

Supporting Information

Ligand-Controlled Regioselectivity in the Hydrothiolation of Alkynes by Rhodium N-Heterocyclic Carbene Catalysts

Andrea Di Giuseppe, Ricardo Castarlenas,* Jesús J. Pérez-Torrente, Marcello Crucianelli, Victor Polo, Rodrigo Sancho, Fernando J. Lahoz, and Luis A. Oro

X-ray determination of complex 2

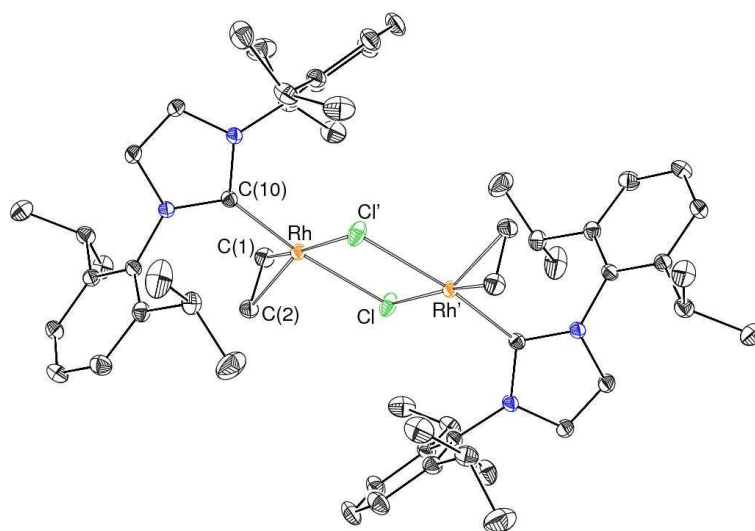
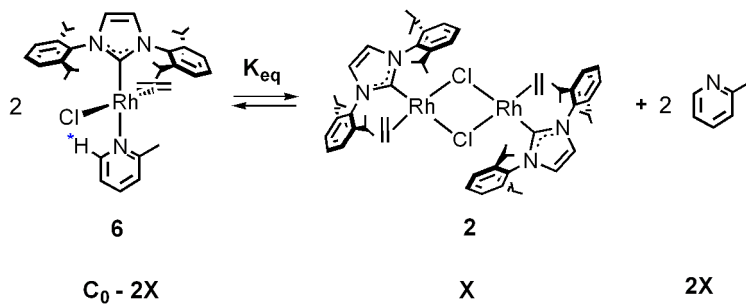


Figure 1. Molecular diagram of 2. Selected bond lengths (Å) and angles (°): Rh-Cl 2.4303(3), Rh-Cl' 2.3945(3), Rh-C(1) 2.1038(13), Rh-C(2) 2.0907(13), Rh-C(10) 1.9495(12); Cl-Rh-Cl' 83.963(11), Cl-Rh-C(10) 173.05(3), Cl-Rh-Ct 89.02(4), Cl'-Rh-C(10) 93.50(3), Cl'-Rh-Ct 168.10(4).

Determination of thermodynamic parameters for the equilibrium



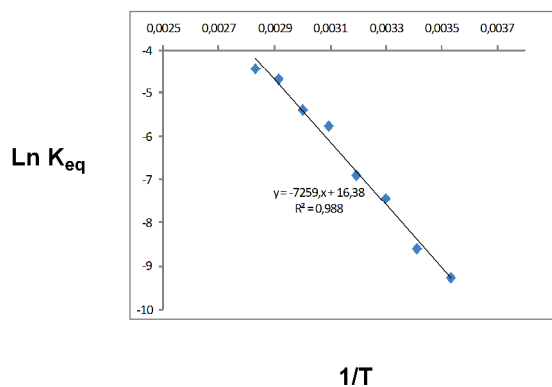
$$K_{eq} = \frac{[\text{Me-py}]^2 \cdot [2]}{[6]^2}$$

$$[6] = C_0 - 2X$$

$$[\text{Me-py}] = 2X$$

$$C_0 = 0.4 \text{ M}$$

$$I_6 / I_{py} = [6] / [\text{Me-py}]$$



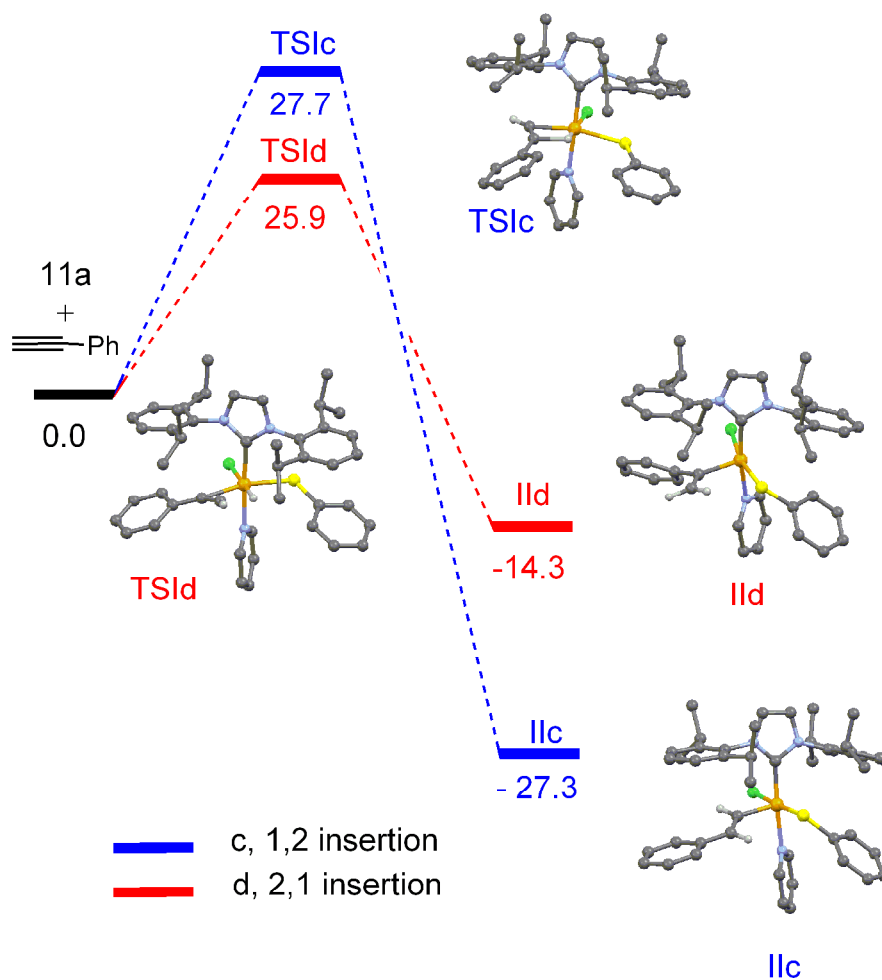
$$\Delta H^\circ = 14.4 \pm 0.5 \text{ kcal mol}^{-1} \text{ and } \Delta S^\circ = 32.5 \pm 1.3 \text{ cal K}^{-1} \text{ mol}^{-1}$$

DFT Calculations

Full reference 51:

Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Alkyne insertion into Rh-H bond



Cartesian coordinates (in Å) for the B3LYP optimized structures

11a

N 1.912845 -1.449222 -1.863511
N -1.317869 1.786935 0.541929
N -2.248088 -0.154438 0.775787
C 2.359077 -2.665003 -1.494690
H 1.969060 -3.045815 -0.557115
C 3.276472 -3.388255 -2.251184
H 3.598429 -4.366481 -1.909369
C 3.768232 -2.830121 -3.429637
H 4.490832 -3.366259 -4.038403
C 3.312137 -1.568903 -3.810370
C 2.380716 -0.916381 -3.008575
C -1.124009 0.456118 0.274658
C -3.117900 0.781314 1.329407
H -4.058947 0.490752 1.766261
C -2.536939 1.992667 1.183261
H -2.863744 2.978878 1.468919
C -0.424753 2.894704 0.256615
C 0.503311 3.284010 1.247864
C 1.314593 4.391623 0.971011
H 2.041871 4.713325 1.709202
C 1.199574 5.090161 -0.227025
H 1.839836 5.947412 -0.419137
C 0.256131 4.701468 -1.172907
H 0.162162 5.265129 -2.095373
C -0.583461 3.601096 -0.955406
C -2.537481 -1.577461 0.780018
C -3.278149 -2.126042 -0.291403
C -3.549509 -3.500228 -0.248678
H -4.106348 -3.955612 -1.060686
C -3.128829 -4.288341 0.817223
H -3.349414 -5.352750 0.825671
C -2.447717 -3.711892 1.884940
H -2.152149 -4.332032 2.724478
C -2.144672 -2.344595 1.901790
Rh 0.383722 -0.442128 -0.716188
C -1.502568 -1.728351 3.143927
C -0.457062 -2.637879 3.812781
C -2.589289 -1.341709 4.172589
H -0.983527 -0.813716 2.843157
H 0.293588 -2.976694 3.094313
H 0.061784 -2.079236 4.599677
H -0.917171 -3.513350 4.286782
H -3.310090 -0.626958 3.762905
H -3.146217 -2.227322 4.501888

H -2.129460 -0.883900 5.056508
C 0.597453 2.595495 2.607066
C -0.234875 3.362386 3.658012
C 2.044110 2.422382 3.101750
H 0.179767 1.590385 2.505782
H -1.289478 3.437781 3.371570
H -0.185759 2.852960 4.627839
H 0.148357 4.381343 3.792609
H 2.664510 1.915390 2.358204
H 2.511900 3.382471 3.352115
H 2.048702 1.811783 4.011532
C -3.863001 -1.273922 -1.415375
C -5.311359 -0.862238 -1.069468
C -3.826068 -1.964055 -2.789639
H -3.258633 -0.368315 -1.505412
H -5.366799 -0.297820 -0.132381
H -5.726211 -0.232027 -1.865058
H -5.955968 -1.743831 -0.966293
H -2.814773 -2.294958 -3.038190
H -4.507778 -2.821984 -2.841412
H -4.139856 -1.252444 -3.561164
C -1.662795 3.255797 -1.977902
C -1.169944 3.349930 -3.432252
C -2.903096 4.153175 -1.774279
H -1.960379 2.216317 -1.820724
H -0.282854 2.730260 -3.586610
H -1.950761 2.981324 -4.106336
H -0.941013 4.381271 -3.727627
H -3.322441 4.051067 -0.767191
H -2.653146 5.210624 -1.925153
H -3.687148 3.886077 -2.492794
Cl -0.784742 -0.173666 -2.805265
H 1.048441 0.913921 -0.785676
S 1.496663 -0.906309 1.306216
H 1.971026 0.048151 -3.280601
H 3.662038 -1.091010 -4.719621
C 3.265624 -0.766558 1.103869
C 4.088137 -1.662125 1.813079
C 3.885874 0.233906 0.332795
C 5.477925 -1.558458 1.754808
H 3.627388 -2.441785 2.413868
C 5.277292 0.325063 0.268607
H 3.271310 0.941737 -0.214466
C 6.083369 -0.567304 0.978669
H 6.089981 -2.262214 2.314382
H 5.731885 1.106015 -0.336908

H 7.166218 -0.490630 0.929406

11b

N -1.631129 -0.795121 -1.926778
N -1.352832 0.608784 1.540476
N 0.239965 1.916905 0.879345
C -2.512778 -1.788941 -1.711429
H -2.385628 -2.348980 -0.792371
C -3.522457 -2.109560 -2.614025
H -4.201242 -2.925439 -2.388663
C -3.626292 -1.380558 -3.797573
H -4.395887 -1.613040 -4.528105
C -2.713977 -0.351160 -4.025866
C -1.734062 -0.095372 -3.070301
C -0.349232 0.701894 0.600679
C -0.379732 2.536485 1.962692
H -0.055237 3.498510 2.322724
C -1.367871 1.716974 2.382129
H -2.076879 1.808748 3.188572
C -2.368296 -0.419763 1.615926
C -3.651936 -0.123854 1.101646
C -4.634677 -1.116336 1.202155
H -5.631043 -0.919363 0.818289
C -4.357635 -2.348739 1.787240
H -5.133395 -3.107580 1.848843
C -3.094569 -2.601936 2.314509
H -2.898919 -3.554610 2.795335
C -2.074448 -1.641335 2.260435
C 1.320894 2.583334 0.175052
C 2.591527 2.663997 0.785221
C 3.591297 3.369448 0.101211
H 4.580415 3.442048 0.541386
C 3.345842 3.972041 -1.126327
H 4.141183 4.505357 -1.640291
C 2.074911 3.906423 -1.689778
H 1.890044 4.401916 -2.636721
C 1.031716 3.227328 -1.049918
Rh 0.174007 -0.768778 -0.707739
C -0.379172 3.278333 -1.634773
C -0.404399 3.355030 -3.171762
C -1.169732 4.465795 -1.041728
H -0.897617 2.358392 -1.348549
H 0.225359 2.583963 -3.629304
H -1.431130 3.223037 -3.532348
H -0.060816 4.328241 -3.540490

H -1.249854 4.397481 0.047863
 H -0.680450 5.416574 -1.284941
 H -2.186363 4.494143 -1.453176
 C -4.018688 1.239201 0.513957
 C -4.844821 2.058706 1.529198
 C -4.779168 1.146340 -0.821726
 H -3.092514 1.787585 0.317376
 H -4.317010 2.185851 2.479945
 H -5.064621 3.055407 1.128796
 H -5.799225 1.563701 1.744413
 H -4.219696 0.577909 -1.568502
 H -5.761295 0.674230 -0.702465
 H -4.951282 2.153818 -1.218489
 C 2.909266 2.086067 2.163476
 C 2.899475 3.197465 3.236770
 C 4.256483 1.340820 2.205223
 H 2.135006 1.355415 2.412474
 H 1.940047 3.723754 3.289288
 H 3.101064 2.770481 4.226378
 H 3.673641 3.946572 3.031251
 H 4.308606 0.579998 1.423548
 H 5.107118 2.023938 2.093607
 H 4.367818 0.840898 3.174326
 C -0.750127 -1.895317 2.974592
 C -0.219186 -3.327254 2.793699
 C -0.892758 -1.550826 4.473340
 H 0.005349 -1.230952 2.549884
 H -0.122143 -3.587052 1.735174
 H 0.776423 -3.403110 3.243195
 H -0.857816 -4.073567 3.281993
 H -1.205322 -0.510708 4.622311
 H -1.634902 -2.196290 4.959158
 H 0.065900 -1.690828 4.986151
 Cl 0.713558 -2.633774 -2.101610
 H 0.832228 0.299090 -1.560829
 S 2.064234 -1.039000 0.625057
 H -0.988638 0.673627 -3.222901
 H -2.743307 0.241003 -4.934900
 C 3.326209 -2.019518 -0.179784
 C 3.627133 -3.300402 0.304791
 C 4.107582 -1.486669 -1.217069
 C 4.689397 -4.029953 -0.231936
 H 3.019497 -3.722272 1.099756
 C 5.160442 -2.222777 -1.759102
 H 3.877807 -0.496311 -1.598699
 C 5.459066 -3.495995 -1.266733
 H 4.908930 -5.022547 0.154608
 H 5.751233 -1.799409 -2.568166
 H 6.282676 -4.066940 -1.687989

11c

N -0.818755 -1.401001 -1.816631
 N -1.673102 0.435756 1.399139
 N -0.568007 2.131519 0.643240
 C -1.445910 -2.552680 -1.501221
 H -1.322820 -2.900719 -0.482768
 C -2.198801 -3.274225 -2.423268
 H -2.674155 -4.198550 -2.112719
 C -2.318668 -2.793300 -3.725434
 H -2.894705 -3.336933 -4.468549
 C -1.675379 -1.599920 -4.053509
 C -0.932082 -0.941871 -3.079204
 C -0.670953 0.766067 0.518344
 C -1.466108 2.617231 1.591271
 H -1.527141 3.667035 1.825485
 C -2.153311 1.556916 2.070635
 H -2.931650 1.486409 2.813200
 C -2.275895 -0.870061 1.552968
 C -3.516559 -1.105015 0.916535
 C -4.103751 -2.364953 1.085196
 H -5.058554 -2.575655 0.612117
 C -3.486787 -3.350327 1.851660
 H -3.957297 -4.323484 1.966367
 C -2.278467 -3.083092 2.488988
 H -1.819379 -3.849112 3.105471
 C -1.649851 -1.834463 2.371852
 C 0.277382 3.037421 -0.112346
 C 1.377748 3.647224 0.527398
 C 2.128099 4.566890 -0.219237
 H 2.984427 5.047382 0.242771
 C 1.803425 4.872656 -1.534696
 H 2.406402 5.583424 -2.093671
 C 0.696049 4.277827 -2.133257
 H 0.441174 4.541651 -3.154067
 C -0.098870 3.360404 -1.437284
 Rh 0.567374 -0.588670 -0.438296
 C -1.369843 2.810665 -2.084163
 C -1.274398 2.682748 -3.614938
 C -2.590285 3.681467 -1.711312
 H -1.543542 1.806268 -1.686208
 H -0.357257 2.170509 -3.925883
 H -2.132416 2.115850 -3.994237
 H -1.292326 3.660177 -4.110630
 H -2.742577 3.725955 -0.628301
 H -2.458389 4.707405 -2.075493
 H -3.504153 3.277145 -2.164092
 C -4.257210 -0.033274 0.116651
 C -5.468861 0.495288 0.913918

C -4.706351 -0.516375 -1.274668
 H -3.577063 0.808222 -0.042548
 H -5.170005 0.895734 1.888650
 H -5.973180 1.295712 0.359770
 H -6.199827 -0.301783 1.094313
 H -3.860652 -0.871149 -1.870093
 H -5.438454 -1.329682 -1.210282
 H -5.183512 0.308264 -1.817274
 C 1.746881 3.404620 1.989498
 C 1.263340 4.573930 2.875602
 C 3.258166 3.189491 2.195967
 H 1.251720 2.486603 2.315046
 H 0.181636 4.734436 2.807724
 H 1.507063 4.378214 3.926544
 H 1.753061 5.512104 2.587347
 H 3.632422 2.395223 1.546736
 H 3.833178 4.104782 2.010074
 H 3.445825 2.893981 3.234645
 C -0.395303 -1.537155 3.187927
 C 0.644805 -2.670180 3.137589
 C -0.786435 -1.214158 4.646416
 H 0.090836 -0.653098 2.770544
 H 0.930174 -2.905638 2.107460
 H 1.552613 -2.352303 3.660127
 H 0.285203 -3.586501 3.622251
 H -1.477819 -0.364915 4.701683
 H -1.271424 -2.072168 5.128405
 H 0.107454 -0.960392 5.227646
 Cl 2.204322 0.042997 1.123753
 H 0.955900 0.527203 -1.390848
 S 1.879335 -2.359799 -1.334055
 H -0.389666 -0.033008 -3.300654
 H -1.727719 -1.184385 -5.054547
 C 3.605766 -2.332046 -0.884798
 C 4.434706 -1.235722 -1.173363
 C 4.181440 -3.477710 -0.312764
 C 5.799829 -1.287775 -0.895659
 H 3.998557 -0.342744 -1.609329
 C 5.550340 -3.528753 -0.043400
 H 3.548704 -4.330949 -0.084264
 C 6.366983 -2.434194 -0.332175
 H 6.424922 -0.426752 -1.121802
 H 5.976977 -4.426830 0.397903
 H 7.432556 -2.472446 -0.120180

HCCPh

C 0.000000 0.000000 3.234730
 H 0.000000 0.000000 4.300767
 C 0.000000 0.000000 2.024515

C 0.000000 0.000000 0.594435
 C 0.000000 1.213497 -0.119911
 C 0.000000 -1.213497 -0.119911
 C 0.000000 1.208941 -1.512854
 H 0.000000 2.150349 0.428506
 C 0.000000 -1.208941 -1.512854
 H 0.000000 -2.150349 0.428506
 C 0.000000 0.000000 -2.213299
 H 0.000000 2.151485 -2.053503
 H 0.000000 -2.151485 -2.053503
 H 0.000000 0.000000 -3.299872

TSIa

N 1.601320 -0.594215 2.342431
 N -2.283399 1.321186 -0.579349
 N -2.463682 -0.832239 -0.697539
 C 2.003719 0.339981 3.224175
 H 1.590504 1.329884 3.082653
 C 2.877104 0.063558 4.271992
 H 3.164137 0.858562 4.952939
 C 3.354292 -1.236685 4.429090
 H 4.035086 -1.485823 5.238389
 C 2.930483 -2.210146 3.527353
 C 2.055549 -1.849440 2.504977
 C -1.612261 0.158682 -0.256951
 C -3.629461 -0.297778 -1.236254
 H -4.418840 -0.928156 -1.611018
 C -3.515218 1.044545 -1.166037
 H -4.180017 1.832844 -1.477735
 Rh 0.051747 -0.107136 0.870112
 C 2.184867 1.658191 -0.073177
 C 1.112852 1.863779 0.587370
 Cl -1.260278 0.475993 2.808241
 H -0.430048 -1.597058 1.000122
 H 1.705037 -2.578007 1.786746
 H 3.264406 -3.239808 3.604080
 S 1.529694 -0.430882 -1.011521
 C 2.526590 -1.913248 -0.842406
 C 1.915229 -3.169216 -0.684939
 C 3.924477 -1.847450 -0.948524
 C 2.687865 -4.330042 -0.641149
 H 0.835034 -3.229034 -0.591047
 C 4.691632 -3.013673 -0.898271
 H 4.410854 -0.885188 -1.071583
 C 4.080154 -4.259199 -0.745494
 H 2.196773 -5.293269 -0.524527
 H 5.773795 -2.944266 -0.978824
 H 4.680042 -5.164652 -0.709011
 C -2.259995 -2.266919 -0.730216
 C -1.786562 -2.844375 -1.928939

C -2.656333 -3.041604 0.380041
 C -1.680973 -4.241173 -1.975996
 C -2.528971 -4.43242C 0.273523
 C -2.041965 -5.028547 -0.886426
 H -1.317073 -4.716798 -2.881472
 H -2.824583 -5.056973 1.110912
 H -1.955016 -6.110598 -0.946133
 C -1.843793 2.701012 -0.475717
 C -2.335860 3.505921 0.574097
 C -1.046530 3.226961 -1.518863
 C -1.933774 4.849547 0.598980
 C -0.682257 4.576046 -1.440454
 C -1.107922 5.378925 -0.385896
 H -2.287611 5.491629 1.399184
 H -0.061028 5.006401 -2.218614
 H -0.809977 6.423536 -0.343432
 C -3.261660 -2.425196 1.636478
 C -2.660746 -2.997260 2.931848
 C -4.796603 -2.586177 1.626765
 H -3.031251 -1.358020 1.640395
 H -1.574282 -2.872689 2.941005
 H -3.062461 -2.452545 3.792709
 H -2.898325 -4.059685 3.068695
 H -5.247144 -2.127331 0.738772
 H -5.086690 -3.644421 1.638146
 H -5.233511 -2.107116 2.510892
 C -1.458456 -2.019023 -3.172966
 C -2.634803 -2.052145 -4.173295
 C -0.164213 -2.463793 -3.878248
 H -1.309642 -0.981563 -2.858973
 H -3.562479 -1.677206 -3.729479
 H -2.408547 -1.433889 -5.050413
 H -2.820681 -3.075475 -4.521329
 H 0.684035 -2.483043 -3.189657
 H -0.264720 -3.457392 -4.331069
 H 0.072139 -1.762839 -4.687286
 C -3.342298 3.011951 1.611033
 C -4.769803 3.464339 1.231422
 C -3.013341 3.475257 3.041623
 H -3.312303 1.920334 1.621006
 H -5.071264 3.103394 0.241991
 H -5.493734 3.082632 1.961244
 H -4.846834 4.558637 1.221977
 H -2.000540 3.180350 3.324931
 H -3.119138 4.560764 3.160182
 H -3.706354 3.001857 3.746304
 C -0.649246 2.404113 -2.743394
 C 0.720554 2.791160 -3.325558
 C -1.727049 2.515121 -3.845205

H -0.580846 1.355512 -2.439812
 H 1.489723 2.820269 -2.550336
 H 1.020435 2.053362 -4.078510
 H 0.694866 3.767972 -3.823618
 H -2.705338 2.165200 -3.502227
 H -1.836247 3.555768 -4.174432
 H -1.442810 1.913783 -4.717407
 H 0.766617 2.768001 1.076918
 C 3.542762 1.964988 -0.458646
 C 4.045876 1.771505 -1.759779
 C 4.385697 2.549215 0.509848
 C 5.342682 2.162450 -2.082018
 H 3.411686 1.302993 -2.504333
 C 5.680863 2.943963 0.178967
 H 4.008762 2.689476 1.518136
 C 6.165058 2.752017 -1.116519
 H 5.714349 2.007116 -3.091365
 H 6.315635 3.393580 0.937958
 H 7.177500 3.052930 -1.371732

TSIb

N -0.812138 2.580657 -1.226425
 N 1.224959 -2.058701 0.367042
 N -0.828116 -2.380921 -0.239733
 C -0.807257 3.727561 -0.524087
 H -0.418130 3.662224 0.482844
 C -1.256766 4.938905 -1.043915
 H -1.221359 5.829885 -0.425339
 C -1.744706 4.975837 -2.347536
 H -2.105062 5.904177 -2.782069
 C -1.757997 3.790178 -3.080347
 C -1.283910 2.622512 -2.489762
 C 0.096731 -1.376787 -0.030333
 C -0.274723 -3.633680 -0.001699
 H -0.848643 -4.536558 -0.127827
 C 1.003254 -3.433545 0.378804
 H 1.780642 -4.123771 0.661014
 Rh -0.203939 0.590139 -0.446312
 C 0.937456 2.131788 1.779511
 C 1.616549 1.870417 0.751200
 Cl 0.876978 0.222347 -2.572108
 H -1.517327 0.064945 -1.053504
 H -1.252572 1.687375 -3.033277
 H -2.124804 3.758992 -4.101389
 S -1.112734 0.903722 1.751774
 H 0.703563 2.632835 2.697991
 C -2.574721 1.928700 1.745341
 C -3.479913 1.955806 0.670941

C -2.866407 2.685287 2.895405
 C -4.646443 2.717408 0.751112
 H -3.263507 1.373127 -0.218426
 C -4.031011 3.449863 2.964951
 H -2.183162 2.660366 3.740523
 C -4.927122 3.471205 1.893392
 H -5.338668 2.721892 -0.087513
 H -4.238914 4.028678 3.861650
 H -5.834060 4.067173 1.948784
 C 2.921918 2.268276 0.222879
 C 3.121415 2.508724 -1.147683
 C 4.002481 2.479975 1.104545
 C 4.354009 2.970132 -1.614066
 H 2.311490 2.316765 -1.841276
 C 5.235785 2.918902 0.630486
 H 3.862495 2.288272 2.163989
 C 5.416421 3.173819 -0.732181
 H 4.484203 3.158974 -2.676773
 H 6.055700 3.073077 1.328080
 H 6.376987 3.524367 -1.101089
 C -2.229146 -2.287083 -0.609134
 C -3.198635 -2.314695 0.418086
 C -2.576890 -2.309392 -1.977815
 C -4.546374 -2.294466 0.034735
 C -3.940336 -2.293322 -2.297582
 C -4.916446 -2.273996 -1.305940
 H -5.316215 -2.304377 0.799565
 H -4.240957 -2.304649 -3.340451
 H -5.968630 -2.260107 -1.578898
 C 2.519505 -1.571233 0.815259
 C 3.598112 -1.573192 -0.094869
 C 2.689529 -1.301450 2.192417
 C 4.863701 -1.239786 0.406391
 C 3.978475 -0.977411 2.632023
 C 5.054718 -0.941230 1.750049
 H 5.712599 -1.222054 -0.269256
 H 4.144279 -0.762158 3.682843
 H 6.046817 -0.687125 2.114130
 C -1.537081 -2.415973 -3.088897
 C -1.859453 -1.527159 -4.302531
 C -1.370180 -3.885283 -3.533226
 H -0.579408 -2.066903 -2.697411
 H -2.038056 -0.492137 -3.996634
 H -1.009317 -1.527230 -4.992600
 H -2.737045 -1.881945 -4.856904
 H -1.059199 -4.529053 -2.703063
 H -2.309062 -4.286642 -3.934752
 H -0.607778 -3.959551 -4.317741
 C -2.842180 -2.451050 1.897892

C -2.944141 -3.927022 2.343558
 C -3.709239 -1.573268 2.818207
 H -1.806222 -2.126141 2.028795
 H -2.279778 -4.579487 1.767946
 H -2.674477 -4.024572 3.402070
 H -3.968128 -4.300043 2.220568
 H -3.707282 -0.528700 2.498413
 H -4.748252 -1.921736 2.856961
 H -3.317190 -1.615620 3.840936
 C 3.457866 -2.000153 -1.554130
 C 3.923670 -3.460751 -1.739558
 C 4.219240 -1.080132 -2.525096
 H 2.402516 -1.934528 -1.827315
 H 3.350633 -4.160075 -1.121195
 H 3.804095 -3.765718 -2.786107
 H 4.982523 -3.572995 -1.475440
 H 3.943328 -0.033970 -2.376951
 H 5.306739 -1.175847 -2.416467
 H 3.968258 -1.352486 -3.556433
 C 1.555409 -1.435790 3.207807
 C 1.603136 -0.373672 4.320619
 C 1.550349 -2.845816 3.839278
 H 0.606494 -1.300021 2.680875
 H 1.694144 0.632686 3.903797
 H 0.680538 -0.416795 4.910357
 H 2.438671 -0.539475 5.011200
 H 1.429244 -3.632245 3.087992
 H 2.488415 -3.033223 4.375910
 H 0.726338 -2.938566 4.557170

Ia

N 1.121179 -0.932785 2.366447
 N -2.679078 1.197972 -0.257743
 N -2.557193 -0.744064 -1.207181
 C 1.289657 -2.224066 2.705668
 H 0.690447 -2.937531 2.154598
 C 2.163175 -2.623232 3.712544
 H 2.268091 -3.678592 3.941487
 C 2.879098 -1.653382 4.412523
 H 3.563372 -1.934753 5.207807
 C 2.698473 -0.314669 4.069673
 C 1.819091 0.000649 3.037512
 C -1.903767 0.062484 -0.308939
 C -3.722121 -0.135189 -1.668041
 H -4.373332 -0.625256 -2.372810
 C -3.801642 1.075114 -1.072501
 H -4.539888 1.856747 -1.143259
 C -2.350245 2.431038 0.430706
 C -2.772513 2.614946 1.765124

C -2.421049 3.820237 2.390399
 H -2.722569 3.990125 3.418704
 C -1.710778 4.806897 1.714874
 H -1.449601 5.732035 2.222380
 C -1.358959 4.623876 0.380180
 H -0.835002 5.414921 -0.146459
 C -1.678033 3.441597 -0.298218
 C -2.117731 -2.022152 -1.735299
 C -1.202616 -2.019030 -2.813800
 C -0.829138 -3.258221 -3.346151
 H -0.120917 -3.294113 -4.166919
 C -1.356252 -4.446421 -2.847221
 H -1.052408 -5.397165 -3.277760
 C -2.280703 -4.416933 -1.809605
 H -2.698362 -5.348296 -1.440919
 C -2.688688 -3.207941 -1.228582
 Rh -0.366723 -0.385072 0.914516
 C 2.230108 0.504569 -0.531420
 C 0.986592 0.744838 -0.044410
 C -3.758711 -3.217814 -0.140345
 C -3.518130 -4.301736 0.925380
 C -5.161793 -3.387422 -0.762758
 H -3.721358 -2.258570 0.381582
 H -2.526276 -4.196673 1.371274
 H -4.254186 -4.192058 1.729317
 H -3.624723 -5.314620 0.517955
 H -5.395089 -2.594628 -1.482540
 H -5.245847 -4.346273 -1.289192
 H -5.929140 -3.364952 0.020058
 C -3.669797 1.614968 2.488354
 C -5.148525 2.033455 2.333518
 C -3.316376 1.435476 3.974045
 H -3.542796 0.635848 2.021702
 H -5.445378 2.100568 1.280626
 H -5.801545 1.299534 2.819959
 H -5.334535 3.011266 2.795063
 H -2.268872 1.147463 4.098591
 H -3.509776 2.341250 4.562135
 H -3.926191 0.630685 4.397051
 C -0.685348 -0.727439 -3.446132
 C -1.638107 -0.252752 -4.566018
 C 0.746361 -0.838459 -3.997896
 H -0.665107 0.041907 -2.668286
 H -2.653307 -0.075912 -4.197273
 H -1.272433 0.683113 -5.005798
 H -1.695457 -1.000753 -5.366119
 H 1.438532 -1.242306 -3.253905
 H 0.793131 -1.470142 -4.893324
 H 1.105008 0.155848 -4.286860
 C -1.384564 3.324345 -1.794480
 C -0.030126 3.922101 -2.215077
 C -2.512806 3.993305 -2.612188
 H -1.366598 2.261699 -2.055904
 H 0.802797 3.517339 -1.634978
 H 0.157518 3.696805 -3.270982

H -0.016425 5.013698 -2.113546
H -3.493308 3.557306 -2.398781
H -2.567753 5.065311 -2.387878
H -2.321811 3.882298 -3.686085
Cl -1.950998 -1.504944 2.442459
H 0.049408 -1.469059 -0.055829
H 1.661370 1.027543 2.725737
H 3.229663 0.479330 4.584562
S 2.784590 -1.199506 -0.723258
H 0.670431 1.789954 -0.146840
C 3.111521 1.586528 -1.060071
C 3.883763 1.424610 -2.224531
C 3.183280 2.825062 -0.394351
C 4.669499 2.465674 -2.716422
H 3.860783 0.472846 -2.745750
C 3.967669 3.867899 -0.887797
H 2.622180 2.961836 0.526353
C 4.714982 3.694680 -2.054035
H 5.250627 2.315048 -3.622872
H 4.005554 4.812397 -0.350364
H 5.334049 4.502303 -2.435502
C 4.457381 -1.254480 -0.091096
C 4.966219 -0.355904 0.856730
C 5.272568 -2.303093 -0.545660
C 6.270461 -0.503291 1.330653
H 4.346987 0.457065 1.218066
C 6.568221 -2.453937 -0.052994
H 4.890161 -2.997455 -1.289560
C 7.076952 -1.551877 0.884097
H 6.655753 0.207184 2.058077
H 7.185556 -3.272580 -0.414409
H 8.090943 -1.662496 1.258415

Ib

N 0.436595 -1.640796 2.573568
N -1.372577 1.338134 -1.500991
N -2.068466 -0.711316 -1.505387
C 1.677100 -2.165595 2.489312
H 2.256631 -1.874654 1.622914
C 2.193288 -3.033837 3.446623
H 3.197718 -3.426062 3.322976
C 1.405231 -3.381801 4.542620
H 1.780799 -4.057846 5.305803
C 0.123972 -2.841638 4.633752
C -0.324192 -1.980600 3.635230
C -1.263112 0.161663 -0.801688
C -2.660834 -0.084804 -2.595564
H -3.324100 -0.612629 -3.260348
C -2.232852 1.194378 -2.590159
H -2.455711 2.024314 -3.239697
C -0.778106 2.643469 -1.268386

C -1.454752 3.554972 -0.430664
C -0.956608 4.863179 -0.365837
H -1.453304 5.586187 0.272907
C 0.148022 5.255146 -1.112954
H 0.508834 6.278961 -1.054368
C 0.790234 4.338334 -1.940148
H 1.648098 4.657836 -2.523346
C 0.346116 3.013764 -2.041159
C -2.336583 -2.107265 -1.205461
C -1.447886 -3.089575 -1.700480
C -1.748789 -4.429977 -1.431221
H -1.083010 -5.208085 -1.788776
C -2.894312 -4.785307 -0.725369
H -3.107047 -5.832842 -0.527463
C -3.778884 -3.802929 -0.295525
H -4.683113 -4.093772 0.228605
C -3.533411 -2.443096 -0.531045
Rh -0.369495 -0.480778 0.902068
C 2.481195 0.393618 0.242466
C 1.309440 0.624869 0.874696
C -4.590897 -1.414389 -0.134085
C -5.235868 -1.702866 1.233516
C -5.691833 -1.328076 -1.215110
H -4.103741 -0.439517 -0.052631
H -4.476521 -1.816965 2.009777
H -5.876876 -0.860648 1.516838
H -5.868382 -2.598889 1.210174
H -5.293577 -1.054881 -2.197669
H -6.210066 -2.288942 -1.322253
H -6.436569 -0.573569 -0.935334
C -2.728638 3.195558 0.327640
C -3.971458 3.681968 -0.448524
C -2.743281 3.739711 1.766946
H -2.787031 2.108848 0.413962
H -4.023463 3.242075 -1.451112
H -4.885574 3.402441 0.088474
H -3.966218 4.773388 -0.561424
H -1.844062 3.440737 2.312226
H -2.823686 4.833795 1.796214
H -3.607002 3.328897 2.299972
C -0.249278 -2.744312 -2.581799
C -0.657901 -2.758508 -4.071580
C 0.957625 -3.671786 -2.360563
H 0.075956 -1.730527 -2.332498
H -1.462305 -2.045909 -4.281328
H 0.197967 -2.494154 -4.704265
H -1.004902 -3.755085 -4.370608
H 1.235413 -3.721939 -1.303656
H 0.765231 -4.690058 -2.718976

H 1.820735 -3.291012 -2.917080
C 1.047759 2.057719 -3.006021
C 2.581148 2.197066 -2.976623
C 0.546484 2.254977 -4.453779
H 0.810544 1.033388 -2.700816
H 2.971525 2.136212 -1.957483
H 3.036432 1.388025 -3.557598
H 2.912876 3.143768 -3.419116
H -0.528219 2.074061 -4.548233
H 0.747573 3.276981 -4.797237
H 1.062211 1.564418 -5.131917
Cl -2.417527 0.094241 2.225243
H 0.485630 -1.372430 -0.015305
H -1.311564 -1.531289 3.659813
H -0.532300 -3.076631 5.465720
S 2.829055 -0.900417 -0.925037
C 4.608999 -1.046180 -0.812899
C 5.301370 -1.443494 -1.967136
C 5.322868 -0.841729 0.377405
C 6.681759 -1.637444 -1.928441
H 4.756469 -1.590559 -2.895804
C 6.707366 -1.017394 0.401855
H 4.798580 -0.548465 1.281746
C 7.392939 -1.419358 -0.746169
H 7.204174 -1.945341 -2.830576
H 7.249490 -0.847960 1.328816
H 8.470012 -1.559188 -0.720684
H 3.329709 1.056534 0.402185
C 1.264134 1.823486 1.768066
C 1.842448 3.043304 1.362123
C 0.706146 1.770197 3.060934
C 1.887121 4.145890 2.214342
H 2.240771 3.131883 0.357305
C 0.749612 2.873890 3.912435
H 0.230401 0.859844 3.401396
C 1.343811 4.067686 3.497394
H 2.337699 5.072351 1.866622
H 0.314277 2.797499 4.905643
H 1.373802 4.927502 4.161768

TSIIa

7 -1.102724 -1.992827 -1.425833
7 2.328521 1.703513 -0.110876
7 2.980609 -0.142650 0.805719
C -1.263028 -3.225802 -0.914001
H -0.737111 -3.423745 0.012519
C -2.047697 -4.196190 -1.529787
H -2.141818 -5.177232 -1.075616

C -2.698422 -3.881456 -2.722026
 H -3.319781 -4.616505 -3.225601
 C -2.534558 -2.603750 -3.253355
 C -1.727666 -1.692850 -2.577269
 C 1.935008 0.403002 0.098533
 C 3.993716 0.789550 1.010143
 H 4.893869 0.539477 1.547293
 C 3.590044 1.942256 0.431731
 H 4.066674 2.905748 0.352154
 C 1.542632 2.778560 -0.680961
 C 1.528646 2.962221 -2.079097
 C 0.777236 4.034345 -2.579710
 H 0.742621 4.201569 -3.651566
 C 0.088206 4.895774 -1.731059
 H -0.486754 5.720624 -2.144314
 C 0.149894 4.713993 -0.352604
 H -0.376555 5.402017 0.301631
 C 0.882402 3.659278 0.206879
 C 3.042908 -1.475025 1.373206
 C 2.381226 -1.710364 2.599416
 C 2.485730 -2.989244 3.158392
 H 1.986275 -3.202683 4.098318
 C 3.232542 -3.987282 2.538689
 H 3.302901 -4.973220 2.991164
 C 3.903401 -3.717726 1.350690
 H 4.498503 -4.497675 0.886737
 C 3.831688 -2.458543 0.739030
 Rh 0.352148 -0.654278 -0.591980
 C -2.373436 0.393961 0.700800
 C -1.096656 0.511995 0.229464
 C 4.646799 -2.188631 -0.523756
 C 4.555515 -3.329502 -1.553132
 C 6.124558 -1.918538 -0.165365
 H 4.236291 -1.298600 -1.007350
 H 3.514740 -3.543839 -1.806029
 H 5.068284 -3.030735 -2.474495
 H 5.036618 -4.248279 -1.195626
 H 6.237906 -1.070445 0.518934
 H 6.578099 -2.793974 0.315698
 H 6.700849 -1.696767 -1.071498
 C 2.359248 2.103272 -3.026310
 C 3.683689 2.820310 -3.366067
 C 1.606247 1.716211 -4.310049
 H 2.601562 1.166706 -2.520544
 H 4.265811 3.043765 -2.464371
 H 4.300091 2.188552 -4.016307
 H 3.500522 3.767605 -3.888689
 H 0.658617 1.223362 -4.073804
 H 1.403995 2.581397 -4.953637

H 2.209039 1.006916 -4.886366
 C 1.646112 -0.610804 3.362432
 C 2.564035 -0.010932 4.449373
 C 0.315934 -1.079768 3.977892
 H 1.404342 0.188378 2.657003
 H 3.485427 0.396291 4.018400
 H 2.051808 0.799857 4.981639
 H 2.846753 -0.772752 5.185772
 H -0.330618 -1.544861 3.227121
 H 0.468178 -1.799810 4.790396
 H -0.219978 -0.222850 4.401797
 C 0.996093 3.548627 1.728144
 C -0.357309 3.650393 2.455705
 C 1.969248 4.617118 2.272450
 H 1.416595 2.567677 1.969345
 H -1.068181 2.897917 2.104923
 H -0.207914 3.501547 3.531749
 H -0.821036 4.634919 2.326453
 H 2.960814 4.539073 1.813991
 H 1.590454 5.626925 2.074815
 H 2.088698 4.508490 3.356965
 Cl 1.715989 -1.411448 -2.426558
 H -0.292032 -0.579333 0.872553
 H -1.553652 -0.694505 -2.961897
 H -3.016686 -2.309466 -4.179935
 S -2.932771 -1.166138 1.381053
 H -0.753801 1.542947 0.142388
 C -3.264478 1.581446 0.818600
 C -4.188448 1.725994 1.869991
 C -3.190019 2.613839 -0.137747
 C -4.982499 2.866667 1.975847
 H -4.273303 0.938598 2.612106
 C -3.981338 3.756583 -0.026902
 H -2.510861 2.511192 -0.978987
 C -4.882673 3.890512 1.030828
 H -5.682459 2.955772 2.802885
 H -3.902949 4.536825 -0.779994
 H -5.507763 4.775869 1.112014
 C -4.483227 -1.542724 0.569402
 C -4.903623 -0.946285 -0.626322
 C -5.291175 -2.519809 1.172157
 C -6.117577 -1.323054 -1.203888
 H -4.290301 -0.187331 -1.099079
 C -6.494806 -2.899344 0.580204
 H -4.978063 -2.977244 2.107472
 C -6.917001 -2.300727 -0.609561
 H -6.436729 -0.846149 -2.127378
 H -7.109457 -3.658197 1.057925
 H -7.860236 -2.590109 -1.064586

TSIIb

7 0.034817 -0.846653 3.096563
 7 1.021304 -0.200149 -2.043492
 7 1.654716 1.593037 -0.991531
 C -0.604525 0.020798 3.902954
 H -0.961950 0.930110 3.432271
 C -0.796982 -0.210979 5.261748
 H -1.315439 0.528015 5.864377
 C -0.310431 -1.393576 5.817535
 H -0.443452 -1.606299 6.874604
 C 0.353859 -2.293910 4.986845
 C 0.510329 -1.982845 3.638741
 C 1.061629 0.361344 -0.779639
 C 1.922347 1.793302 -2.342705
 H 2.360835 2.709961 -2.700643
 C 1.542581 0.675984 -2.995957
 H 1.604630 0.408292 -4.037181
 C 0.715151 -1.573612 -2.410801
 C 1.668102 -2.580543 -2.117595
 C 1.368604 -3.893323 -2.505203
 H 2.075283 -4.684390 -2.278611
 C 0.201270 -4.199931 -3.196331
 H -0.007787 -5.226093 -3.487636
 C -0.680199 -3.183238 -3.541052
 H -1.570036 -3.422349 -4.114187
 C -0.444635 -1.851838 -3.170337
 C 2.177750 2.533415 -0.008111
 C 1.318978 3.478646 0.588168
 C 1.875497 4.404191 1.480330
 H 1.230007 5.139204 1.951505
 C 3.237160 4.410448 1.757733
 H 3.650467 5.137069 2.452638
 C 4.072237 3.494788 1.127340
 H 5.137479 3.518410 1.333701
 C 3.573546 2.541727 0.230553
 Rh 0.464967 -0.332680 1.021019
 C -2.595507 -0.249549 -0.211040
 C -1.559139 -0.766460 0.495745
 C 4.567332 1.624256 -0.482354
 H 4.009419 0.797143 -0.927941
 C 3.039721 -2.280901 -1.518462
 H 2.968733 -1.377226 -0.912640
 C -0.156004 3.581575 0.235688
 C -1.405223 -0.778079 -3.674843
 H -1.263003 0.122995 -3.073094
 Cl 2.739199 -0.699038 1.637785
 H -0.996089 0.363054 1.045710

H 1.036423 -2.643779 2.961999
H 0.754596 -3.226911 5.369640
S -2.683315 1.350820 -0.969020
C -4.405344 1.782396 -0.746213
C -4.990313 2.630960 -1.698588
C -5.165301 1.349327 0.349108
C -6.314367 3.042506 -1.551311
H -4.409253 2.960194 -2.555953
C -6.496396 1.749627 0.476913
H -4.716001 0.704529 1.097808
C -7.075851 2.599289 -0.467194
H -6.755741 3.700638 -2.295244
H -7.078207 1.402101 1.326890
H -8.110651 2.912285 -0.360436
H -3.471778 -0.865988 -0.401287
C -1.819709 -2.133145 1.063205
C -1.090955 -3.256296 0.633227
C -2.832703 -2.325020 2.018605
C -1.367213 -4.523816 1.145593
H -0.312001 -3.127005 -0.110145
C -3.098895 -3.592271 2.541682
H -3.405594 -1.467392 2.361739
C -2.366996 -4.698114 2.107108
H -0.798915 -5.379541 0.789399
H -3.882801 -3.713818 3.285395
H -2.575647 -5.686278 2.508894
H -0.449319 2.654902 -0.255563
C -2.885359 -1.187525 -3.551883
H -3.526979 -0.319023 -3.734292
H -3.157308 -1.954933 -4.286157
H -3.113662 -1.575629 -2.556345
C -1.106640 -0.422381 -5.148801
H -1.786760 0.365720 -5.493570
H -0.082178 -0.067188 -5.296766
H -1.248918 -1.296829 -5.795182
C -1.061121 3.735694 1.469372
H -0.860763 2.944007 2.199115
H -0.922439 4.701669 1.969617
H -2.112252 3.665433 1.169379
C -0.397488 4.732452 -0.762678
H 0.195752 4.602798 -1.675223
H -1.455160 4.773189 -1.049881
H -0.128201 5.701358 -0.324256
C 5.609485 1.004130 0.467697
H 6.208068 0.265088 -0.078813
H 6.305951 1.755810 0.858019
H 5.123527 0.500718 1.305460
C 5.294132 2.384783 -1.614174
H 5.879756 3.217966 -1.207134

H 5.984635 1.714832 -2.140411
H 4.600978 2.799594 -2.353126
C 4.057587 -2.025303 -2.652706
H 4.170803 -2.912913 -3.287705
H 3.752586 -1.190693 -3.293580
H 5.040786 -1.783630 -2.231186
C 3.558434 -3.380179 -0.576713
H 2.826234 -3.611648 0.202219
H 3.811616 -4.304501 -1.110913
H 4.466414 -3.028363 -0.077131

II

N 0.771536 3.082590 -0.958770
N -1.283375 -1.326681 0.653913
N 0.843993 -1.713637 0.683124
C 2.020994 3.587558 -0.998748
H 2.814126 2.910184 -0.700022
C 2.301465 4.887561 -1.407677
H 3.329424 5.235908 -1.422848
C 1.246919 5.713242 -1.798490
H 1.431011 6.733489 -2.123223
C -0.046427 5.193982 -1.771785
C -0.242705 3.879586 -1.355121
C -0.074111 -0.742210 0.336257
C 0.223720 -2.841042 1.219181
H 0.788405 -3.697709 1.551603
C -1.105627 -2.596244 1.200219
H -1.942239 -3.192843 1.525614
C -2.600175 -0.743227 0.520427
C -3.049083 0.157409 1.506892
C -4.349992 0.662484 1.385695
H -4.722026 1.359310 2.131620
C -5.177458 0.275431 0.336781
H -6.185114 0.676375 0.261895
C -4.717538 -0.633187 -0.611791
H -5.373487 -0.933080 -1.423006
C -3.423459 -1.163021 -0.546773
C 2.276418 -1.624090 0.546403
C 2.907155 -2.328133 -0.495092
C 4.308794 -2.293285 -0.542428
H 4.826077 -2.823930 -1.336673
C 5.046350 -1.589092 0.402848
H 6.131973 -1.582729 0.349721
C 4.395911 -0.880242 1.413892
H 4.982892 -0.321904 2.136413
C 3.001922 -0.881342 1.504167
45 0.343049 1.080858 -0.310498
C 2.257643 -0.014686 2.512746

C 1.904162 1.335252 1.841497
C 2.994909 0.206353 3.841449
H 1.314618 -0.519072 2.746476
H 1.868484 1.172922 0.720430
H 0.998415 1.787437 2.251591
H 2.723617 2.058785 1.941956
H 3.253666 -0.745139 4.319106
H 3.917938 0.782660 3.710143
H 2.357770 0.770242 4.532401
C -2.206190 0.555165 2.714806
C -2.791897 -0.035411 4.013701
C -2.039548 2.082031 2.825596
H -1.206216 0.132793 2.583787
H -2.867249 -1.127395 3.957071
H -2.157220 0.217448 4.872007
H -3.795914 0.357320 4.213286
H -1.593893 2.485375 1.910065
H -2.998857 2.585803 2.992373
H -1.386625 2.332897 3.671434
C 2.128113 -3.073163 -1.574356
C 2.511726 -4.563980 -1.638592
C 2.300386 -2.387605 -2.944743
H 1.064994 -3.019443 -1.324314
H 2.364431 -5.060485 -0.672154
H 1.895008 -5.081404 -2.382579
H 3.560687 -4.702043 -1.926625
H 1.956253 -1.349200 -2.906708
H 3.348746 -2.395620 -3.267684
H 1.711250 -2.913240 -3.705587
C -2.975042 -2.192436 -1.581647
C -3.339085 -1.793704 -3.023064
C -3.557279 -3.585357 -1.255810
H -1.883945 -2.256597 -1.536208
H -2.948990 -0.800974 -3.258059
H -2.899113 -2.512414 -3.724805
H -4.423191 -1.800819 -3.190189
H -3.263149 -3.936492 -0.260621
H -4.653525 -3.567999 -1.289320
H -3.211112 -4.324861 -1.988103
Cl -0.914794 0.792581 -2.273516
H -1.223769 3.420384 -1.348031
H -0.900740 5.790097 -2.076550

TS1c

N -0.326960 1.962338 -2.470100
N 1.900617 -1.543639 0.629120

N -0.163763 -2.156574 0.849891
 C 0.524487 2.077306 -3.505289
 H 1.333519 1.357822 -3.532239
 C 0.361499 3.030143 -4.507751
 H 1.072871 3.070220 -5.326427
 C -0.720269 3.905762 -4.438859
 H -0.875041 4.659845 -5.205618
 C -1.603338 3.786416 -3.367702
 C -1.377571 2.799886 -2.410548
 C 0.607833 -1.150024 0.312352
 C 0.622556 -3.139937 1.439249
 H 0.178178 -4.004864 1.901953
 C 1.906251 -2.760696 1.299789
 H 2.826428 -3.226865 1.609392
 Rh 0.074962 0.422944 -0.950067
 C 1.117973 2.094568 0.135475
 C 1.890390 1.460500 -0.652849
 Cl 0.632839 -1.092411 -2.784138
 H -2.058209 2.664200 -1.580748
 H -2.467088 4.435563 -3.267820
 C -1.603629 -2.341412 0.982200
 C -2.244495 -1.785725 2.107732
 C -2.241925 -3.246488 0.109170
 C -3.587261 -2.126475 2.317172
 C -3.577908 -3.561395 0.379235
 C -4.248233 -3.003950 1.464471
 H -4.118723 -1.706766 3.165117
 H -4.102973 -4.248722 -0.276768
 H -5.288970 -3.257359 1.648885
 C 3.186894 -0.884552 0.461296
 C 4.014777 -1.257475 -0.620164
 C 3.636627 -0.020121 1.489585
 C 5.273044 -0.643383 -0.710907
 C 4.905842 0.552332 1.347101
 C 5.710961 0.261890 0.248949
 H 5.924795 -0.896661 -1.540830
 H 5.272778 1.231342 2.109274
 H 6.691129 0.722710 0.156445
 C -1.527321 -3.899563 -1.072163
 C -2.363218 -3.873649 -2.365308
 C -1.123068 -5.352515 -0.739820
 H -0.619788 -3.325188 -1.279160
 H -2.680136 -2.855398 -2.601396
 H -1.755652 -4.244695 -3.198555
 H -3.250388 -4.515374 -2.294606
 H -0.460019 -5.413779 0.130269
 H -2.007329 -5.966653 -0.528336
 H -0.597934 -5.802504 -1.590795
 C -1.513728 -0.910161 3.124987
 C -0.980063 -1.759503 4.299773
 C -2.376671 0.241828 3.670601
 H -0.652626 -0.458099 2.621457
 H -0.289699 -2.538813 3.962590
 H -0.446942 -1.126611 5.020239
 H -1.807370 -2.247915 4.828619
 H -2.848075 0.809079 2.863361
 H -3.170411 -0.122719 4.333222
 H -1.753488 0.921694 4.264890
 C 3.646440 -2.346570 -1.623824

C 4.344631 -3.672878 -1.249362
 C 3.984278 -1.969692 -3.077071
 H 2.566192 -2.496726 -1.584010
 H 4.076602 -4.012713 -0.243037
 H 4.057314 -4.461178 -1.954988
 H 5.436271 -3.569417 -1.285224
 H 3.518715 -1.021259 -3.355497
 H 5.065930 -1.903249 -3.248511
 H 3.592044 -2.737593 -3.752437
 C 2.826859 0.251792 2.757149
 C 3.031097 1.667032 3.328549
 C 3.161732 -0.783937 3.854997
 H 1.765594 0.146460 2.509244
 H 2.928847 2.440440 2.563880
 H 2.283820 1.861644 4.105642
 H 4.016561 1.775286 3.796993
 H 2.944290 -1.807851 3.540092
 H 4.223484 -0.729137 4.124079
 H 2.573993 -0.580870 4.758233
 H 2.880168 1.408112 -1.071505
 C 0.857043 3.257241 0.968594
 C -0.120496 3.282660 1.977063
 C 1.655741 4.402637 0.770740
 C -0.292219 4.416807 2.769367
 H -0.740376 2.406867 2.142760
 C 1.481153 5.530881 1.567951
 H 2.405766 4.395424 -0.014481
 C 0.506457 5.544515 2.569937
 H -1.053315 4.417147 3.544810
 H 2.103050 6.406109 1.400182
 H 0.368472 6.428593 3.185985
 S -2.229934 -0.272388 -1.429076
 C -3.507048 0.608953 -0.572559
 C -4.839898 0.240873 -0.873865
 C -3.329562 1.672378 0.333870
 C -5.922066 0.901760 -0.302710
 H -5.012611 -0.576144 -1.568951
 C -4.420842 2.338228 0.902262
 H -2.323732 1.985524 0.593740
 C -5.726186 1.960689 0.592309
 H -6.931688 0.588311 -0.559891
 H -4.239347 3.159128 1.593525
 H -6.573633 2.478277 1.033422
 H -0.348406 1.365332 0.292664

TSId

N -0.232437 3.002368 -0.519377
 N 1.201262 -2.077904 -0.014646
 N -0.935915 -2.123545 0.336379
 C -0.261742 3.879747 0.498829
 H -0.109078 3.465193 1.488892
 C -0.462543 5.244588 0.320363
 H -0.481043 5.901536 1.184059
 C -0.640492 5.732834 -0.973216
 H -0.800698 6.792777 -1.150199
 C -0.609847 4.828306 -2.031167
 C -0.409705 3.474413 -1.768130
 C 0.091553 -1.252814 0.028887

C -0.470565 -3.425737 0.472384
 H -1.136640 -4.234840 0.719357
 C 0.856014 -3.398762 0.246127
 H 1.595617 -4.180998 0.248762
 Rh -0.001720 0.800270 -0.220026
 C 0.762165 1.135498 1.812584
 C 1.698299 1.382355 0.978054
 Cl 1.028063 0.657951 -2.439500
 H -0.380841 2.736104 -2.558116
 H -0.742775 5.153194 -3.057988
 H 0.484646 0.954829 2.838176
 C 3.000820 1.978810 0.774234
 C 3.677392 1.873325 -0.453563
 C 3.593363 2.724619 1.817949
 C 4.922418 2.478851 -0.621038
 H 3.205067 1.328437 -1.262939
 C 4.833447 3.330225 1.639838
 H 3.066061 2.830034 2.762363
 C 5.504896 3.205324 0.419146
 H 5.435064 2.388530 -1.574932
 H 5.275504 3.902991 2.450961
 H 6.472515 3.680428 0.279788
 C -2.356143 -1.912821 0.578473
 C -2.769104 -1.526213 1.868578
 C -3.273610 -2.302392 -0.423889
 C -4.146944 -1.454975 2.117176
 C -4.634780 -2.216475 -0.114648
 C -5.071861 -1.785026 1.135150
 H -4.496635 -1.148909 3.098175
 H -5.366356 -2.493458 -0.866917
 H -6.135723 -1.717799 1.345365
 C 2.620624 -1.785935 -0.159878
 C 3.222327 -1.906723 -1.433084
 C 3.381446 -1.606948 1.019980
 C 4.606916 -1.703563 -1.507434
 C 4.761477 -1.415822 0.878887
 C 5.367027 -1.440937 -0.372458
 H 5.099421 -1.768987 -2.471792
 H 5.371033 -1.257584 1.762718
 H 6.438940 -1.284112 -0.460404
 C -2.844735 -2.874651 -1.775582
 C -3.620569 -2.282285 -2.966324
 C -2.990593 -4.413164 -1.786768
 H -1.789866 -2.627014 -1.927957
 H -3.531753 -1.194298 -2.982874
 H -3.208118 -2.675439 -3.903139
 H -4.682714 -2.554103 -2.940101
 H -2.407472 -4.897294 -0.996668
 H -4.038795 -4.705440 -1.650386
 H -2.651685 -4.819088 -2.747368
 C -1.788410 -1.297306 3.016693
 C -1.715713 -2.547232 3.920414
 C -2.118698 -0.051416 3.858753
 H -0.793235 -1.148759 2.588501
 H -1.403986 -3.432877 3.356326
 H -0.996646 -2.394783 4.734909
 H -2.693086 -2.761974 4.368250
 H -2.234717 0.838256 3.232101
 H -3.047285 -0.177084 4.426536

H -1.321140 0.132690 4.589836
 C 2.463852 -2.369585 -2.677105
 C 2.557368 -3.906447 -2.817664
 C 2.956011 -1.713531 -3.979302
 H 1.414602 -2.091353 -2.556114
 H 2.129401 -4.433029 -1.959016
 H 2.014662 -4.235032 -3.712026
 H 3.601414 -4.226715 -2.920785
 H 2.977812 -0.625581 -3.890586
 H 3.952314 -2.070553 -4.269012
 H 2.271599 -1.970472 -4.795435
 C 2.790633 -1.740856 2.425343
 C 3.350939 -0.723966 3.436768
 C 3.021995 -3.168308 2.972181
 H 1.710924 -1.576941 2.360230
 H 3.290810 0.299860 3.062890
 H 2.786158 -0.787385 4.374790
 H 4.398981 -0.930602 3.682059
 H 2.574349 -3.935002 2.333571
 H 4.094546 -3.381924 3.050407
 H 2.584033 -3.268673 3.972798
 S -2.082883 0.649676 -1.469051
 C -3.444148 1.419424 -0.627500
 C -4.685437 1.440373 -1.302594
 C -3.391186 2.028458 0.639662
 C -5.809657 2.031091 -0.732553
 H -4.757016 0.987555 -2.287813
 C -4.521566 2.619034 1.209078
 H -2.452206 2.039022 1.181849
 C -5.741048 2.624734 0.532123
 H -6.748853 2.027741 -1.281799
 H -4.442559 3.080363 2.191791
 H -6.619180 3.086724 0.975453
 H -0.650598 0.934549 1.261929

Ис

N -0.611027 2.451143 -1.514049
 N 0.895824 -2.279831 0.344136
 N -1.263433 -2.236574 0.199396
 C -1.260990 2.543035 -2.691049
 H -1.530866 1.603032 -3.156381
 C -1.542639 3.762937 -3.298422
 H -2.069978 3.776930 -4.246812
 C -1.130311 4.940097 -2.676365
 H -1.331299 5.907528 -3.128060
 C -0.452882 4.847058 -1.462594
 C -0.216808 3.589528 -0.914964
 C -0.149131 -1.435976 0.071076
 C -0.905431 -3.542586 0.516348
 H -1.645030 -4.315625 0.641117
 C 0.440259 -3.568487 0.612315
 H 1.124937 -4.366627 0.847057
 C 2.314968 -1.997254 0.471065
 C 3.166537 -2.290509 -0.613434
 C 4.542446 -2.109988 -0.415712
 H 5.227546 -2.321465 -1.230747
 C 5.046387 -1.671332 0.803607
 H 6.116540 -1.532359 0.930810

C 4.181789 -1.410970 1.862866
 H 4.588765 -1.075620 2.811148
 C 2.798631 -1.573177 1.727476
 C -2.662981 -1.852929 0.109608
 C -3.352120 -1.538560 1.306491
 C -4.709651 -1.212606 1.199655
 H -5.264011 -0.950244 2.094254
 C -5.363354 -1.221362 -0.028677
 H -6.416723 -0.958807 -0.084234
 C -4.678097 -1.594889 -1.179558
 H -5.209151 -1.641662 -2.124568
 C -3.319711 -1.941253 -1.139495
 Rh -0.257702 0.483975 -0.622654
 C 2.314692 1.765240 0.333550
 C 1.673325 0.934457 -0.504160
 C -2.649270 -2.508477 -2.387790
 C -3.069206 -1.800962 -3.687357
 C -2.935967 -4.022801 -2.498785
 H -1.570719 -2.369287 -2.292869
 H -2.926504 -0.719096 -3.617153
 H -2.447836 -2.160297 -4.514175
 H -4.115074 -2.001295 -3.950525
 H -2.579534 -4.573660 -1.621731
 H -4.011366 -4.214533 -2.599649
 H -2.434020 -4.437902 -3.380744
 C 2.658505 -2.843341 -1.942998
 C 2.893022 -4.367258 -2.022238
 C 3.288729 -2.145884 -3.162039
 H 1.583254 -2.657059 -2.002264
 H 2.397355 -4.901856 -1.204180
 H 2.502311 -4.763642 -2.966985
 H 3.962842 -4.604870 -1.973662
 H 3.129442 -1.064745 -3.126719
 H 4.364943 -2.341389 -3.240134
 H 2.818694 -2.516316 -4.079666
 C -2.712684 -1.636651 2.691268
 C -2.986500 -3.025591 3.312120
 C -3.183263 -0.542690 3.666485
 H -1.632417 -1.517325 2.575056
 H -2.597626 -3.842321 2.696376
 H -2.514601 -3.097525 4.299288
 H -4.063494 -3.187509 3.441250
 H -3.083038 0.453772 3.232127
 H -4.226114 -0.688694 3.973051
 H -2.572926 -0.579815 4.576024
 C 1.884346 -1.350448 2.930693
 C 2.265257 -0.112032 3.761018
 C 1.854993 -2.605102 3.830538
 H 0.868994 -1.180787 2.560915
 H 2.343408 0.778139 3.131619
 H 1.495751 0.074120 4.518403
 H 3.217287 -0.247160 4.287966
 H 1.506551 -3.489556 3.286461
 H 2.854397 -2.825359 4.225011
 H 1.182816 -2.447895 4.682716
 Cl 0.085014 -0.395958 -2.875893
 H 0.297733 3.471881 0.029121
 H -0.109457 5.731124 -0.935502
 H 2.189631 0.466248 -1.339267

C 3.739087 2.147337 0.239900
 C 4.343799 2.782101 1.341145
 C 4.532045 1.927793 -0.903304
 C 5.685257 3.162501 1.314568
 H 3.748074 2.973850 2.231175
 C 5.872140 2.305015 -0.929937
 H 4.090700 1.468297 -1.782717
 C 6.460057 2.922322 0.178792
 H 6.124237 3.648958 2.182414
 H 6.460646 2.125702 -1.826649
 H 7.504796 3.220696 0.151874
 S -0.785100 1.278229 1.547073
 C -2.191308 2.367525 1.399977
 C -3.260575 2.137350 0.514543
 C -2.266295 3.484213 2.254676
 C -4.349841 3.008571 0.468844
 H -3.245521 1.264980 -0.132081
 C -3.368131 4.338923 2.221161
 H -1.449877 3.676060 2.945888
 C -4.413246 4.112564 1.322016
 H -5.160537 2.811525 -0.228826
 H -3.403336 5.192640 2.893994
 H -5.267277 4.783800 1.290609
 H 1.784801 2.187849 1.183092

Ид

N 1.094727 2.726821 0.107782
 N -1.642637 -1.841171 0.095360
 N 0.400464 -2.192523 0.717324
 C 1.240379 3.474796 -1.002808
 H 0.824617 3.053725 -1.909902
 C 1.881221 4.710124 -0.990857
 H 1.968496 5.273956 -1.913834
 C 2.401261 5.193089 0.208122
 H 2.910888 6.151762 0.246303
 C 2.250911 4.419734 1.358514
 C 1.590901 3.198144 1.269268
 C -0.423819 -1.213227 0.193555
 C -0.305223 -3.363744 0.966946
 H 0.173102 -4.227925 1.396446
 C -1.575560 -3.147830 0.575012
 H -2.443762 -3.785341 0.580582
 C -2.923926 -1.413269 -0.446126
 C -3.944451 -1.055152 0.458351
 C -5.229771 -0.852968 -0.065413
 H -6.035322 -0.576895 0.607763
 C -5.490239 -1.005333 -1.421199
 H -6.495291 -0.847414 -1.804266
 C -4.463839 -1.368111 -2.291724
 H -4.682535 -1.493398 -3.346949
 C -3.163080 -1.596325 -1.828190
 C 1.834296 -2.179674 0.970931
 C 2.697442 -2.689889 -0.030273
 C 4.062378 -2.758108 0.270396
 H 4.752109 -3.126921 -0.480970
 C 4.553545 -2.370707 1.513694
 H 5.618960 -2.433181 1.719545
 C 3.678394 -1.928032 2.497928

H 4.064594 -1.667502 3.478291
 C 2.298312 -1.838270 2.261266
 Rh 0.201496 0.748347 0.040222
 C -1.350406 1.383013 -2.416270
 C -1.305924 1.542364 -1.083193
 C 1.366282 -1.497125 3.420549
 C 1.867117 -0.318819 4.274126
 C 1.147155 -2.740583 4.309999
 H 0.400101 -1.194727 3.013057
 H 2.067428 0.560934 3.655795
 H 1.097444 -0.041000 5.001596
 H 2.777636 -0.567162 4.832957
 H 0.724115 -3.578009 3.744233
 H 2.090422 -3.081551 4.754287
 H 0.454326 -2.504428 5.126302
 C -3.729764 -0.945964 1.965974
 C -4.366709 -2.146936 2.697691
 C -4.267472 0.376804 2.542183
 H -2.655089 -0.954842 2.160893
 H -3.959950 -3.104488 2.353025
 H -4.180929 -2.073296 3.775726
 H -5.452812 -2.174003 2.546127
 H -3.818328 1.236818 2.041412
 H -5.358583 0.449512 2.454020
 H -4.016885 0.438904 3.607162
 C 2.197754 -3.246926 -1.363126
 C 1.985143 -4.774984 -1.266253
 C 3.133824 -2.941614 -2.546813
 H 1.236319 -2.775965 -1.583943
 H 1.258372 -5.046924 -0.495153
 H 1.619093 -5.166919 -2.222813
 H 2.928376 -5.283863 -1.033435
 H 3.378946 -1.879093 -2.601716
 H 4.067537 -3.514183 -2.488110
 H 2.641043 -3.227030 -3.483365
 C -2.089283 -2.101773 -2.791988
 C -2.227535 -1.533124 -4.216057
 C -2.091059 -3.645829 -2.860490
 H -1.115182 -1.781494 -2.409421
 H -2.337695 -0.445605 -4.209868
 H -1.333739 -1.782396 -4.798896
 H -3.086849 -1.961826 -4.745465
 H -1.900495 -4.104219 -1.885778
 H -3.057567 -4.014398 -3.225385
 H -1.314641 -3.995050 -3.551862
 Cl -0.732563 1.075592 2.263068
 H 1.418528 2.576967 2.140616
 H 2.632909 4.751047 2.318726
 H -2.121535 1.893843 -2.993983
 C -2.355217 2.398895 -0.446379
 C -3.690377 2.223692 -0.862795
 C -2.093615 3.441951 0.459966
 C -4.709959 3.064196 -0.415804
 H -3.926086 1.412352 -1.541630
 C -3.111573 4.283988 0.905021
 H -1.089490 3.594835 0.827773
 C -4.426424 4.103651 0.469958
 H -5.728786 2.896536 -0.756893
 H -2.873623 5.083655 1.602116

H -5.218195 4.758881 0.824126
 S 1.557499 0.253984 -1.856673
 C 3.200293 0.876743 -1.553619
 C 3.835124 0.828918 -0.299438
 C 3.926634 1.391463 -2.645694
 C 5.138376 1.302588 -0.140766
 H 3.313917 0.402549 0.551825
 C 5.237441 1.840277 -2.486938
 H 3.450317 1.437096 -3.621418
 C 5.849542 1.808015 -1.231231
 H 5.605154 1.257471 0.840557
 H 5.777849 2.228426 -3.347254
 H 6.868073 2.165743 -1.105973
 H -0.649939 0.780960 -2.977640