242507
C 0.536662 -5.459701 -0.204279
H 1.498127 -5.167496 -2.109026
H -0.563404 -5.474207 1.652034
H 1.000416 -6.428524 -0.031021
C -2.504961 2.558241 -1.380237
C -2.905900 3.747540 -0.753990
C -3.291851 2.057353 -2.425037
C -4.071551 4.398193 -1.143502
H -2.290549 4.188718 0.028774
C -4.457187 2.710097 -2.814301
H -3.007118 1.152059 -2.956786

C -4.855440 3.876152 -2.168575
 H -4.361853 5.323386 -0.649815
 H -5.048458 2.309038 -3.635171
 H -5.765682 4.387103 -2.474591
 C 0.106097 2.968264 -0.248568
 C 0.838660 2.826072 0.933876
 C 0.234418 4.146181 -0.997257
 C 1.661024 3.855377 1.379259
 H 0.744100 1.903505 1.508297
 C 1.065591 5.168120 -0.554165
 H -0.340630 4.284492 -1.912277
 C 1.769279 5.028902 0.639418
 H 2.212370 3.743938 2.312832
 H 1.150683 6.084078 -1.135068
 H 2.402968 5.840176 0.993257
 RTS1-2full
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 H -1.040746 1.023904 0.456423
 F -2.819486 1.853786 0.991245
 C -3.910609 1.769723 0.178082
 F -4.965020 1.575130 0.965030
 F -4.026579 2.937118 -0.417158
 O -2.882400 0.972995 -1.859941
 C -5.097121 0.296743 -1.516340
 O -5.424376 -0.837263 -1.783650
 O -5.754559 1.390603 -1.814208
 C -7.025500 1.232167 -2.511890

H -7.171795 2.200020 -2.998470
H -6.897284 0.456682 -3.274497
P 1.651108 1.804857 -0.706808
P 1.674639 -1.300577 -1.218218
C 1.768652 1.192014 -2.450469
C 1.174054 -0.203116 -2.647194
H 2.835472 1.208349 -2.708818
H 0.081956 -0.136201 -2.490577
Ir 1.293491 -0.030981 0.733316
C 2.935858 -0.379240 2.155957
C 2.242286 0.805683 2.626134
C 2.033585 -1.505349 2.321195
C 0.892484 0.439933 2.899854
C 0.771818 -1.001130 2.722548
H 1.303547 1.912077 -3.137212
C -3.743412 0.604856 -0.815529
H -1.970707 0.982099 -1.507260
H -2.993871 -1.780941 -2.094932
C -3.218489 -1.793324 -1.033773
C -3.235582 -0.672891 -0.141764
C -3.679784 -1.256641 1.148622
C -3.733983 -2.649119 0.970243
H -3.436087 -3.837362 -0.798909
C -3.901555 -0.750833 2.431907
C -3.993453 -3.553801 1.990050
C -4.185312 -1.639648 3.463382
H -3.876626 0.316860 2.631206

C -4.227255 -3.022357 3.251579
H -4.034218 -4.626484 1.807896
H -4.384257 -1.249010 4.459103
H -4.454661 -3.687982 4.080839
N -3.452789 -2.913925 -0.379619
H -1.932736 -0.417558 0.006727
C -0.202785 1.295306 3.438039
H -1.160098 1.095795 2.935177
H -0.354928 1.092468 4.507851
H 0.011367 2.364587 3.336345
C 2.881042 2.126707 2.870425
H 2.149492 2.938565 2.953603
H 3.425360 2.084871 3.825074
H 3.607562 2.397031 2.094213
C 4.402717 -0.505658 1.917191
H 4.868630 0.468229 1.731994
H 4.893488 -0.941374 2.799555
H 4.624373 -1.157563 1.060574
C 2.423796 -2.936174 2.218283
H 3.319671 -3.070692 1.603027
H 2.661340 -3.313789 3.223589
H 1.624803 -3.569024 1.812977
C -0.449201 -1.784170 3.054184
H -0.364212 -2.835141 2.752335
H -0.624765 -1.770425 4.139851
H -1.347672 -1.361237 2.583264
C -8.126839 0.904783 -1.538643

H -9.085483 0.868239 -2.068507
H -7.964154 -0.072335 -1.070160
H -8.201181 1.669439 -0.757177
C 1.451527 -0.749538 -4.040857
H 0.901575 -1.678225 -4.229860
H 1.129722 -0.025037 -4.799850
H 2.520589 -0.942958 -4.200131
C 3.163369 2.792727 -0.482020
C 3.145444 4.185495 -0.366133
C 4.389972 2.115854 -0.438366
C 4.336934 4.885422 -0.193928
H 2.206341 4.733609 -0.414905
C 5.575647 2.818912 -0.270785
H 4.420961 1.028445 -0.520879
C 5.549312 4.206453 -0.141285
H 4.313935 5.969353 -0.105594
H 6.523187 2.283952 -0.237503
H 6.477298 4.757405 -0.004518
C 0.271368 2.991559 -0.640959
C -0.561955 3.262785 -1.729588
C 0.047008 3.660562 0.570161
C -1.577823 4.207467 -1.616283
H -0.435510 2.745676 -2.680211
C -0.960727 4.610195 0.678248
H 0.692231 3.454353 1.425117
C -1.770948 4.888650 -0.419735
H -2.225763 4.403213 -2.467662

H -1.112614 5.135563 1.619077
 H -2.563808 5.628741 -0.336869
 C 3.385067 -1.903132 -1.463797
 C 3.733981 -3.170188 -0.973456
 C 4.387918 -1.114465 -2.042475
 C 5.047459 -3.622476 -1.041240
 H 2.973268 -3.823794 -0.548183
 C 5.699510 -1.572469 -2.117331
 H 4.162144 -0.133705 -2.453841
 C 6.034936 -2.823602 -1.609513
 H 5.295715 -4.611001 -0.660279
 H 6.459209 -0.949315 -2.584861
 H 7.060615 -3.180780 -1.669004
 C 0.692169 -2.835206 -1.340454
 C -0.163525 -3.185726 -0.294152
 C 0.908712 -3.753271 -2.379735
 C -0.757048 -4.445824 -0.258031
 H -0.346211 -2.471439 0.509911
 C 0.281799 -4.992584 -2.363392
 H 1.608881 -3.524017 -3.182274
 C -0.536717 -5.349550 -1.291946
 H -1.379208 -4.720236 0.595400
 H 0.458830 -5.698328 -3.172059
 H -0.985726 -6.340529 -1.259973

RTS1-3full

O -0.914654 -0.062383 0.147004

H -1.255230 -0.846228 0.621685
F -6.062625 -0.049017 0.028372
C -5.252865 -0.194118 -1.032612
F -5.641995 -1.238000 -1.738291
F -5.380272 0.880122 -1.800028
O -3.008217 -0.609161 -1.620843
C -3.709545 -1.552852 0.469025
O -2.877389 -1.583224 1.363994
O -4.524019 -2.529071 0.175235
C -4.448459 -3.747143 0.967875
H -4.842184 -4.512156 0.292060
H -3.390321 -3.953546 1.171769
P 1.298048 -1.632362 -1.038838
P 1.817087 1.434069 -0.734181
C 0.920116 -0.550250 -2.514227
C 1.818681 0.681682 -2.426395
H 2.850053 0.402731 -2.685459
H 1.505722 1.432117 -3.165579
Ir 1.187155 -0.206726 0.844455
C 2.811573 -0.155077 2.357188
C 2.235649 -1.476297 2.416271
C 1.799668 0.789090 2.803299
C 0.853113 -1.348375 2.761567
C 0.601721 0.059158 3.019162
H -0.123480 -0.226044 -2.364330
C -3.809984 -0.347984 -0.507677
H -2.083679 -0.499227 -1.313029

H -4.105606 0.572912 2.308723
 C -3.889810 1.248916 1.487342
 C -3.345670 0.937119 0.200074
 C -3.363805 2.236516 -0.514102
 C -3.842956 3.204458 0.376780
 H -4.492545 3.001504 2.417704
 C -3.010120 2.626420 -1.804822
 C -4.031314 4.539835 0.042181
 C -3.199086 3.953925 -2.163742
 H -2.652928 1.895319 -2.527854
 C -3.709330 4.896443 -1.258503
 H -4.428903 5.262978 0.751712
 H -2.962087 4.270179 -3.177457
 H -3.860112 5.923538 -1.583721
 N -4.121978 2.546776 1.588373
 H -2.054769 0.646416 0.364750
 C -0.107501 -2.456431 3.029655
 H -1.136674 -2.187699 2.763446
 H -0.099005 -2.720479 4.097171
 H 0.144801 -3.361286 2.464700
 C 2.999646 -2.744916 2.280166
 H 2.341965 -3.618678 2.224775
 H 3.632601 -2.874408 3.170192
 H 3.664171 -2.754097 1.408068
 C 4.263631 0.156931 2.234020
 H 4.813035 -0.637869 1.715621
 H 4.704842 0.253907 3.237059

H 4.444368 1.100820 1.704086
 C 2.050678 2.217303 3.138062
 H 2.879762 2.630901 2.552640
 H 2.329234 2.300345 4.198678
 H 1.171115 2.852820 2.980248
 C -0.695821 0.604461 3.501081
 H -0.805688 1.671378 3.270198
 H -0.760383 0.497015 4.593653
 H -1.543946 0.059578 3.067585
 C -5.276275 -3.615443 2.218897
 H -5.297252 -4.573334 2.750795
 H -6.308912 -3.342552 1.974805
 H -4.858761 -2.862771 2.897363
 C 1.073814 -1.241866 -3.862567
 H 0.465475 -2.150566 -3.941378
 H 2.120049 -1.522415 -4.042923
 H 0.767256 -0.565810 -4.670636
 C 2.899380 -2.409595 -1.405211
 C 2.999204 -3.551316 -2.210465
 C 4.066283 -1.807571 -0.925944
 C 4.250351 -4.070099 -2.526092
 H 2.102363 -4.040169 -2.590255
 C 5.316549 -2.325205 -1.245187
 H 3.983493 -0.931378 -0.283253
 C 5.407546 -3.460230 -2.046318
 H 4.321528 -4.957967 -3.150587
 H 6.217157 -1.846666 -0.861786

H 6.382003 -3.875005 -2.295187
C 0.087949 -2.991715 -1.034070
C -1.089494 -2.952076 -1.784632
C 0.331575 -4.097694 -0.207592
C -2.020394 -3.984007 -1.692917
H -1.297749 -2.128805 -2.462741
C -0.589143 -5.134744 -0.128839
H 1.264737 -4.162413 0.353731
C -1.768905 -5.076366 -0.869673
H -2.933265 -3.932487 -2.284047
H -0.378959 -5.998373 0.498996
H -2.485063 -5.894594 -0.814863
C 3.464642 2.209614 -0.545252
C 3.574599 3.404516 0.180466
C 4.627099 1.626043 -1.063628
C 4.819477 3.982501 0.404362
H 2.679902 3.902360 0.555899
C 5.869323 2.213483 -0.846948
H 4.582258 0.709798 -1.650016
C 5.969752 3.386140 -0.104864
H 4.888158 4.912951 0.964249
H 6.761807 1.757105 -1.270671
H 6.942157 3.844659 0.061608
C 0.728977 2.889530 -0.786626
C -0.092184 3.179355 0.305529
C 0.912786 3.853661 -1.785218
C -0.686621 4.431276 0.420548

H -0.237259 2.421500 1.078175
C 0.296659 5.093767 -1.681394
H 1.583411 3.660319 -2.623232
C -0.489589 5.388373 -0.569569
H -1.306576 4.663151 1.285371
H 0.451496 5.842735 -2.455257
H -0.948851 6.370738 -0.473982

RTS1-4full

O 0.716890 -0.025259 -0.118255
H 1.126735 0.775288 0.274110
F 5.811680 -0.636531 -0.915018
C 4.863352 -0.310399 -1.790664
F 5.281801 0.678498 -2.558346
F 4.653602 -1.375328 -2.575012
O 2.630929 0.329525 -2.053884
C 3.719928 1.288304 -0.130729
O 2.801563 1.660116 0.579533
O 4.893325 1.862082 -0.196926
C 5.119555 3.028202 0.641343
H 4.312569 3.744191 0.442443
H 5.031466 2.707369 1.687630
P -1.474805 1.818077 -0.699427
P -2.023726 -1.262933 -1.103959
C -1.540339 1.145474 -2.441540
C -2.457820 -0.068878 -2.438950
H -3.494367 0.247591 -2.247596

H -2.476083 -0.571891 -3.416537
Ir -1.265846 -0.046122 0.768606
C -2.745142 -0.156432 2.441130
C -1.798735 0.880714 2.789378
C -2.026675 -1.414444 2.420689
C -0.502947 0.294610 2.856303
C -0.647888 -1.139755 2.630586
H -0.509048 0.805786 -2.636514
C 3.563064 0.054096 -1.050350
H 1.746526 0.327342 -1.629457
H 2.484543 -2.543458 -1.835530
C 2.871979 -2.380722 -0.833574
C 3.103185 -1.128647 -0.183862
C 3.691883 -1.499071 1.122619
C 3.650805 -2.898966 1.210050
H 2.981212 -4.355514 -0.229113
C 4.157714 -0.779759 2.223668
C 4.036315 -3.617910 2.332625
C 4.563021 -1.481168 3.353678
H 4.203703 0.307515 2.211885
C 4.500860 -2.879029 3.412101
H 3.989014 -4.704362 2.365505
H 4.942077 -0.932174 4.212801
H 4.827509 -3.393997 4.312340
N 3.136584 -3.377034 -0.008392
H 1.857414 -0.793486 0.004731
C 0.769612 0.978959 3.218135

H	1.637863	0.507021	2.741669
H	0.928495	0.937915	4.305264
H	0.773421	2.033871	2.918766
C	-2.164643	2.282800	3.126616
H	-1.288010	2.937895	3.174506
H	-2.635612	2.303479	4.120309
H	-2.886584	2.712804	2.420057
C	-4.228081	-0.033180	2.538400
H	-4.566344	1.000042	2.401818
H	-4.556524	-0.349401	3.539731
H	-4.748978	-0.671067	1.813743
C	-2.672637	-2.750481	2.323371
H	-3.537855	-2.744151	1.649663
H	-3.035947	-3.047530	3.318143
H	-1.978959	-3.530390	1.987762
C	0.458866	-2.131434	2.717410
H	0.246479	-3.036642	2.133232
H	0.621007	-2.441831	3.759983
H	1.405013	-1.709370	2.357002
C	6.485207	3.556558	0.306051
H	6.710493	4.429354	0.928592
H	6.542235	3.859948	-0.744968
H	7.255009	2.798738	0.487828
C	-1.970935	2.161256	-3.492299
H	-1.349140	3.064286	-3.487342
H	-3.012125	2.471323	-3.333104
H	-1.903965	1.718374	-4.494247

C -2.945501 2.874375 -0.520938
 C -2.939692 4.223392 -0.898003
 C -4.133496 2.302610 -0.055536
 C -4.105549 4.975783 -0.807405
 H -2.025542 4.690959 -1.261969
 C -5.297730 3.056509 0.035281
 H -4.129616 1.261173 0.262775
 C -5.283268 4.396420 -0.341978
 H -4.093237 6.023043 -1.101478
 H -6.214956 2.601462 0.405791
 H -6.190648 4.992304 -0.271522
 C -0.062577 2.971027 -0.684610
 C 0.844618 3.081164 -1.743647
 C 0.102146 3.791322 0.439444
 C 1.882750 4.007143 -1.686001
 H 0.756790 2.458036 -2.632094
 C 1.139011 4.712136 0.496721
 H -0.613955 3.735123 1.259935
 C 2.024972 4.828080 -0.572413
 H 2.571687 4.092260 -2.524235
 H 1.242822 5.357721 1.366369
 H 2.818759 5.572840 -0.541857
 C -3.545082 -2.268215 -0.965302
 C -3.587150 -3.649098 -1.178697
 C -4.733120 -1.599456 -0.636842
 C -4.785285 -4.345175 -1.039074
 H -2.693834 -4.196107 -1.471422

C -5.926841 -2.295812 -0.500601
H -4.734448 -0.518866 -0.493404
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H -4.803602 -5.418820 -1.213329
H -6.840833 -1.759972 -0.251726
H -6.886403 -4.222952 -0.585079
C -0.771963 -2.394746 -1.808387
C -0.388929 -3.513753 -1.056572
C -0.250002 -2.235258 -3.094682
C 0.428671 -4.492299 -1.612161
H -0.785643 -3.649841 -0.048689
C 0.602025 -3.196038 -3.637026
H -0.517262 -1.371416 -3.701788
C 0.922700 -4.337900 -2.907390
H 0.657858 -5.392466 -1.041802
H 0.992036 -3.063472 -4.643950
H 1.548427 -5.109612 -3.352041

RTS1-5full

O 0.810102 -0.587508 0.462827
H 0.845611 -1.500947 0.794917
F 2.348845 -2.873406 0.868824
C 3.457369 -2.792698 0.083864
F 4.494967 -3.012603 0.884374
F 3.389894 -3.765748 -0.804678
O 2.480506 -1.358237 -1.558310
C 4.838077 -1.334159 -1.421628

O 4.882589 -1.440306 -2.614578
O 5.856973 -1.110082 -0.598444
C 7.157981 -0.939461 -1.224040
H 7.868792 -1.195872 -0.433604
H 7.245864 -1.667319 -2.037472
P -1.922844 -1.307524 -0.868248
P -1.043937 1.632898 -0.717455
C -1.184672 -0.586049 -2.463503
C -0.400528 0.699180 -2.173120
H -2.112424 -0.310628 -2.985986
H 0.644724 0.462660 -1.926729
Ir -1.262796 0.012838 0.989525
C -2.894038 0.504075 2.428596
C -2.626364 -0.914273 2.552637
C -1.715620 1.216009 2.893150
C -1.266424 -1.074634 2.939206
C -0.714161 0.255866 3.173160
C 3.512862 -1.423398 -0.622415
H 1.675019 -1.091929 -1.069708
H 4.061828 -1.142590 2.359265
C 4.033796 -0.314353 1.658313
C 3.418831 -0.254262 0.368904
C 3.795817 1.084421 -0.137982
C 4.508315 1.739118 0.875354
H 5.054635 1.051247 2.839009
C 3.617206 1.725388 -1.363362
C 5.061334 3.004929 0.735493

C 4.165912 2.992606 -1.524726
H 3.104633 1.228253 -2.185640
C 4.879101 3.621746 -0.495178
H 5.622592 3.483543 1.535679
H 4.052412 3.504002 -2.478323
H 5.304001 4.608868 -0.664142
N 4.589676 0.848376 1.959118
H 2.085092 -0.250651 0.613214
C -0.556991 -2.362046 3.191639
H 0.529708 -2.256168 3.072624
H -0.732777 -2.715152 4.217506
H -0.892499 -3.152645 2.506921
C -3.634269 -1.993479 2.388471
H -3.167644 -2.974313 2.244850
H -4.249194 -2.051138 3.298439
H -4.312858 -1.802188 1.547918
C -4.246561 1.118109 2.289636
H -4.985157 0.405393 1.907811
H -4.598044 1.454150 3.276143
H -4.247563 1.993281 1.627354
C -1.632955 2.681977 3.144802
H -2.491136 3.211496 2.717084
H -1.645696 2.874852 4.226892
H -0.719301 3.134340 2.738337
C 0.646779 0.522877 3.712090
H 0.906526 1.586803 3.657164
H 0.700246 0.221853 4.768018

H 1.409373 -0.051058 3.169392
C 7.320673 0.477337 -1.711206
H 8.332911 0.622027 -2.105716
H 6.611156 0.695176 -2.517969
H 7.166527 1.196030 -0.895356
C -3.696760 -1.286967 -1.287168
C -4.226534 -2.202598 -2.207311
C -4.504814 -0.253769 -0.810831
C -5.553116 -2.096104 -2.607368
H -3.609547 -3.008089 -2.606028
C -5.833916 -0.151947 -1.208775
H -4.079604 0.484774 -0.135217
C -6.360251 -1.077178 -2.103653
H -5.960562 -2.814567 -3.315547
H -6.454344 0.654339 -0.820383
H -7.399761 -1.004843 -2.416312
C -1.491579 -3.067471 -0.653480
C -0.179654 -3.534401 -0.811281
C -2.475212 -3.959883 -0.199078
C 0.135601 -4.859849 -0.529975
H 0.609686 -2.883140 -1.180649
C -2.152404 -5.281388 0.087625
H -3.505857 -3.628771 -0.086623
C -0.846632 -5.734172 -0.076583
H 1.154512 -5.211295 -0.676261
H -2.929414 -5.962888 0.427973
H -0.597463 -6.771031 0.138731

C -2.535516 2.511562 -1.277793
C -3.168562 3.371581 -0.371472
C -3.064470 2.364608 -2.561923
C -4.328077 4.045294 -0.731836
H -2.729622 3.531862 0.614995
C -4.225536 3.043247 -2.922972
H -2.580115 1.724931 -3.298106
C -4.862417 3.874297 -2.008178
H -4.807837 4.718524 -0.024066
H -4.628594 2.925478 -3.926599
H -5.768089 4.405416 -2.293202
C 0.142795 2.968746 -0.383328
C 0.977540 2.898479 0.734995
C 0.174187 4.104603 -1.199656
C 1.802810 3.968473 1.060113
H 0.962094 2.000973 1.356614
C 1.018388 5.163005 -0.884697
H -0.481602 4.174296 -2.068383
C 1.817828 5.103264 0.254355
H 2.437856 3.917898 1.943954
H 1.034544 6.048068 -1.517241
H 2.455920 5.946168 0.513827
H -0.368753 1.348938 -3.060892
C -0.420155 -1.536897 -3.377420
H 0.588714 -1.763320 -3.012787
H -0.951485 -2.484769 -3.525186
H -0.303571 -1.069394 -4.363622

RTS1-6full

O 0.657089 -0.351551 -0.026263
H 0.754922 -1.312806 0.100586
F 2.575488 -2.354293 0.172938
C 3.636100 -1.979729 -0.593441
F 4.734918 -2.284512 0.091819
F 3.593847 -2.713973 -1.686404
O 2.675225 -0.222296 -1.945920
C 4.937927 0.044017 -1.402046
O 5.366056 1.132091 -1.091123
O 5.496236 -0.812565 -2.223971
C 6.801796 -0.461374 -2.766423
H 6.869238 -1.056786 -3.680578
H 6.788880 0.602722 -3.025065
P -2.123283 -1.438202 -0.847770
P -1.319127 1.596464 -1.089214
C -2.428669 -0.517864 -2.439094
C -1.355374 0.549220 -2.614829
H -3.369061 0.005926 -2.190182
H -0.365831 0.098103 -2.776388
Ir -1.329428 0.117202 0.767136
C -2.877038 0.414788 2.350179
C -2.202686 -0.836157 2.637791
C -1.910758 1.478706 2.505654
C -0.825947 -0.552499 2.848491
C -0.642306 0.892360 2.770485

C 3.565728 -0.468333 -0.890669
H 1.770079 -0.321724 -1.586498
H 2.952883 2.272129 -0.804455
C 3.200401 1.751147 0.115684
C 3.160922 0.340931 0.346965
C 3.706943 0.196975 1.720659
C 3.898569 1.494130 2.227550
H 3.629693 3.407735 1.278138
C 3.924198 -0.878800 2.585712
C 4.292089 1.772318 3.528596
C 4.330321 -0.622259 3.890947
H 3.796062 -1.905066 2.254147
C 4.513373 0.683227 4.360260
H 4.426380 2.793314 3.880686
H 4.518638 -1.458170 4.561146
H 4.835664 0.847280 5.385802
N 3.554343 2.398769 1.210954
H 1.821428 0.096712 0.351230
C 0.247595 -1.530374 3.176857
H 1.222154 -1.213396 2.781477
H 0.358753 -1.624817 4.266443
H 0.031155 -2.529441 2.779180
C -2.895680 -2.140580 2.817087
H -2.201420 -2.988332 2.809583
H -3.396532 -2.147109 3.796412
H -3.670278 -2.314711 2.058628
C -4.357254 0.590319 2.379802

H -4.884497 -0.214614 1.854558
H -4.698219 0.568298 3.425919
H -4.675591 1.552682 1.962957
C -2.238851 2.929901 2.509933
H -2.883730 3.221115 1.670872
H -2.782519 3.175276 3.434000
H -1.338093 3.553864 2.492771
C 0.623972 1.611255 3.073933
H 0.748106 2.508618 2.453190
H 0.646723 1.927120 4.127145
H 1.494702 0.965873 2.913535
C 7.885205 -0.798858 -1.776001
H 8.867925 -0.618077 -2.226134
H 7.806333 -0.177138 -0.876946
H 7.833983 -1.854466 -1.485755
C -3.719215 -2.277325 -0.578738
C -3.865436 -3.668403 -0.591264
C -4.855207 -1.475054 -0.401411
C -5.119531 -4.240409 -0.394278
H -3.007203 -4.314985 -0.763266
C -6.104421 -2.049765 -0.206951
H -4.767035 -0.388087 -0.416524
C -6.236095 -3.436672 -0.192525
H -5.221870 -5.323304 -0.406789
H -6.978551 -1.415556 -0.072799
H -7.213124 -3.889544 -0.038310
C -0.883441 -2.755812 -1.075289

C -0.068277 -2.872471 -2.206136
C -0.701199 -3.660075 -0.016514
C 0.865519 -3.900456 -2.297662
H -0.154631 -2.169832 -3.031401
C 0.227915 -4.688804 -0.113591
H -1.315051 -3.573922 0.881666
C 1.006489 -4.816598 -1.261483
H 1.485577 -3.981493 -3.187417
H 0.340125 -5.396621 0.705256
H 1.732775 -5.622334 -1.342742
C -2.748123 2.703637 -1.315071
C -2.668116 3.810708 -2.168620
C -3.963376 2.402540 -0.695579
C -3.792238 4.597342 -2.391915
H -1.728852 4.064228 -2.661228
C -5.085598 3.194384 -0.915568
H -4.015679 1.540990 -0.031180
C -4.998595 4.293335 -1.764667
H -3.726091 5.455855 -3.056719
H -6.027091 2.954871 -0.423867
H -5.872801 4.916349 -1.940397
C 0.111810 2.707104 -1.293927
C 0.307189 3.714153 -0.339850
C 0.934145 2.668741 -2.424047
C 1.300275 4.670846 -0.516388
H -0.354833 3.775677 0.525645
C 1.930116 3.628490 -2.599639

H 0.805276 1.903023 -3.186898
C 2.111407 4.631335 -1.650799
H 1.421757 5.468133 0.215402
H 2.556638 3.597330 -3.488483
H 2.875519 5.391335 -1.802316
H -1.580348 1.187138 -3.482591
C -2.704605 -1.361142 -3.678484
H -1.800221 -1.804973 -4.107370
H -3.408572 -2.174196 -3.459809
H -3.158865 -0.733096 -4.454770

RTS1-7full

O -0.909889 -0.010534 0.233738
H -1.315540 -0.738448 0.744123
F -6.047753 0.299282 0.013953
C -5.241611 0.065752 -1.033997
F -5.691345 -0.974034 -1.708535
F -5.294492 1.121378 -1.836000
O -3.026586 -0.522879 -1.585886
C -3.801392 -1.323536 0.537903
O -2.961964 -1.386035 1.424964
O -4.712111 -2.229118 0.308742
C -4.758692 -3.391474 1.183319
H -5.282384 -4.139937 0.582554
H -3.728187 -3.723893 1.359382
P 1.035971 -1.658744 -1.084918
P 1.954417 1.308419 -0.653303

C 0.738658 -0.440453 -2.439157
C 1.821193 0.632363 -2.399354
H 2.786126 0.125598 -2.556673
H 0.750071 -0.950574 -3.413957
Ir 1.196195 -0.358015 0.870377
C 2.874093 -0.506631 2.310349
C 2.191811 -1.779040 2.325942
C 1.958742 0.492876 2.839119
C 0.843818 -1.560515 2.756966
C 0.717322 -0.151701 3.076762
H -0.255123 0.011912 -2.296333
C -3.814569 -0.161194 -0.491934
H -2.103292 -0.539742 -1.259646
H -4.091864 0.950130 2.263381
C -3.810440 1.557667 1.408735
C -3.273953 1.125601 0.153734
C -3.168851 2.374790 -0.634934
C -3.570911 3.432975 0.188563
H -4.273673 3.409124 2.221788
C -2.750396 2.653261 -1.934340
C -3.606673 4.760056 -0.221057
C -2.777039 3.973343 -2.364471
H -2.465382 1.845842 -2.606050
C -3.206147 5.011877 -1.524603
H -3.941577 5.559179 0.437688
H -2.480672 4.208268 -3.384680
H -3.229619 6.031247 -1.903181

N -3.932552 2.875080 1.427892
H -2.014680 0.767878 0.363801
C -0.183046 -2.592726 3.089020
H -1.138059 -2.434582 2.570036
H -0.392242 -2.574364 4.168162
H 0.167239 -3.603446 2.853542
C 2.834902 -3.094418 2.062756
H 2.121602 -3.855856 1.728913
H 3.296409 -3.462470 2.990709
H 3.624914 -3.027963 1.306862
C 4.340209 -0.311143 2.134999
H 4.783933 -1.059461 1.467940
H 4.840720 -0.409582 3.109482
H 4.582366 0.681592 1.737896
C 2.311218 1.888993 3.217029
H 3.203125 2.238955 2.686390
H 2.533360 1.935467 4.292802
H 1.496587 2.597157 3.018497
C -0.515412 0.469039 3.631463
H -0.561406 1.546576 3.430113
H -0.536685 0.340756 4.723705
H -1.418011 -0.008568 3.229334
C -5.497497 -3.066407 2.454945
H -5.611466 -3.973832 3.058539
H -6.498741 -2.679821 2.234722
H -4.952098 -2.328564 3.054409
C 1.643559 1.669477 -3.497668

H 1.570779 1.169631 -4.471891
H 2.498877 2.354242 -3.551207
H 0.729913 2.261695 -3.354538
C 2.499204 -2.595773 -1.618428
C 2.384897 -3.654723 -2.526327
C 3.764655 -2.209015 -1.168511
C 3.527501 -4.308987 -2.974290
H 1.405068 -3.974739 -2.881992
C 4.905885 -2.861556 -1.621205
H 3.847705 -1.391250 -0.452221
C 4.785415 -3.913983 -2.524899
H 3.435034 -5.133117 -3.678302
H 5.887182 -2.551280 -1.264387
H 5.674244 -4.432664 -2.877804
C -0.341941 -2.842951 -1.144524
C -1.279395 -2.852984 -2.180801
C -0.436056 -3.800275 -0.128003
C -2.308359 -3.791820 -2.184633
H -1.224917 -2.130448 -2.994021
C -1.452452 -4.745912 -0.140168
H 0.302873 -3.810324 0.672582
C -2.393118 -4.739013 -1.170301
H -3.040490 -3.780706 -2.988889
H -1.507615 -5.495379 0.647891
H -3.188653 -5.481892 -1.186218
C 3.696006 1.856318 -0.503578
C 3.999657 2.951389 0.318701

C 4.748076 1.181509 -1.135961
 C 5.318202 3.345450 0.517829
 H 3.199287 3.516049 0.796635
 C 6.065729 1.583245 -0.940646
 H 4.561458 0.333927 -1.793196
 C 6.355229 2.659795 -0.108661
 H 5.535089 4.201071 1.154088
 H 6.869204 1.056189 -1.451540
 H 7.386254 2.972557 0.041280
 C 1.035380 2.876619 -0.493387
 C 0.114230 3.021704 0.548794
 C 1.376836 3.999925 -1.259928
 C -0.440140 4.265313 0.831997
 H -0.149340 2.150990 1.149793
 C 0.798983 5.234332 -0.993229
 H 2.125473 3.923980 -2.046206
 C -0.101107 5.371287 0.060683
 H -1.133796 4.371490 1.665566
 H 1.073142 6.099138 -1.593742
 H -0.534019 6.345265 0.282176

RTS1-8full

O -0.739715 -0.293943 -0.019687
 H -1.101610 -0.942156 0.616552
 F -5.835470 -0.571933 -1.048471
 C -4.854255 -1.263335 -1.619606
 F -5.201261 -2.534697 -1.717949

F -4.696199 -0.785628 -2.859568
O -2.584057 -1.761703 -1.604477
C -3.604015 -1.763078 0.566633
O -2.589262 -1.922476 1.225090
O -4.802352 -2.129522 0.937052
C -4.943183 -2.882731 2.176132
H -5.892539 -3.407312 2.043588
H -4.129150 -3.614502 2.219415
P 1.926905 -1.532049 -0.946314
P 1.514075 1.582353 -0.995170
C 2.284689 -0.604454 -2.516475
C 1.515825 0.707826 -2.654401
H 2.060221 1.363648 -3.351797
H 3.367663 -0.436093 -2.494203
Ir 1.291552 -0.008782 0.736047
C 2.865045 0.423575 2.232322
C 2.420660 -0.927884 2.492575
C 1.760256 1.314127 2.550664
C 1.029074 -0.883733 2.804459
C 0.629069 0.513398 2.850118
H 2.112411 -1.249815 -3.388185
C -3.536527 -1.101391 -0.831163
H -1.708685 -1.638560 -1.184325
H -2.720133 0.799530 -2.857628
C -3.119643 1.137053 -1.907911
C -3.185954 0.396233 -0.681291
C -3.902494 1.309238 0.238236

C -4.150695 2.501624 -0.454580
H -3.635519 3.065035 -2.465071
C -4.284695 1.228967 1.575795
C -4.787642 3.602622 0.099203
C -4.922042 2.320962 2.154665
H -4.104232 0.330230 2.162186
C -5.179773 3.489695 1.425961
H -4.974310 4.508318 -0.475102
H -5.240317 2.263736 3.193476
H -5.694567 4.318436 1.906276
N -3.631428 2.342723 -1.751384
H -1.917276 0.298091 -0.328030
C 0.179840 -2.015848 3.272956
H -0.833787 -1.989198 2.852821
H 0.078734 -1.974822 4.367577
H 0.622855 -2.988711 3.031630
C 3.285045 -2.134653 2.559855
H 2.751309 -3.053457 2.290244
H 3.638802 -2.252331 3.594742
H 4.168751 -2.058655 1.918445
C 4.274097 0.861734 2.027628
H 4.883443 0.070083 1.577819
H 4.734959 1.125248 2.990660
H 4.335223 1.743866 1.377829
C 1.863538 2.792429 2.675532
H 2.675454 3.196075 2.061066
H 2.088994 3.049723 3.720686

H 0.935784 3.310060 2.402847
C -0.726634 0.972801 3.259082
H -0.885354 2.040454 3.065645
H -0.868633 0.811404 4.337438
H -1.516507 0.410500 2.740836
C -4.961799 -1.975025 3.378198
H -5.201274 -2.560199 4.273458
H -5.731030 -1.200764 3.270648
H -3.984438 -1.501758 3.539027
C 0.107930 0.466400 -3.183714
H 0.162497 -0.040430 -4.156161
H -0.434455 1.407690 -3.332691
H -0.471674 -0.173821 -2.505201
C 3.474004 -2.462935 -0.698939
C 3.482185 -3.853856 -0.568379
C 4.683326 -1.758232 -0.617637
C 4.682272 -4.527407 -0.353155
H 2.554532 -4.420423 -0.641557
C 5.878326 -2.434279 -0.409933
H 4.694650 -0.669261 -0.702121
C 5.877554 -3.821985 -0.272820
H 4.680571 -5.610984 -0.257438
H 6.813771 -1.880640 -0.355786
H 6.813707 -4.351523 -0.109516
C 0.670203 -2.803441 -1.289329
C 0.370988 -3.255916 -2.578048
C 0.059416 -3.422005 -0.190916

C -0.530981 -4.299934 -2.761240
H 0.837711 -2.809415 -3.454430
C -0.835312 -4.468501 -0.376297
H 0.294476 -3.081481 0.818988
C -1.132477 -4.907387 -1.664046
H -0.760853 -4.641088 -3.768126
H -1.304238 -4.937862 0.486632
H -1.836621 -5.722841 -1.813502
C 3.026135 2.612743 -0.972249
C 2.990950 3.885465 -0.385702
C 4.245616 2.136114 -1.469954
C 4.149935 4.648163 -0.283474
H 2.050101 4.295870 -0.018636
C 5.400385 2.905172 -1.376010
H 4.309466 1.163648 -1.955265
C 5.356742 4.159279 -0.773646
H 4.103998 5.636706 0.168874
H 6.335688 2.525755 -1.782360
H 6.260014 4.760913 -0.700840
C 0.199615 2.844376 -1.038527
C -0.639274 2.983678 0.068218
C 0.143170 3.793553 -2.067462
C -1.488559 4.080405 0.179081
H -0.603842 2.229517 0.853017
C -0.732717 4.869907 -1.974461
H 0.813143 3.720290 -2.925509
C -1.534265 5.024812 -0.842366

H -2.117931 4.188788 1.062381
H -0.764653 5.610867 -2.770955
H -2.187780 5.891703 -0.755476

STS1-1full

O 0.864003 0.201681 -0.611599
H 1.302726 -0.118736 -1.423988
F 5.846894 0.154860 0.698581
C 5.205420 1.128575 0.046844
F 5.915615 1.483459 -1.015707
F 5.116286 2.168502 0.863536
O 3.147176 1.803585 -0.824386
C 3.866834 -0.380497 -1.525384
O 2.943637 -0.516462 -2.308059
O 4.964347 -1.100271 -1.516139
C 5.233848 -1.964713 -2.658210
H 4.296272 -2.444548 -2.960297
H 5.919449 -2.716574 -2.258402
P -1.632500 1.612869 0.475396
P -1.106561 -1.484863 0.980884
C -1.500199 0.996021 2.221016
C -0.670909 -0.281950 2.349539
H -2.521181 0.852393 2.601282
H 0.373515 -0.018376 2.103904
Ir -1.248738 -0.199268 -0.991256
C -3.081349 -0.728084 -2.092256
C -2.586983 0.498594 -2.688931

C -2.123968 -1.773426 -2.401607
C -1.283226 0.242010 -3.205263
C -1.006958 -1.176760 -3.040758
H -1.053194 1.777651 2.851003
C 3.798332 0.660936 -0.379234
H 2.188036 1.612550 -0.870046
H 3.747641 -2.131521 0.723008
C 3.412624 -1.267803 1.289700
C 3.059415 0.033907 0.811066
C 2.790700 0.807082 2.045499
C 2.859388 -0.087846 3.122606
H 3.356962 -2.185034 3.144581
C 2.428252 2.130957 2.283039
C 2.590541 0.269122 4.437467
C 2.164455 2.508842 3.594707
H 2.390674 2.849334 1.466351
C 2.241839 1.595501 4.655818
H 2.661465 -0.444415 5.256099
H 1.910064 3.545593 3.808558
H 2.040458 1.933392 5.669882
N 3.237306 -1.337456 2.597833
H 1.888384 -0.094380 0.273688
C -0.397249 1.176510 -3.955055
H 0.651867 1.085872 -3.638480
H -0.426789 0.948007 -5.030201
H -0.703032 2.222075 -3.837672
C -3.349703 1.765124 -2.841701

H -2.706383 2.652370 -2.798316
H -3.839032 1.763240 -3.826537
H -4.134820 1.878254 -2.086771
C -4.459390 -0.976903 -1.579995
H -4.945337 -0.052809 -1.248178
H -5.085806 -1.412228 -2.371993
H -4.457925 -1.680207 -0.735487
C -2.343532 -3.229481 -2.198832
H -3.061416 -3.429394 -1.396517
H -2.758943 -3.660465 -3.121692
H -1.414934 -3.770191 -1.977133
C 0.167018 -1.881983 -3.627056
H 0.258954 -2.908816 -3.254293
H 0.044878 -1.946739 -4.718308
H 1.116647 -1.362645 -3.444902
C 5.855868 -1.152011 -3.763373
H 6.172162 -1.810305 -4.580146
H 5.144842 -0.423646 -4.170467
H 6.737255 -0.615145 -3.394822
C -0.715086 -0.837070 3.767066
H 0.027590 -1.630804 3.912501
H -0.481086 -0.041448 4.486458
H -1.703408 -1.240862 4.023084
C -3.265078 2.422133 0.407282
C -3.402794 3.748936 -0.013868
C -4.411575 1.685775 0.731744
C -4.666369 4.325810 -0.104509

H -2.525811 4.340238 -0.274524
C -5.670802 2.265909 0.643406
H -4.326129 0.642952 1.040704
C -5.799240 3.588408 0.222316
H -4.762792 5.359370 -0.429967
H -6.554684 1.687099 0.904764
H -6.784881 4.043333 0.151030
C -0.465798 3.003735 0.328894
C -0.324577 3.927240 1.371168
C 0.180969 3.243366 -0.886507
C 0.472473 5.054735 1.205398
H -0.859748 3.792370 2.311715
C 0.981187 4.370052 -1.050601
H 0.054722 2.537398 -1.706812
C 1.132820 5.272767 -0.001941
H 0.570911 5.772500 2.017660
H 1.490316 4.541527 -1.996845
H 1.758021 6.153863 -0.128388
C -2.584813 -2.437066 1.470078
C -2.691464 -3.790993 1.125249
C -3.671497 -1.819038 2.103028
C -3.860565 -4.498054 1.389816
H -1.856604 -4.305536 0.650535
C -4.834926 -2.529789 2.375542
H -3.615263 -0.775801 2.406927
C -4.935078 -3.869409 2.010702
H -3.925725 -5.549388 1.117268

H -5.662107 -2.036883 2.882308
H -5.845402 -4.425919 2.222608
C 0.224703 -2.744009 0.965738
C 0.994158 -2.925379 -0.187338
C 0.443979 -3.589698 2.063169
C 1.967642 -3.919705 -0.247719
H 0.822186 -2.279827 -1.046332
C 1.427780 -4.572813 2.009524
H -0.183889 -3.517540 2.950807
C 2.191231 -4.741185 0.854348
H 2.538724 -4.059876 -1.165387
H 1.576267 -5.234337 2.861054
H 2.940376 -5.529232 0.806842

STS1-2full

O 0.763532 -0.166222 0.201211
H 1.217371 -0.743452 0.847090
F 5.688129 -0.224910 -1.417856
C 4.661530 -0.917758 -1.901686
F 5.024719 -2.170584 -2.107527
F 4.343696 -0.386163 -3.089341
O 2.427204 -1.494904 -1.625728
C 3.717485 -1.507428 0.412690
O 2.842996 -1.587926 1.260816
O 4.932954 -1.962517 0.555397
C 5.257954 -2.648741 1.797131

H 4.529430 -3.457571 1.930426
H 5.121811 -1.932650 2.617720
P -1.666764 -1.632166 -0.836732
P -1.510024 1.536033 -0.858442
C -1.657777 -0.745187 -2.469327
C -0.979020 0.622565 -2.396604
H -2.697986 -0.668545 -2.812537
H 0.085145 0.437445 -2.165082
Ir -1.309280 -0.051410 0.882740
C -3.020071 0.226643 2.239954
C -2.464035 -1.075834 2.541794
C -2.034225 1.221780 2.631111
C -1.114172 -0.892043 2.970609
C -0.857002 0.537676 3.029293
H -1.141191 -1.360185 -3.217915
C 3.447669 -0.828014 -0.952861
H 1.614346 -1.440907 -1.081837
H 2.404129 1.188460 -2.792146
C 2.885061 1.467050 -1.859793
C 3.078841 0.650796 -0.696650
C 3.848070 1.522410 0.220375
C 4.011032 2.762449 -0.411872
H 3.316831 3.441047 -2.328230
C 4.335150 1.369654 1.518011
C 4.665995 3.844255 0.159542
C 4.995989 2.440272 2.110242
H 4.205366 0.436196 2.063917

C	5.169661	3.658298	1.439317
H	4.779462	4.790768	-0.365991
H	5.396656	2.328752	3.115456
H	5.702362	4.469502	1.929845
N	3.384980	2.673431	-1.666849
H	1.861228	0.486702	-0.227081
C	-0.184901	-1.926185	3.510177
H	0.839796	-1.810432	3.131035
H	-0.131543	-1.843368	4.605520
H	-0.521098	-2.944032	3.283294
C	-3.202175	-2.366150	2.504800
H	-2.551759	-3.214620	2.261074
H	-3.637319	-2.556281	3.496644
H	-4.024003	-2.357154	1.780236
C	-4.443851	0.519791	1.908692
H	-4.921040	-0.322252	1.394475
H	-5.016324	0.715507	2.826773
H	-4.540105	1.403770	1.264159
C	-2.271429	2.688327	2.710619
H	-3.110137	2.998082	2.078227
H	-2.528880	2.958503	3.744931
H	-1.389110	3.276688	2.427960
C	0.408903	1.138834	3.533414
H	0.451985	2.219566	3.355965
H	0.495350	0.981060	4.617994
H	1.294015	0.678745	3.070499
C	6.671588	-3.140993	1.675344

H 6.959561 -3.668450 2.591228
H 6.774238 -3.834723 0.834029
H 7.367909 -2.309001 1.525333
C -1.087518 1.394772 -3.703439
H -0.466264 2.298868 -3.691411
H -0.747018 0.773536 -4.541987
H -2.121249 1.697774 -3.915683
C -3.241740 -2.543605 -0.807891
C -3.280009 -3.937409 -0.712010
C -4.441808 -1.821424 -0.832284
C -4.504579 -4.597061 -0.644365
H -2.356624 -4.514967 -0.691302
C -5.661105 -2.484147 -0.771677
H -4.424305 -0.731017 -0.879141
C -5.692344 -3.874763 -0.674353
H -4.527754 -5.682178 -0.571992
H -6.589517 -1.916432 -0.796305
H -6.646894 -4.394159 -0.622909
C -0.393860 -2.929920 -0.968076
C -0.152754 -3.597263 -2.175922
C 0.275620 -3.350915 0.184335
C 0.760519 -4.643653 -2.228150
H -0.693846 -3.329339 -3.082820
C 1.188981 -4.398103 0.130991
H 0.079050 -2.852543 1.131917
C 1.435361 -5.042246 -1.077200
H 0.941808 -5.152937 -3.172037

H 1.706617 -4.708555 1.037015
 H 2.149215 -5.861828 -1.124202
 C -3.139813 2.313882 -1.125413
 C -3.440542 3.521415 -0.478470
 C -4.138548 1.696726 -1.889126
 C -4.710912 4.079204 -0.576365
 H -2.672946 4.044648 0.090651
 C -5.406113 2.259679 -1.990848
 H -3.935915 0.774913 -2.429424
 C -5.697944 3.447427 -1.327060
 H -4.925333 5.019900 -0.073211
 H -6.164142 1.773123 -2.601155
 H -6.688974 3.888606 -1.407994
 C -0.374940 2.960476 -0.700442
 C 0.529469 2.998404 0.365350
 C -0.443012 4.053014 -1.576367
 C 1.337434 4.111649 0.572053
 H 0.590580 2.142442 1.035240
 C 0.382812 5.156393 -1.382257
 H -1.170213 4.068507 -2.387944
 C 1.264633 5.191985 -0.302984
 H 2.025450 4.129634 1.417530
 H 0.315038 6.005234 -2.059963
 H 1.884547 6.071717 -0.136473

STS1-3full

O -0.782764 -0.218409 0.419678

H -0.982102 -1.068150 0.849761
 F -2.468123 -2.301981 1.131562
 C -3.723575 -1.988229 0.727064
 F -4.224023 -3.051333 0.123269
 F -4.424720 -1.762747 1.837676
 O -2.834884 -1.097574 -1.294996
 C -5.112248 -0.674661 -0.873153
 O -5.337747 -0.888398 -2.030311
 O -5.989028 -0.315666 0.060560
 C -7.386461 -0.326876 -0.344293
 H -7.876159 0.339064 0.371788
 H -7.454852 0.106247 -1.347941
 P 1.480648 -1.606870 -0.956576
 P 1.688459 1.513499 -0.819534
 C 0.905901 -0.642582 -2.449731
 C 1.674121 0.676429 -2.467448
 H 2.715944 0.486105 -2.763199
 H 1.256940 1.351945 -3.226947
 Ir 1.392392 -0.104383 0.874912
 C 3.154229 0.078869 2.202532
 C 2.615411 -1.245945 2.414457
 C 2.177315 1.036288 2.696571
 C 1.273262 -1.109577 2.878549
 C 1.019407 0.312192 3.072024
 H -0.158954 -0.424784 -2.255430
 C -3.699256 -0.792061 -0.250621
 H -1.928622 -0.928634 -0.971889

H -3.883039 0.364230 2.586096
 C -3.803915 0.949243 1.676543
 C -3.301133 0.547089 0.397761
 C -3.529905 1.739274 -0.453915
 C -4.074207 2.747452 0.351754
 H -4.536022 2.726473 2.453369
 C -3.366256 1.977014 -1.817399
 C -4.474522 3.987167 -0.126392
 C -3.759417 3.213761 -2.317176
 H -2.984697 1.198285 -2.474854
 C -4.307647 4.201839 -1.487955
 H -4.910828 4.744461 0.522163
 H -3.660003 3.412870 -3.382103
 H -4.620973 5.149726 -1.920249
 N -4.176365 2.218483 1.650846
 H -1.967965 0.370255 0.552617
 C 0.348564 -2.208606 3.282112
 H -0.689537 -1.859561 3.344173
 H 0.613942 -2.596023 4.276033
 H 0.368015 -3.052150 2.579146
 C 3.388819 -2.510273 2.288348
 H 2.758078 -3.390748 2.451238
 H 4.172294 -2.527300 3.059716
 H 3.892105 -2.609640 1.317678
 C 4.582560 0.403418 1.927288
 H 5.109913 -0.433744 1.455453
 H 5.099479 0.620335 2.873821

H 4.693032 1.287578 1.285305
C 2.442605 2.486181 2.892136
H 3.155561 2.869541 2.153552
H 2.889647 2.642496 3.884835
H 1.535247 3.099249 2.840496
C -0.241153 0.865440 3.637475
H -0.292984 1.955980 3.542562
H -0.314208 0.622745 4.706979
H -1.120148 0.432618 3.141040
C -7.928556 -1.731396 -0.289679
H -8.996918 -1.730544 -0.533287
H -7.807140 -2.159767 0.712219
H -7.418968 -2.374650 -1.016386
C 1.068059 -1.372873 -3.777353
H 0.541590 -2.333376 -3.802283
H 2.127783 -1.566861 -3.989996
H 0.671437 -0.757559 -4.594685
C 3.110168 -2.284827 -1.398571
C 3.225939 -3.489903 -2.103393
C 4.267207 -1.567917 -1.078242
C 4.480098 -3.955169 -2.483543
H 2.338365 -4.070237 -2.354036
C 5.520222 -2.034953 -1.459449
H 4.183336 -0.642615 -0.510000
C 5.626021 -3.230844 -2.164065
H 4.562883 -4.891818 -3.030585
H 6.413430 -1.468334 -1.199372

H 6.603728 -3.603208 -2.462335
C 0.396893 -3.059816 -0.796093
C -0.775970 -3.222490 -1.538325
C 0.756526 -4.050526 0.130794
C -1.589770 -4.334353 -1.335094
H -1.082734 -2.495069 -2.286492
C -0.052726 -5.161420 0.326079
H 1.696080 -3.968165 0.678231
C -1.235195 -5.299278 -0.400490
H -2.504119 -4.436658 -1.915691
H 0.243731 -5.928633 1.038681
H -1.870311 -6.168672 -0.245552
C 3.229762 2.500420 -0.809431
C 3.235313 3.769727 -0.214035
C 4.426578 1.997468 -1.336547
C 4.413036 4.505072 -0.131659
H 2.312404 4.197983 0.178199
C 5.599728 2.740506 -1.260849
H 4.462118 1.021594 -1.819083
C 5.597501 3.991574 -0.650886
H 4.400119 5.491151 0.327979
H 6.518130 2.342241 -1.687499
H 6.515507 4.572436 -0.594207
C 0.404493 2.799967 -0.844235
C -0.322764 3.056192 0.320533
C 0.310651 3.685978 -1.923719
C -1.105587 4.201411 0.420182

H -0.249723 2.355165 1.153007
C -0.494635 4.813794 -1.832381
H 0.901104 3.526865 -2.826609
C -1.190087 5.080110 -0.654924
H -1.644866 4.415382 1.342307
H -0.559620 5.502034 -2.672496
H -1.797900 5.979582 -0.576639

STS1-4full

O 0.747220 0.181222 0.099102
H 0.944605 1.067821 0.451671
F 2.812495 1.990259 0.767846
C 3.844120 1.732152 -0.079835
F 3.849758 2.698496 -0.979924
F 4.959710 1.796856 0.638454
O 2.770975 0.420276 -1.797273
C 5.005804 -0.129671 -1.362615
O 5.347771 -1.289780 -1.334409
O 5.634854 0.850679 -1.964712
C 6.873502 0.507789 -2.649186
H 7.550304 0.063765 -1.909641
H 6.639194 -0.258696 -3.397167
P -1.669915 1.764812 -0.608719
P -1.705725 -1.309952 -1.286418
C -1.241587 1.233551 -2.347057
C -2.013101 -0.056705 -2.606700
H -3.095322 0.146605 -2.607481

H -1.789369 -0.475249 -3.597868
Ir -1.333788 -0.166019 0.749476
C -2.943567 -0.624159 2.214357
C -2.236332 0.537274 2.711940
C -2.020300 -1.742670 2.240341
C -0.875178 0.173427 2.915253
C -0.748699 -1.255278 2.639950
H -0.166060 0.997291 -2.308748
C 3.672438 0.343386 -0.722507
H 1.871026 0.340100 -1.420848
H 2.905247 -2.296635 -1.279981
C 3.163505 -2.022240 -0.262062
C 3.205292 -0.705270 0.288668
C 3.712811 -0.914097 1.667965
C 3.797800 -2.303230 1.868105
H 3.445592 -3.926640 0.499771
C 3.968914 -0.081199 2.760500
C 4.125566 -2.897654 3.078051
C 4.311676 -0.656891 3.979016
H 3.923754 0.999933 2.672909
C 4.390910 -2.044614 4.140390
H 4.181224 -3.978842 3.188642
H 4.534669 -0.011201 4.825571
H 4.668413 -2.460009 5.106245
N 3.435252 -2.925879 0.662593
H 1.879167 -0.411624 0.351017
C 0.210452 1.058568 3.425656

H 1.205511 0.685472 3.149142
H 0.181855 1.114715 4.522965
H 0.114625 2.082799 3.040324
C -2.856159 1.847768 3.041189
H -2.106361 2.641953 3.125579
H -3.363397 1.773473 4.014187
H -3.609554 2.153887 2.304356
C -4.425162 -0.777312 2.138121
H -4.941580 0.187956 2.096255
H -4.782403 -1.292264 3.042267
H -4.738322 -1.383073 1.278123
C -2.419374 -3.156705 2.005179
H -3.095591 -3.263437 1.146311
H -2.956778 -3.533540 2.887807
H -1.556284 -3.814553 1.851771
C 0.488344 -2.052902 2.846392
H 0.501993 -2.960110 2.229086
H 0.569706 -2.366798 3.897386
H 1.389176 -1.472244 2.616382
C 7.412646 1.773036 -3.253009
H 8.351344 1.561477 -3.776608
H 7.614649 2.523333 -2.480604
H 6.706435 2.197375 -3.975285
C -1.500067 2.277700 -3.422738
H -0.978968 3.220650 -3.216983
H -2.572133 2.491456 -3.520986
H -1.145070 1.910638 -4.394137

C -3.345998 2.467820 -0.708391
C -3.573020 3.744177 -1.242712
C -4.436294 1.702855 -0.289276
C -4.871131 4.228547 -1.354812
H -2.737349 4.367045 -1.559840
C -5.734440 2.189262 -0.398717
H -4.253034 0.721899 0.143303
C -5.951313 3.454770 -0.934850
H -5.040205 5.219682 -1.770243
H -6.574221 1.583112 -0.061906
H -6.963195 3.844666 -1.021938
C -0.601753 3.181009 -0.198796
C 0.647379 3.386402 -0.797012
C -1.050613 4.089706 0.773589
C 1.417416 4.492270 -0.443464
H 1.039837 2.697059 -1.546404
C -0.272193 5.182658 1.129588
H -2.034127 3.963987 1.226124
C 0.961957 5.387608 0.516234
H 2.383229 4.642927 -0.919389
H -0.638057 5.887512 1.873407
H 1.565694 6.251994 0.784362
C -3.130964 -2.446848 -1.429015
C -2.992964 -3.815215 -1.684609
C -4.420437 -1.915626 -1.277758
C -4.116222 -4.634623 -1.756175
H -2.012022 -4.255970 -1.845076

C -5.538777 -2.736328 -1.353084
H -4.563675 -0.847025 -1.115899
C -5.387883 -4.102144 -1.581435
H -3.991536 -5.696066 -1.959562
H -6.532275 -2.306417 -1.241024
H -6.262988 -4.745803 -1.636479
C -0.266869 -2.301948 -1.821591
C 0.102125 -3.397372 -1.027721
C 0.409511 -2.081407 -3.023875
C 1.063862 -4.298885 -1.469387
H -0.410473 -3.574323 -0.080316
C 1.403957 -2.962536 -3.446390
H 0.164614 -1.229482 -3.656542
C 1.713185 -4.086309 -2.685646
H 1.293541 -5.181663 -0.873447
H 1.916744 -2.781790 -4.388563
H 2.456809 -4.796435 -3.042200

STS1-5full

O 1.003099 -0.462330 0.020855
H 1.358910 -1.296671 0.388615
F 6.091847 -0.029386 -0.892092
C 5.195120 -0.663267 -1.651380
F 5.663365 -1.858918 -1.977366
F 5.033172 0.040096 -2.763505
O 2.935388 -1.247523 -1.840560
C 3.938217 -1.809926 0.270135

O 2.932401 -2.350267 0.695383
O 5.144525 -1.966726 0.758720
C 5.329002 -2.928164 1.837475
H 6.355210 -3.278063 1.701757
H 4.637320 -3.760520 1.675705
P -1.810428 -1.211747 -1.113947
P -1.187322 1.633793 -0.245904
C -1.178459 -0.097296 -2.514633
C -0.604422 1.209067 -1.942492
H -2.109058 0.134636 -3.052913
H 0.481509 1.105426 -1.822227
Ir -1.004851 -0.394178 0.946147
C -2.423233 -0.455297 2.669139
C -2.133693 -1.820212 2.290281
C -1.196022 0.129080 3.181827
C -0.730117 -2.035859 2.439651
C -0.162010 -0.825636 3.017919
C 3.854759 -0.795330 -0.897313
H 2.046713 -1.096138 -1.462086
H 4.393049 0.556799 1.720863
C 4.036206 1.092666 0.844667
C 3.412259 0.561620 -0.330696
C 3.262502 1.739692 -1.218736
C 3.655609 2.865057 -0.484429
H 4.477649 3.013887 1.492330
C 2.808445 1.913691 -2.526201
C 3.597416 4.164704 -0.969637

C 2.752576 3.205263 -3.034322
 H 2.552101 1.053849 -3.142368
 C 3.131931 4.316001 -2.267031
 H 3.906474 5.018065 -0.369339
 H 2.425852 3.359762 -4.060545
 H 3.076736 5.311046 -2.702499
 N 4.119663 2.407849 0.760261
 H 2.184446 0.259618 0.032830
 C -0.010143 -3.324848 2.235072
 H 1.056790 -3.174481 2.030782
 H -0.087801 -3.954844 3.133026
 H -0.428448 -3.891935 1.394065
 C -3.130167 -2.855870 1.908846
 H -2.701679 -3.612236 1.240111
 H -3.473003 -3.376347 2.814799
 H -4.012156 -2.427972 1.418755
 C -3.775661 0.129741 2.908954
 H -4.578931 -0.517053 2.540002
 H -3.933844 0.249127 3.990619
 H -3.898177 1.120996 2.451177
 C -1.127748 1.430779 3.900173
 H -1.731060 2.206136 3.413915
 H -1.524838 1.305729 4.918359
 H -0.106216 1.813766 3.994103
 C 1.268087 -0.680719 3.405878
 H 1.523646 0.355242 3.659731
 H 1.483995 -1.300350 4.288159

H 1.936966 -1.020424 2.602320
C 5.123327 -2.259819 3.171377
H 5.324398 -2.972087 3.979506
H 5.809193 -1.413310 3.297098
H 4.087786 -1.911174 3.284487
C -3.610498 -1.096319 -1.379463
C -4.164870 -1.505582 -2.601404
C -4.431417 -0.493270 -0.429181
C -5.519974 -1.323423 -2.846814
H -3.539560 -1.976184 -3.362651
C -5.789959 -0.317030 -0.671258
H -3.991798 -0.129813 0.494881
C -6.334742 -0.732306 -1.881032
H -5.944788 -1.648536 -3.794188
H -6.415443 0.161783 0.081260
H -7.395857 -0.594671 -2.078429
C -1.363634 -2.954452 -1.395041
C -0.013907 -3.329773 -1.441741
C -2.345606 -3.953557 -1.421018
C 0.346849 -4.667473 -1.525793
H 0.767135 -2.576619 -1.410553
C -1.979544 -5.294569 -1.498211
H -3.401286 -3.689948 -1.380186
C -0.636657 -5.653912 -1.550188
H 1.400220 -4.936805 -1.569088
H -2.751705 -6.060557 -1.522883
H -0.355680 -6.703009 -1.612262

C -2.818723 2.417528 -0.420501
C -3.394866 3.018356 0.706091
C -3.529778 2.403518 -1.623086
C -4.668223 3.569039 0.636523
H -2.831144 3.081802 1.638714
C -4.802869 2.961564 -1.692777
H -3.103591 1.959064 -2.521746
C -5.376689 3.535015 -0.563538
H -5.104412 4.040081 1.515287
H -5.346490 2.945336 -2.635188
H -6.371983 3.970776 -0.619782
C -0.125103 2.995572 0.337914
C 0.740003 2.792447 1.413824
C -0.252257 4.276044 -0.213824
C 1.434440 3.863927 1.968610
H 0.842661 1.786149 1.825199
C 0.464382 5.338889 0.322857
H -0.942573 4.450509 -1.040133
C 1.290887 5.138176 1.427652
H 2.066192 3.707725 2.843907
H 0.354892 6.334333 -0.102725
H 1.812325 5.983195 1.874209
H -0.766362 2.051631 -2.631830
C -0.227061 -0.743610 -3.511354
H 0.742957 -0.997796 -3.067213
H -0.644284 -1.659815 -3.946672
H -0.033351 -0.043900 -4.335590

STS1-6full

O -0.711940 0.116108 -0.078386
H -1.037647 1.004343 0.178346
F -5.822136 -0.331766 -0.936888
C -4.835044 -0.203385 -1.819562
F -5.175042 0.669877 -2.749432
F -4.670686 -1.391095 -2.417527
O -2.566492 0.267607 -2.114535
C -3.625829 1.570010 -0.396201
O -2.692249 1.992600 0.263327
O -4.760302 2.193994 -0.579646
C -4.924166 3.498646 0.040051
H -4.087335 4.129295 -0.283819
H -4.842691 3.365174 1.126664
P 1.888956 1.624955 -0.726319
P 1.568271 -1.491424 -1.068248
C 2.398640 0.804764 -2.325157
C 1.531745 -0.422339 -2.577001
H 3.403841 0.439003 -2.049178
H 0.487935 -0.151649 -2.795493
Ir 1.250646 -0.075519 0.804556
C 2.715211 -0.204469 2.503217
C 1.865834 0.944444 2.739324
C 1.883695 -1.384374 2.576899
C 0.523592 0.486847 2.843000
C 0.532559 -0.968714 2.746208

C -3.532376 0.199690 -1.105929
H -1.700981 0.375385 -1.668110
H -2.625625 -2.565811 -1.435637
C -3.014713 -2.209985 -0.485544
C -3.158965 -0.854941 -0.050328
C -3.799895 -0.971661 1.280377
C -3.881687 -2.339436 1.583631
H -3.291656 -4.050300 0.411173
C -4.213809 -0.052751 2.245663
C -4.347858 -2.839047 2.791417
C -4.696668 -0.532667 3.458105
H -4.156619 1.019844 2.068671
C -4.762792 -1.904533 3.730565
H -4.395750 -3.907251 2.992602
H -5.037267 0.173713 4.211978
H -5.149195 -2.244309 4.688509
N -3.380864 -3.040921 0.473098
H -1.897373 -0.545106 0.114307
C -0.678628 1.327400 3.099437
H -1.593791 0.860951 2.714536
H -0.816329 1.477307 4.179784
H -0.593872 2.317043 2.633142
C 2.353857 2.330986 2.967862
H 1.556686 3.074745 2.854365
H 2.728776 2.415298 3.998556
H 3.181099 2.602096 2.300264
C 4.198768 -0.197377 2.654242

H 4.657619 0.698980 2.222293
H 4.449873 -0.200600 3.725854
H 4.672534 -1.083547 2.216246
C 2.405429 -2.778601 2.591947
H 3.115381 -2.972432 1.777132
H 2.940965 -2.954352 3.536247
H 1.603356 -3.522878 2.538040
C -0.659709 -1.840222 2.928532
H -0.879267 -1.984227 3.996559
H -1.552486 -1.395565 2.473619
H -0.514885 -2.832618 2.483552
C -6.265018 4.025862 -0.385040
H -6.434391 5.011804 0.061551
H -6.320389 4.127527 -1.474257
H -7.070865 3.359435 -0.059144
C 3.360201 2.644116 -0.368806
C 3.380985 4.038304 -0.478952
C 4.548410 1.972090 -0.052314
C 4.557734 4.742040 -0.235409
H 2.485988 4.586606 -0.765522
C 5.720767 2.676465 0.188701
H 4.559390 0.883713 0.006921
C 5.723763 4.067006 0.107970
H 4.560507 5.826298 -0.322965
H 6.635270 2.139822 0.434811
H 6.639203 4.622053 0.300954
C 0.516941 2.790309 -1.026595

C -0.297541 2.715173 -2.161061
C 0.245215 3.777495 -0.067248
C -1.314627 3.642795 -2.366270
H -0.137926 1.943103 -2.911473
C -0.757697 4.715008 -0.281711
H 0.850723 3.843129 0.838233
C -1.526651 4.659622 -1.441457
H -1.927004 3.577430 -3.263411
H -0.930921 5.496979 0.454852
H -2.292492 5.411894 -1.623357
C 3.135394 -2.412585 -1.215592
C 3.247037 -3.501150 -2.090297
C 4.257881 -1.998776 -0.494424
C 4.464711 -4.155225 -2.233930
H 2.383216 -3.844905 -2.659883
C 5.475011 -2.656600 -0.636726
H 4.165257 -1.158067 0.190963
C 5.577491 -3.736959 -1.507624
H 4.544948 -4.999833 -2.914834
H 6.342191 -2.328507 -0.066026
H 6.526730 -4.256062 -1.621533
C 0.316239 -2.785313 -1.373320
C 0.126942 -3.755860 -0.383919
C -0.333014 -2.929687 -2.604094
C -0.682131 -4.861818 -0.623064
H 0.649701 -3.658087 0.568693
C -1.147671 -4.035908 -2.842829

H -0.197729 -2.196741 -3.397277
 C -1.317422 -5.005686 -1.856689
 H -0.791047 -5.630594 0.141089
 H -1.633764 -4.148286 -3.809936
 H -1.927415 -5.884167 -2.059559
 H 1.916838 -0.994122 -3.434662
 C 2.579786 1.723083 -3.527567
 H 1.632101 2.071868 -3.950288
 H 3.175569 2.606299 -3.263848
 H 3.117989 1.189157 -4.320668

STS1-7full

O 0.795222 -0.258955 -0.606819
 H 1.086128 -1.082866 -1.027234
 F 5.046462 -1.455256 -2.111171
 C 3.984670 -0.840424 -1.630027
 F 3.787191 0.288945 -2.312953
 F 2.909348 -1.630667 -1.888779
 O 3.893294 -1.857844 0.510937
 C 5.549218 -0.224705 0.246709
 O 6.198106 -0.772398 1.090774
 O 5.910295 0.819359 -0.496644
 C 7.307511 1.218766 -0.395932
 H 7.313570 2.257042 -0.739524
 H 7.597422 1.183651 0.659497
 P -1.262309 -1.599758 0.914785
 P -1.636769 1.483960 0.563575

C -0.615757 -0.482338 2.230721
C -1.505826 0.755333 2.287853
H -2.534629 0.411609 2.483021
H -0.616735 -1.004378 3.200067
Ir -1.363590 -0.267666 -1.013596
C -3.169821 -0.218632 -2.294721
C -2.613158 -1.547197 -2.399560
C -2.221920 0.704347 -2.900450
C -1.287506 -1.432223 -2.922180
C -1.066436 -0.033463 -3.258122
H 0.422290 -0.202570 1.996203
C 4.102580 -0.632613 -0.107470
H 3.052894 -2.242110 0.210701
H 3.340326 2.151486 -1.044347
C 3.191564 1.800959 -0.029402
C 3.149502 0.444316 0.436490
C 3.015048 0.587468 1.909235
C 2.805207 1.948522 2.176157
H 2.743943 3.628427 0.830808
C 3.051478 -0.302346 2.985005
C 2.576999 2.464681 3.444923
C 2.830537 0.195465 4.264974
H 3.296956 -1.350210 2.830651
C 2.584025 1.555012 4.494389
H 2.425718 3.529888 3.612460
H 2.877097 -0.483799 5.113368
H 2.424891 1.908830 5.510422

N	2.928068	2.634661	0.958437
H	1.945831	0.167343	-0.018671
C	-0.353321	-2.543254	-3.263375
H	0.691895	-2.210665	-3.244417
H	-0.549484	-2.916413	-4.278844
H	-0.444419	-3.394265	-2.576442
C	-3.345322	-2.810831	-2.114751
H	-2.684772	-3.683159	-2.165005
H	-4.127480	-2.955009	-2.873810
H	-3.839549	-2.803967	-1.135458
C	-4.590502	0.113879	-1.989110
H	-5.089525	-0.686036	-1.429692
H	-5.148903	0.246295	-2.927562
H	-4.687909	1.046041	-1.416948
C	-2.510799	2.131093	-3.207278
H	-3.221483	2.562923	-2.493289
H	-2.968766	2.204437	-4.204414
H	-1.610762	2.757161	-3.214875
C	0.167698	0.480038	-3.911252
H	0.158068	1.571065	-4.012256
H	0.262039	0.057683	-4.921348
H	1.069528	0.192571	-3.353892
C	8.159624	0.321356	-1.254709
H	9.200865	0.662083	-1.233939
H	7.816383	0.334383	-2.295777
H	8.136448	-0.710433	-0.885439
C	-1.108768	1.705313	3.404793

H -1.125220 1.173039 4.364831
H -1.806987 2.548084 3.489742
H -0.090818 2.091438 3.263214
C -2.799084 -2.265115 1.625258
C -2.742394 -3.240356 2.628984
C -4.039641 -1.755438 1.232446
C -3.913906 -3.695812 3.222072
H -1.782930 -3.650774 2.946465
C -5.211254 -2.214056 1.826809
H -4.080760 -0.993168 0.454439
C -5.147255 -3.186989 2.820049
H -3.864485 -4.454803 3.999808
H -6.173855 -1.816517 1.509166
H -6.061505 -3.552983 3.282419
C -0.144611 -3.028961 0.819468
C 1.108734 -3.028884 1.438804
C -0.557599 -4.163996 0.111468
C 1.940624 -4.143558 1.340589
H 1.429059 -2.168630 2.026315
C 0.276833 -5.270980 0.007719
H -1.553283 -4.197101 -0.333003
C 1.529710 -5.259722 0.617220
H 2.910170 -4.139320 1.837693
H -0.055725 -6.151668 -0.537841
H 2.179507 -6.128904 0.544008
C -3.226744 2.387329 0.563376
C -3.348661 3.593471 -0.140651

C -4.361492 1.856823 1.192334
C -4.575695 4.243683 -0.222660
H -2.478405 4.039868 -0.622285
C -5.583326 2.516875 1.118254
H -4.311604 0.919699 1.745641
C -5.695439 3.706925 0.405464
H -4.652406 5.180859 -0.770023
H -6.451518 2.098478 1.623484
H -6.653044 4.219648 0.346477
C -0.425836 2.840167 0.306421
C 0.277679 2.874661 -0.902147
C -0.357508 3.954244 1.156082
C 1.003619 4.004168 -1.275650
H 0.243164 2.005365 -1.557493
C 0.397560 5.068187 0.802126
H -0.931774 3.978605 2.079637
C 1.066160 5.104261 -0.423636
H 1.512884 4.027245 -2.239118
H 0.428152 5.931038 1.464917
H 1.615288 5.996877 -0.718627

STS1-8full

O -0.745581 -0.181266 0.288732
H -1.016918 -0.721886 1.047302
F -3.896834 -2.765357 1.142545
C -3.823440 -1.452221 1.191864
F -4.872768 -0.973374 1.847303

F -2.725598 -1.158161 1.957120
O -2.866276 -1.600507 -1.022199
C -5.064969 -0.841054 -0.936898
O -5.389304 0.038279 -1.701713
O -5.747726 -1.926122 -0.659432
C -7.028544 -2.091768 -1.334764
H -7.593116 -2.744809 -0.664303
H -7.515252 -1.111957 -1.382520
P 1.699328 -1.754800 -0.820939
P 1.577923 1.358093 -1.214383
C 1.942328 -1.060585 -2.525041
C 1.286409 0.302421 -2.737703
H 1.790405 0.811139 -3.574395
H 3.030289 -1.008720 -2.650029
Ir 1.409626 0.010965 0.714075
C 3.184732 0.425956 1.962071
C 2.635287 -0.820746 2.454323
C 2.230225 1.478219 2.278485
C 1.307104 -0.568754 2.901044
C 1.063396 0.863290 2.797596
H 1.599871 -1.779716 -3.281181
C -3.691161 -0.814714 -0.207322
H -1.941365 -1.488544 -0.723998
H -2.972072 0.810719 -2.396713
C -3.204540 1.266025 -1.440587
C -3.184877 0.634064 -0.155482
C -3.683186 1.694110 0.757020

C -3.869262 2.854162 -0.011064
 H -3.556737 3.197344 -2.109300
 C -3.885383 1.783714 2.136642
 C -4.290168 4.070744 0.506784
 C -4.302530 2.994943 2.677282
 H -3.749998 0.922148 2.785303
 C -4.515607 4.122647 1.875289
 H -4.438309 4.941556 -0.129874
 H -4.485382 3.063180 3.747476
 H -4.862401 5.048453 2.328434
 N -3.529606 2.541285 -1.336263
 H -1.847741 0.438495 0.069323
 C 0.396527 -1.523631 3.595369
 H -0.654740 -1.398165 3.304018
 H 0.441726 -1.359630 4.681944
 H 0.676580 -2.568143 3.419790
 C 3.371162 -2.103568 2.592332
 H 2.716398 -2.978929 2.512249
 H 3.836290 -2.132685 3.588761
 H 4.172432 -2.212213 1.854480
 C 4.600512 0.656454 1.558137
 H 5.061611 -0.256919 1.165423
 H 5.194698 0.977568 2.426041
 H 4.687334 1.435759 0.790115
 C 2.509551 2.936962 2.205832
 H 3.277410 3.169717 1.460363
 H 2.891080 3.275584 3.180154

H 1.617600 3.533230 1.978835
C -0.184745 1.525075 3.269240
H -0.212289 2.592520 3.021566
H -0.268153 1.440984 4.362067
H -1.081522 1.054804 2.838979
C -6.830058 -2.697894 -2.698657
H -7.804528 -2.872401 -3.168847
H -6.308861 -3.659277 -2.628918
H -6.256957 -2.026327 -3.347780
C -0.198763 0.161285 -3.051524
H -0.329964 -0.461657 -3.945947
H -0.665521 1.133420 -3.251353
H -0.740518 -0.320670 -2.226818
C 3.169333 -2.811377 -0.618776
C 3.063235 -4.168728 -0.304593
C 4.440177 -2.235427 -0.755872
C 4.212729 -4.934036 -0.122357
H 2.084773 -4.637550 -0.206270
C 5.583596 -3.003505 -0.579197
H 4.543574 -1.173540 -0.990346
C 5.469736 -4.355400 -0.256523
H 4.121722 -5.991211 0.117520
H 6.566188 -2.549974 -0.695019
H 6.364678 -4.957701 -0.116787
C 0.296672 -2.915523 -0.855700
C -0.190073 -3.492034 -2.031807
C -0.231725 -3.330135 0.375146

C -1.197604 -4.451541 -1.975668
H 0.208797 -3.210166 -3.004638
C -1.221014 -4.302998 0.429693
H 0.153336 -2.894458 1.298954
C -1.711336 -4.858674 -0.749767
H -1.575627 -4.886617 -2.898180
H -1.611627 -4.629025 1.391253
H -2.493697 -5.613152 -0.710197
C 3.174147 2.206669 -1.486132
C 3.338093 3.528243 -1.050083
C 4.263218 1.552287 -2.075610
C 4.568519 4.165398 -1.176751
H 2.496332 4.072235 -0.622031
C 5.488437 2.195676 -2.212123
H 4.164924 0.537981 -2.457488
C 5.646533 3.499546 -1.752021
H 4.679564 5.193014 -0.836752
H 6.318728 1.679484 -2.689548
H 6.605670 4.001843 -1.857333
C 0.390851 2.739969 -1.271672
C -0.297364 3.095910 -0.110929
C 0.300588 3.559517 -2.404425
C -1.032491 4.276446 -0.058052
H -0.242536 2.444798 0.760096
C -0.465527 4.719101 -2.363672
H 0.858505 3.314115 -3.309394
C -1.116894 5.087626 -1.185615

H -1.542543 4.554463 0.863914

H -0.525911 5.357039 -3.243256

H -1.682115 6.017864 -1.147676

Absolute energies (atomic units) of the computed structures

	E(gas phase) a.u	G(gas phase, -78 °C) a.u	E(CH ₂ Cl ₂) a.u	G(CH ₂ Cl ₂ , -78 °C) a.u
1-t	-1137.20500231	-1137.021019	-1137.4744395	-1137.29045619
2a-t	-679.12531527	-679.06858	-679.16474673	-679.10801146
3a	-363.53924239	-363.428009	-363.56876104	-363.45752765
ADD1	-1816.37298692	-1816.115815	-1816.64095111	-1816.38377919
ADD2	-2179.96064848	-2179.570308	-2180.2180999	-2179.82775942
ADD3	-2179.97028757	-2179.581388	-2180.24381909	-2179.85491952
TS1	-2179.93076365	-2179.547948	-2180.20629958	-2179.82348393
Product	-1042.70997618	-1042.523524	-1042.77180804	-1042.58535586
RTS1-1full	-3378.48382702	-3377.586027	-3378.76970619	-3377.87190617
RTS1-2full	-3378.48448056	-3377.584022	-3378.76647539	-3377.86601683
RTS1-3full	-3378.48463281	-3377.588189	-3378.76852876	-3377.87208495
RTS1-4full	-3378.49307608	-3377.593292	-3378.77851705	-3377.87873297
RTS1-5full	-3378.47674311	-3377.576835	-3378.76354877	-3377.86364066
RTS1-6full	-3378.48760668	-3377.590248	-3378.77048023	-3377.87312155
RTS1-7full	-3378.48201739	-3377.583396	-3378.76763965	-3377.86901826
RTS1-8full	-3378.49171152	-3377.592554	-3378.77513060	-3377.87597308
STS1-1full	-3378.49405799	-3377.595049	-3378.77828745	-3377.87927846
STS1-2full	-3378.49170019	-3377.594553	-3378.77719385	-3377.88004666
STS1-3full	-3378.47945226	-3377.581842	-3378.76666717	-3377.86905691
STS1-4full	-3378.48845751	-3377.590442	-3378.76990613	-3377.87189062
STS1-5full	-3378.48173972	-3377.583022	-3378.76875813	-3377.87004041
STS1-6full	-3378.49065648	-3377.592729	-3378.77553219	-3377.87760471
STS1-7full	-3378.48214990	-3377.584449	-3378.76636213	-3377.86866123
STS1-8full	-3378.48526723	-3377.587023	-3378.76895773	-3377.87071330