

Cyanide Addition to Diiron and Diruthenium Bis-Cyclopentadienyl Complexes with Bridging Hydrocarbyl Ligands

Alessia Cinci, Gianluca Ciancaleoni, Stefano Zacchini, Fabio Marchetti

Supporting Information

<u>Table of contents</u>	<i>Pages</i>
Figures S1-S3: DFT-optimized structures	S2-S4
Figures S4: X-ray structure of 8bFe	S5
Figures S5-S14: NMR spectra of products	S6-S11
DFT-optimized XYZ coordinates	S12-S20

Figure S1. DFT optimized geometries of potential stereoisomers of **5A**, computed at the RI-DFT/BP86/def2-TZVP level (dichloromethane as continuous medium), and relative Gibbs free energy values (kcal/mol). Hydrogen atoms, except C α H, have been omitted for clarity.

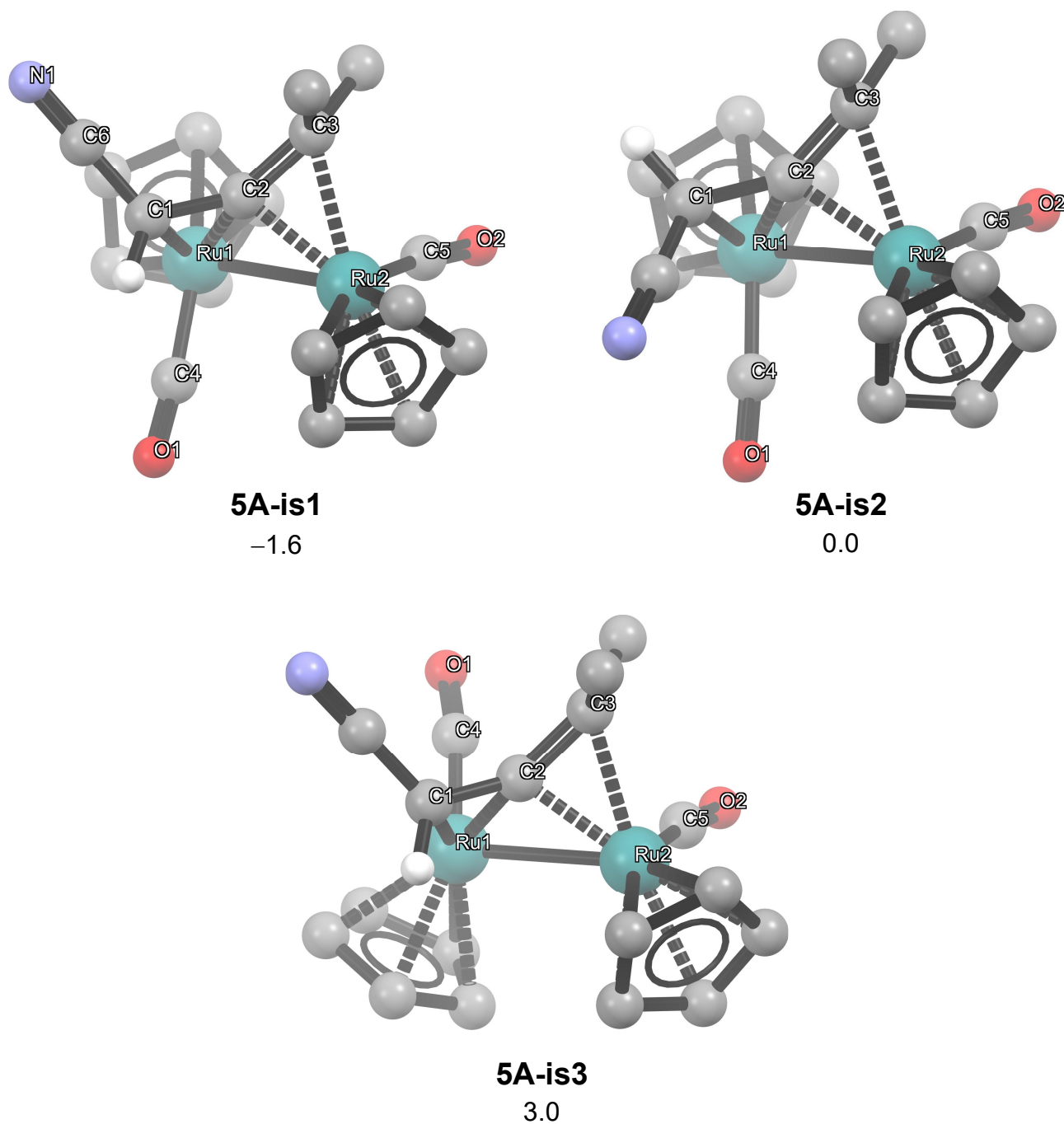


Figure S2. DFT optimized geometries of potential stereoisomers of **5B1** and **5B2**, computed at the RI-DFT/BP86/def2-TZVP level (dichloromethane as continuous medium), and relative Gibbs free energy values (kcal/mol). Hydrogen atoms, except C α H, have been omitted for clarity.

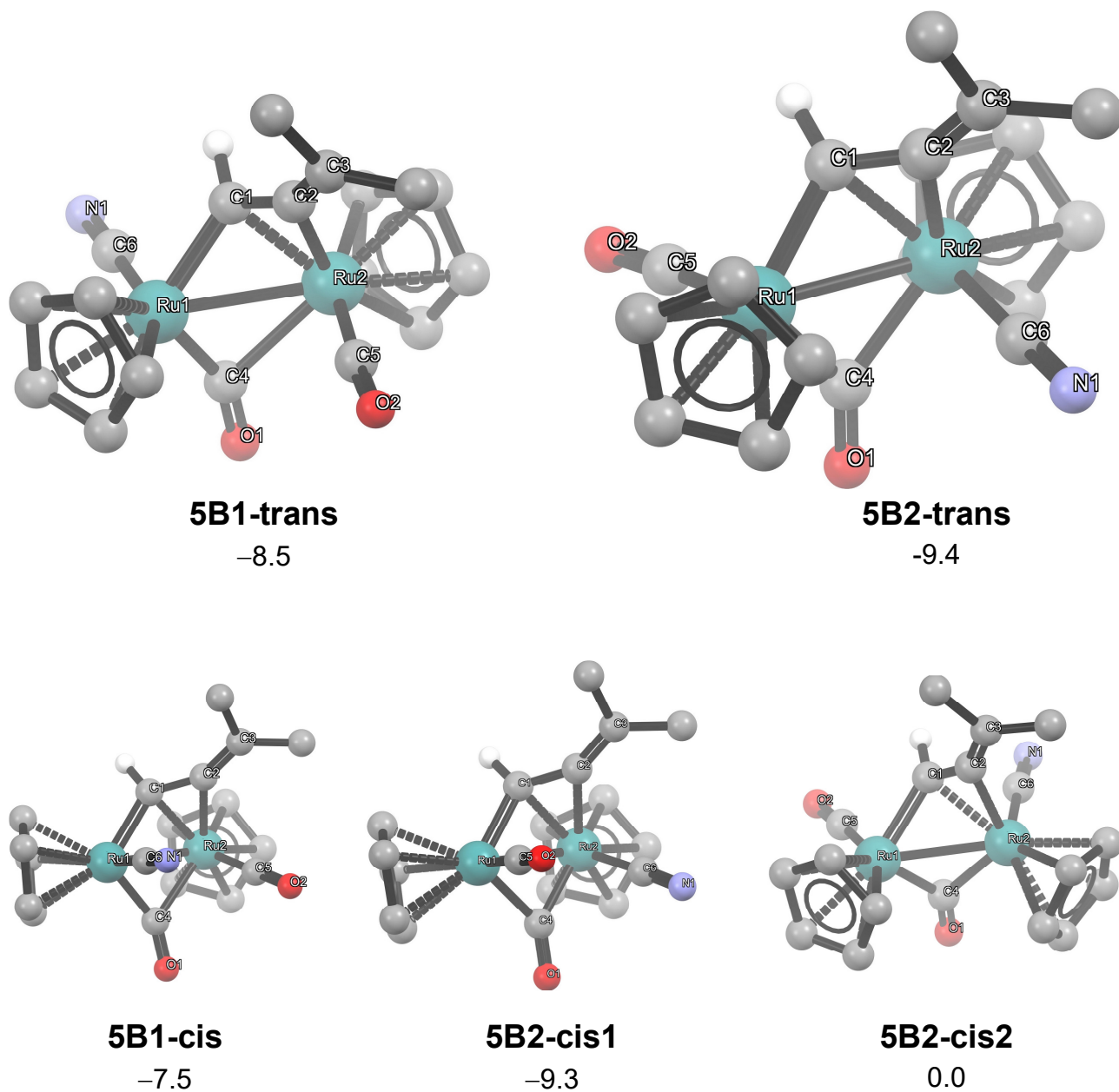
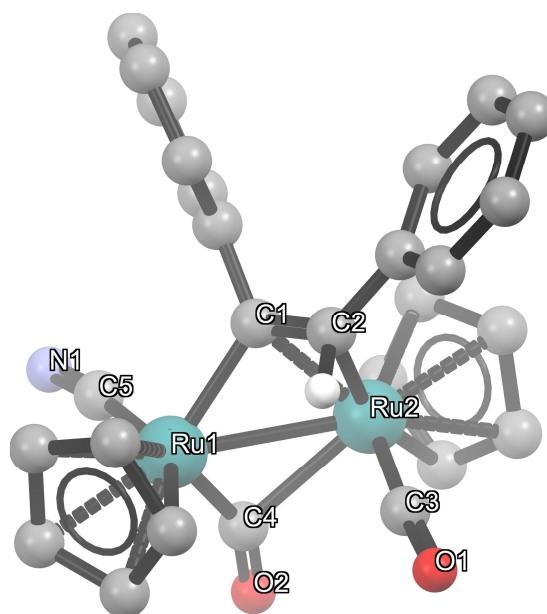
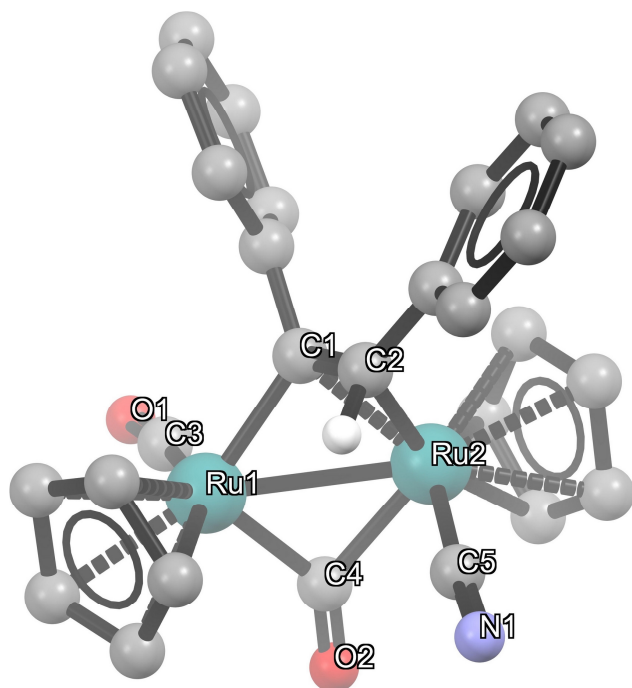


Figure S3. DFT optimized geometries of potential isomers of **6**, computed at the RI-DFT/BP86/def2-TZVP level (dichloromethane as continuous medium), and relative Gibbs free energy values (kcal/mol). Hydrogen atoms, except C α H, have been omitted for clarity.



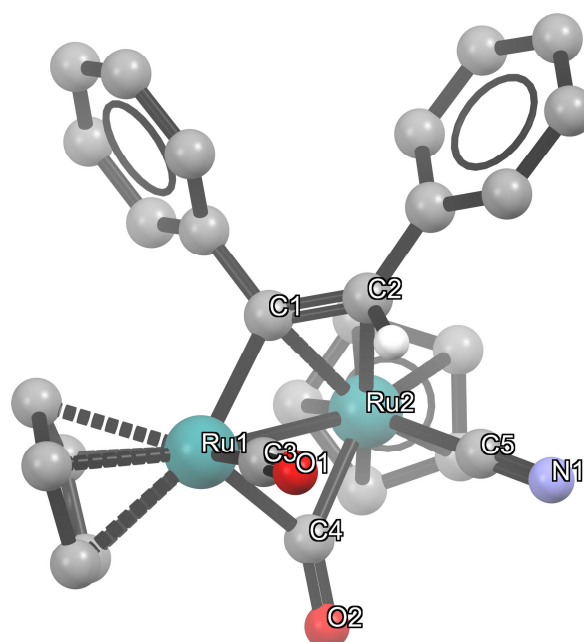
6-1-trans

5.1



6-2-trans

0.0



6-2cis

1.2

Figure S4. View of the molecular structure of **8bFe**. Displacement ellipsoids are at the 30% probability level. H-atoms have been omitted for clarity. Main bond distances (Å) and angles (°): Fe(1)-Fe(2) 2.5219(16), Fe(1)-C(1) 1.910(9), Fe(2)-C(2) 1.762(9), Fe(1)-C(3) 1.856(8), Fe(2)-C(3) 2.028(8), Fe(1)-C(4) 1.857(8), Fe(2)-C(4) 1.871(8), C(1)-N(1) 1.139(10), C(2)-O(2) 1.141(10), C(3)-O(3) 1.163(10), C(4)-N(2) 1.301(10), Fe(1)-C(1)-N(1) 177.9(7), Fe(2)-C(2)-O(2) 176.7(7), Fe(1)-C(3)-Fe(2) 80.8(3), Fe(1)-C(4)-Fe(2) 85.1(3), C(4)-N(2)-C(5) 123.0(8), C(4)-N(2)-C(6) 124.2(7), C(5)-N(2)-C(6) 112.8(7).

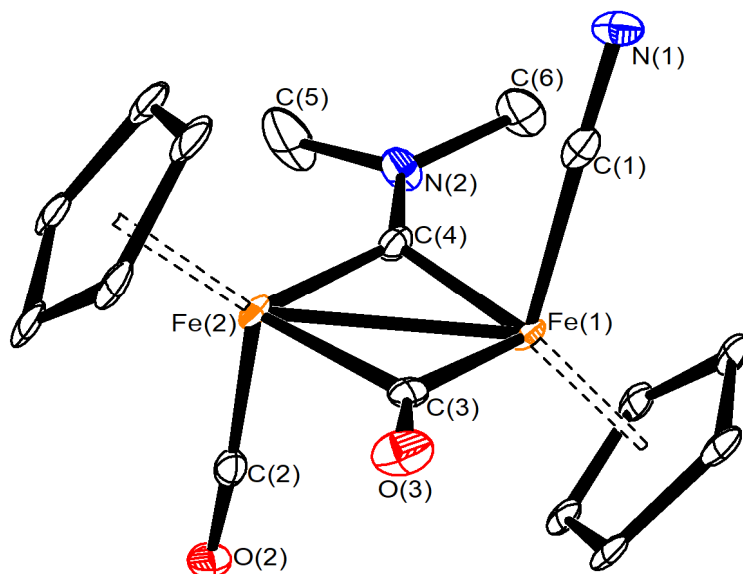


Figure S5. ^1H NMR spectrum (401 MHz, CDCl_3) of **5A**.

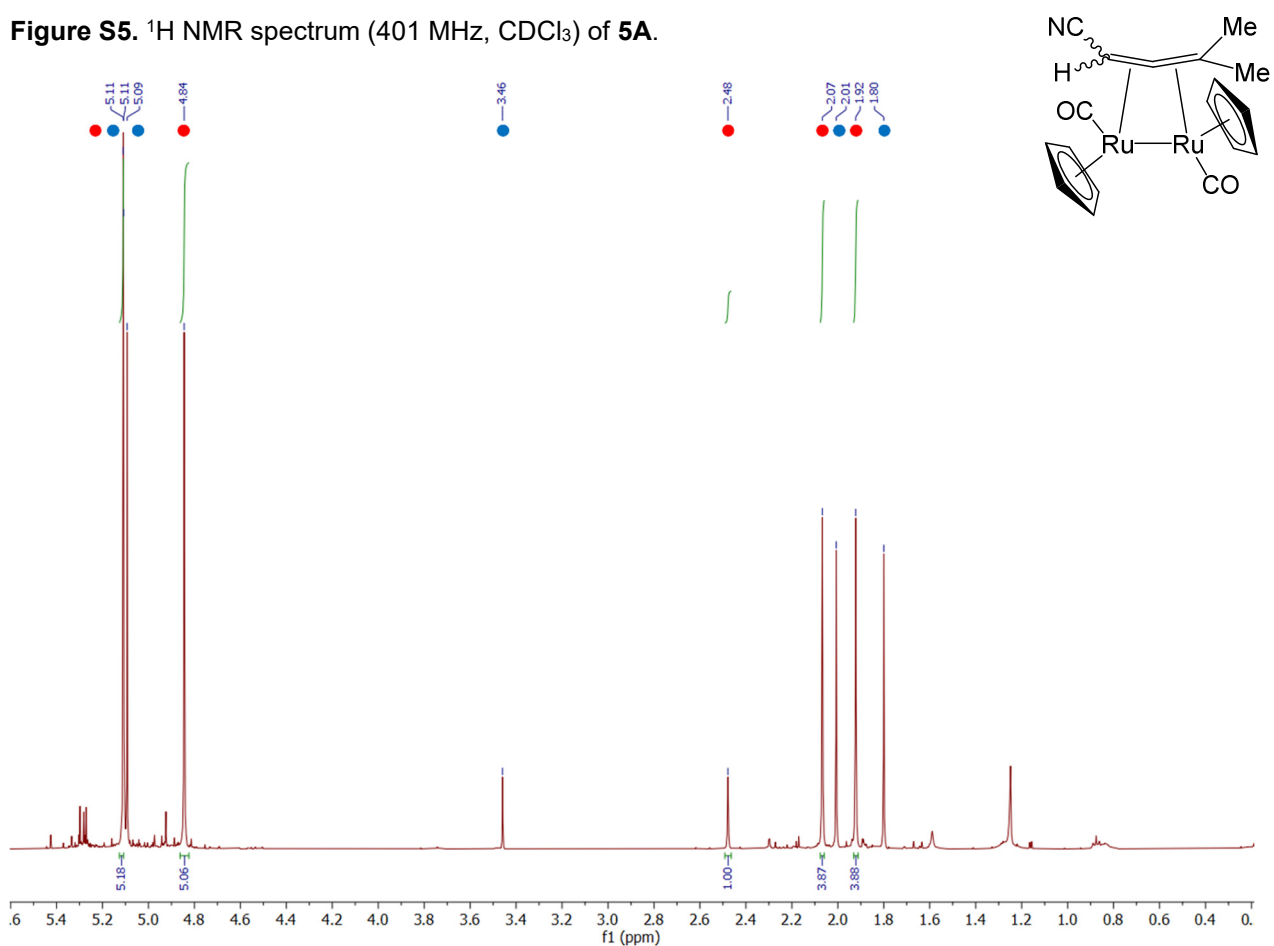


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **5A**.

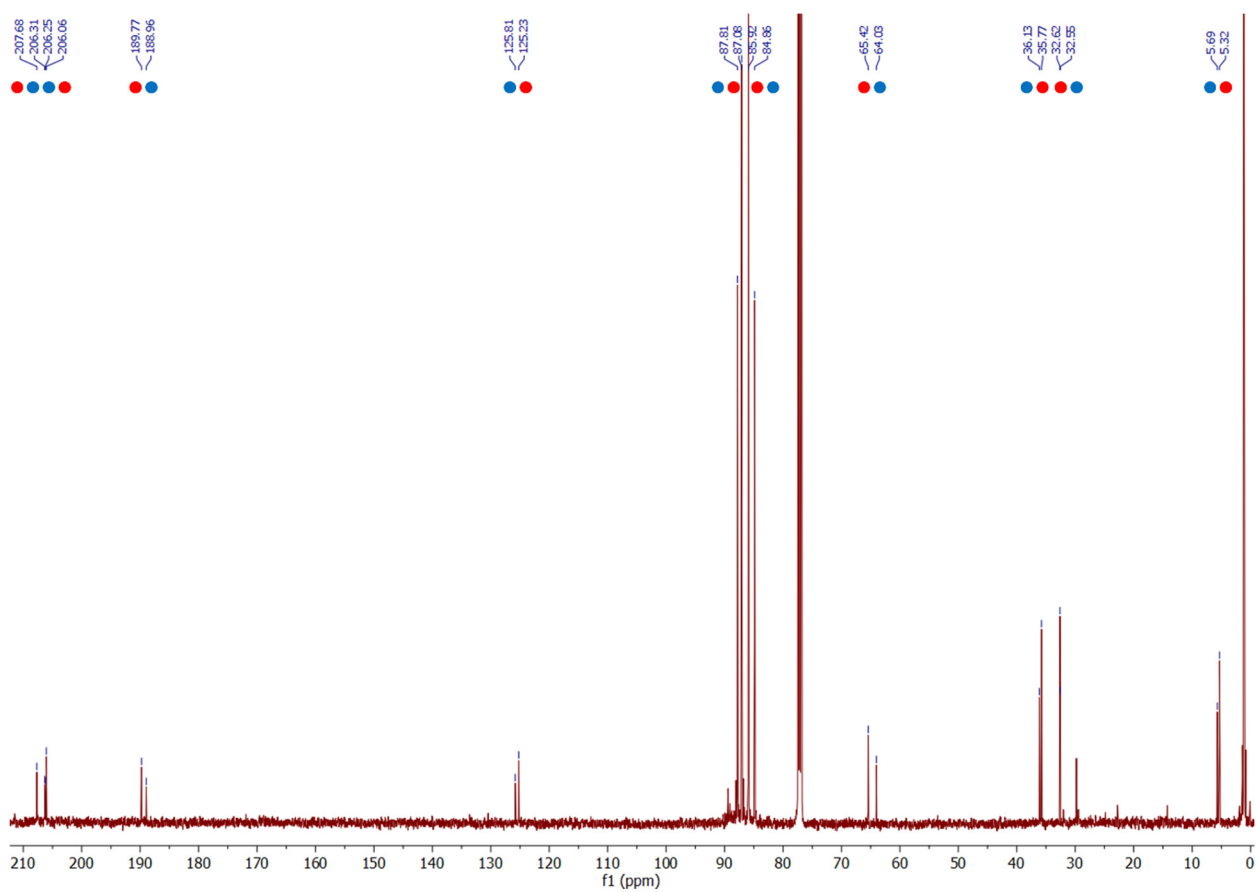


Figure S7. ^1H NMR spectrum (401 MHz, CDCl_3) of **5B1/5B2**.

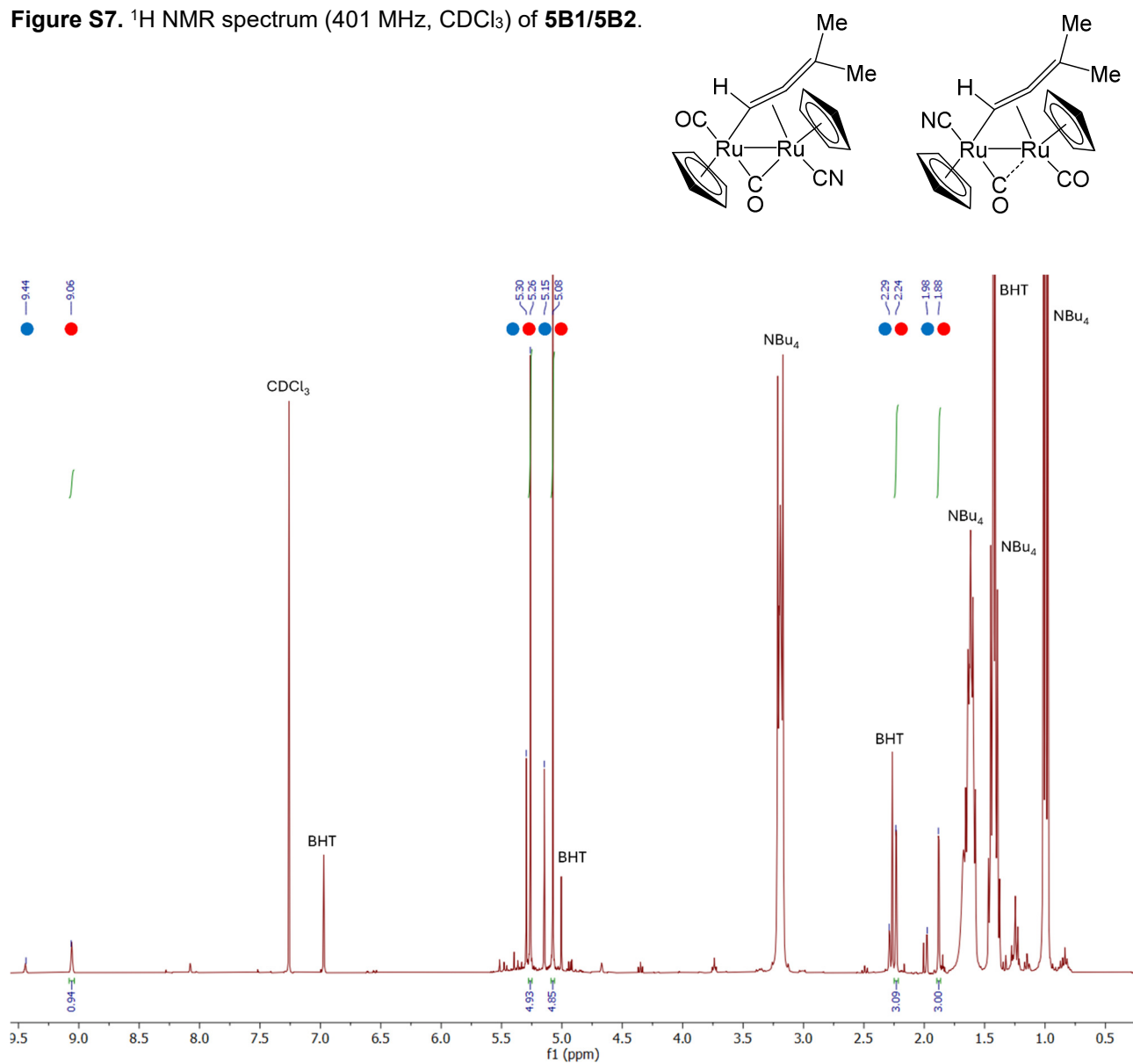


Figure S8. ^1H NMR spectrum (401 MHz, CDCl_3) of **6**.

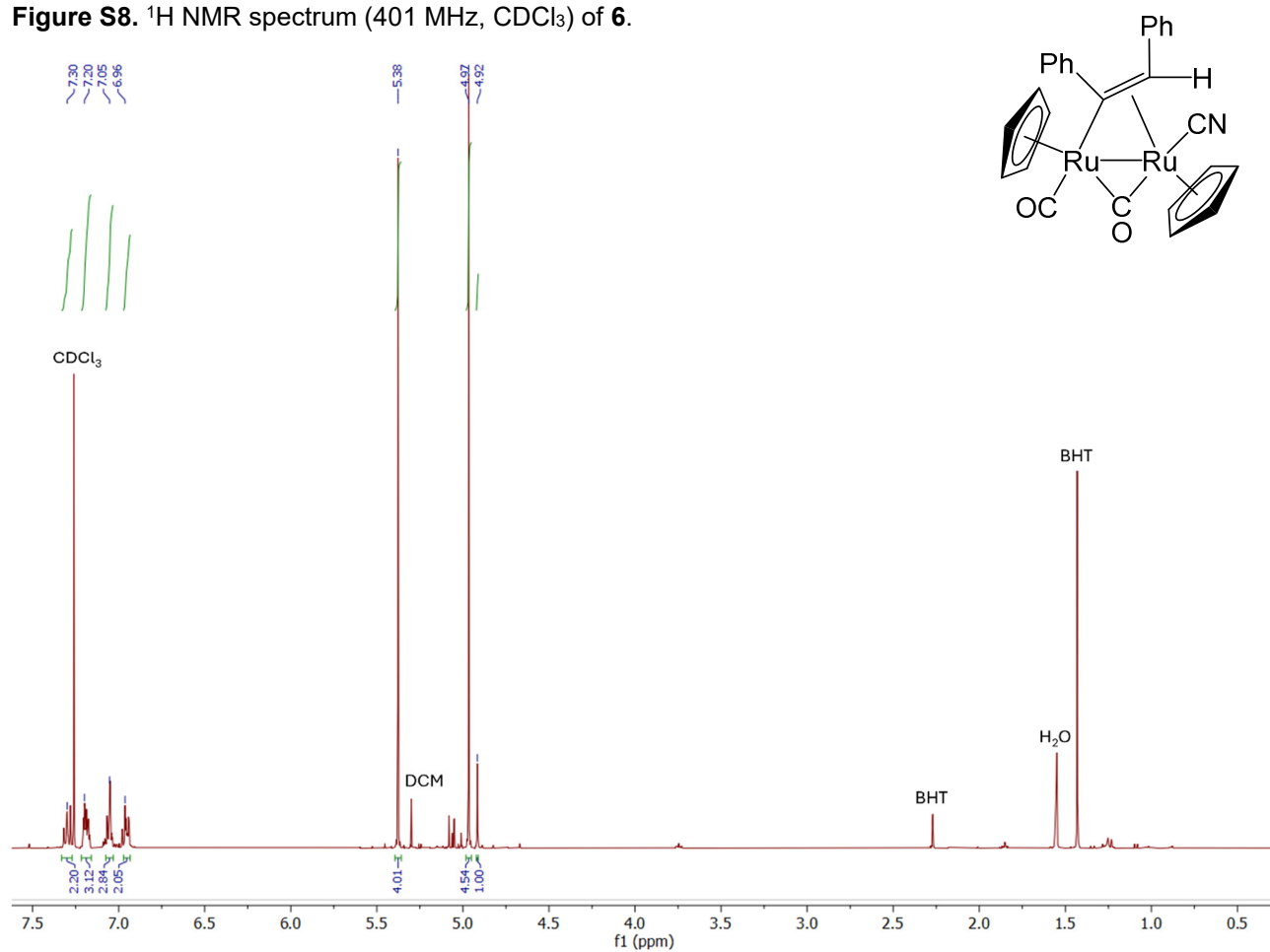


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **6**.

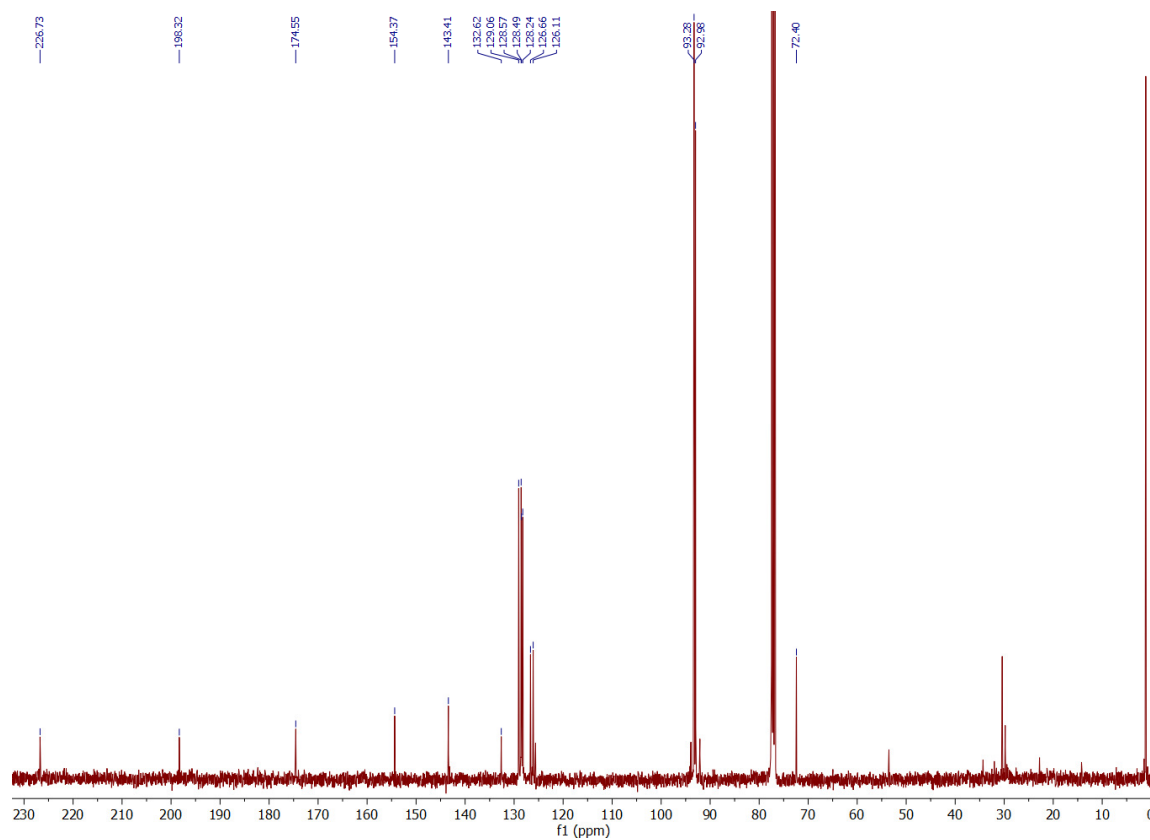


Figure S10. ^1H NMR spectrum (401 MHz, CDCl_3) of **7aRu**.

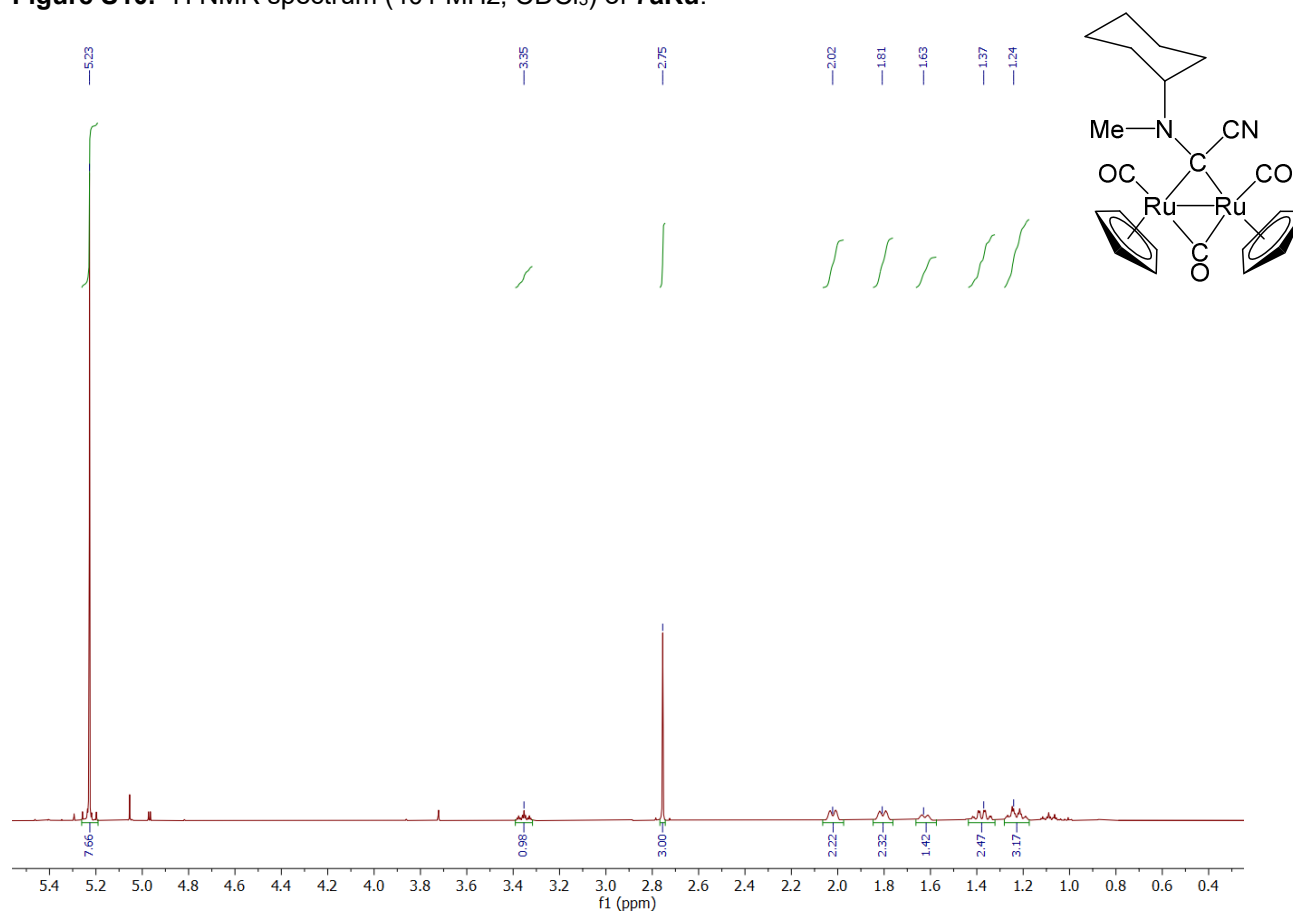


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **7aRu**.

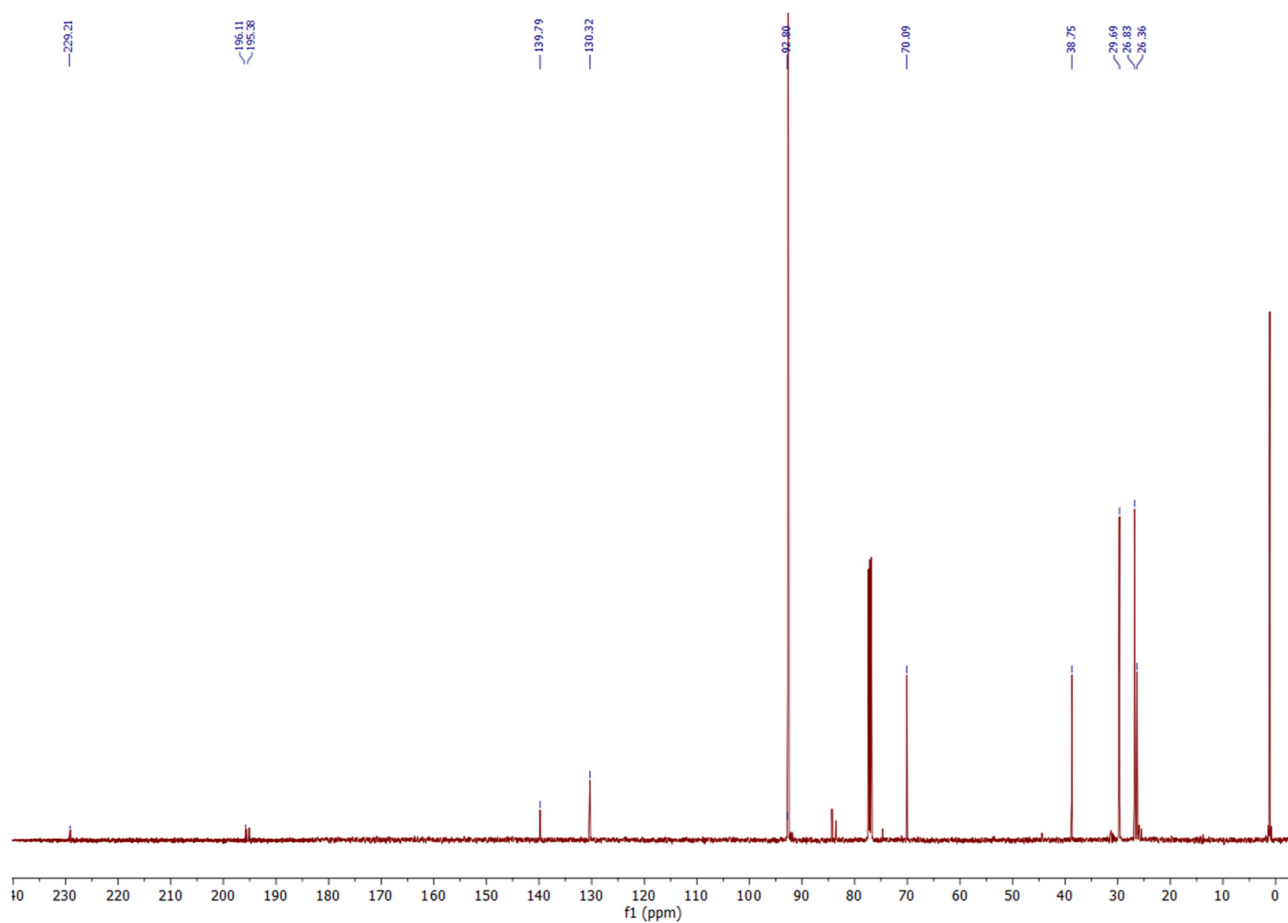


Figure S12. ^1H NMR spectrum (401 MHz, CDCl_3) of **8aRu**.

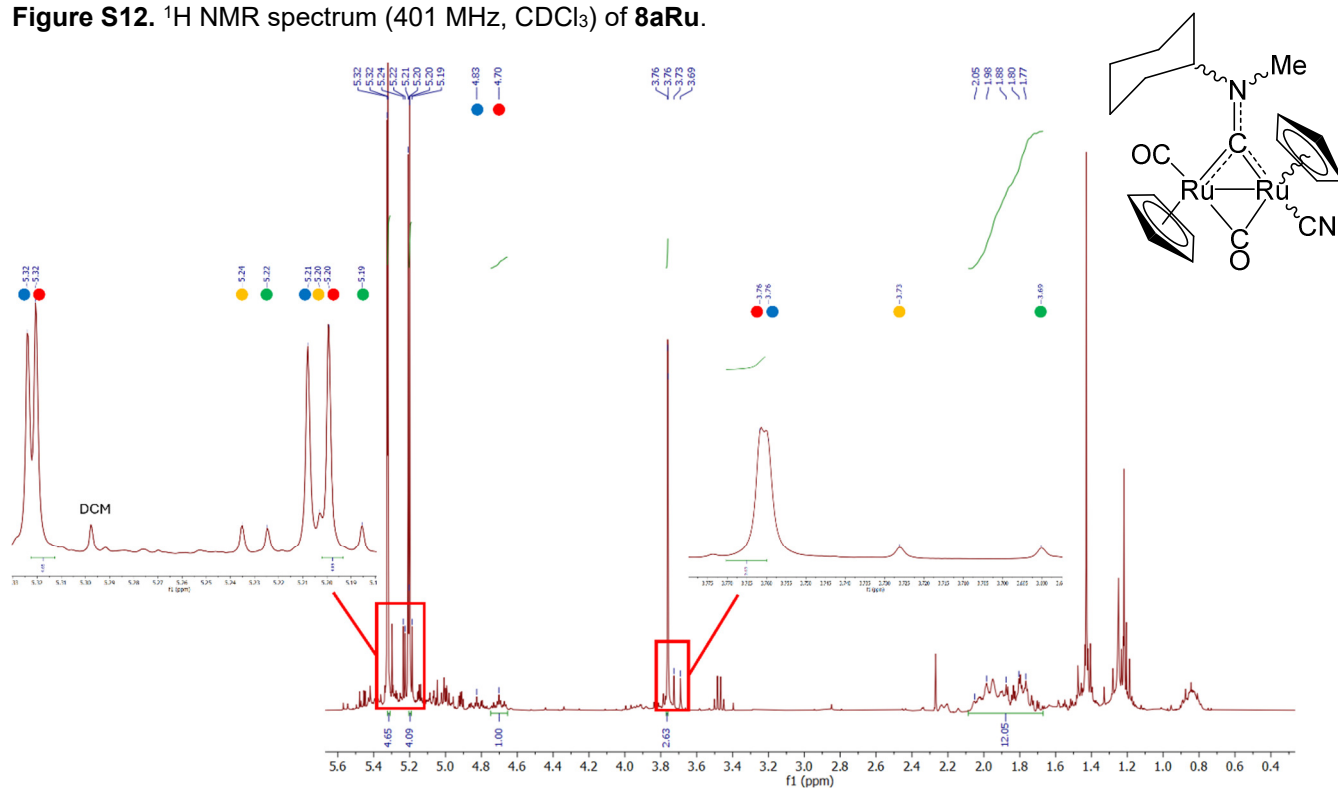


Figure S13. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **8aRu**.

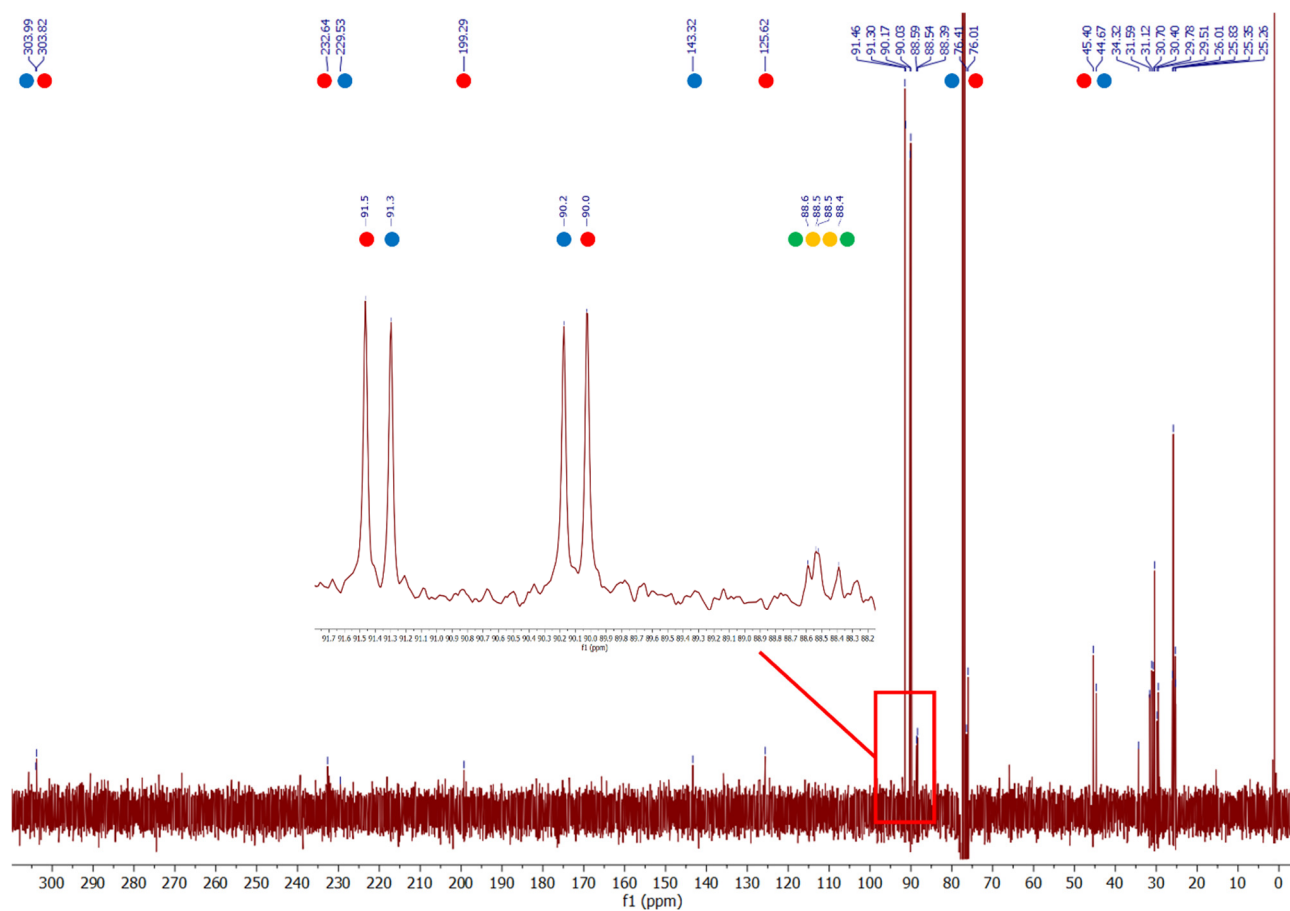
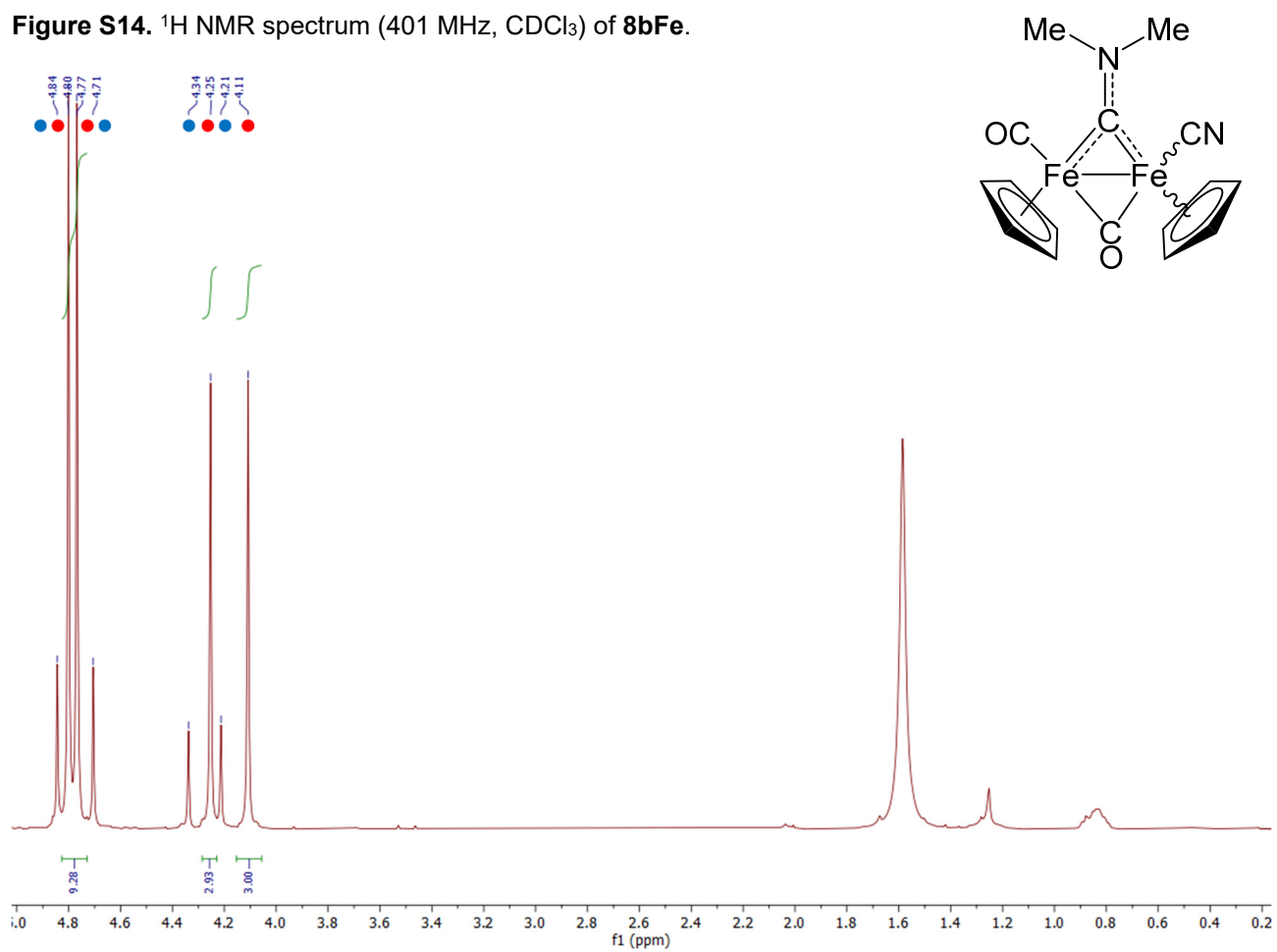


Figure S14. ^1H NMR spectrum (401 MHz, CDCl_3) of **8bFe**.



DFT-optimized XYZ coordinates

40

5A-is1

Ru	4.28878429344132	5.20523157023106	1.65701131138454
Ru	1.73605970088156	6.33371559389664	2.53784381127388
O	5.42864611777354	7.71449685852502	2.88379700339323
O	0.90381199726636	6.35445216111863	-0.35528095644345
C	4.90582398631358	6.76098521819610	2.45064756118155
C	1.27813016248632	6.27903878305563	0.75325415790042
C	3.89715092280299	4.40959843676468	3.68913104211009
C	2.74715514168783	4.58093674688878	2.84360882801567
C	1.44315870299700	4.05781904481861	2.67869293142695
C	5.11792099054339	5.56892346259577	-0.39541840936190
C	6.11212204466830	4.86322460401759	0.37256225636374
C	5.57477846728358	3.58933726559197	0.71444469687413
C	4.26491016153755	3.48567217063970	0.13600114976900
C	3.98619620983136	4.70446441865908	-0.55396969337127
C	0.34866091763737	6.93102510091523	4.21545759482087
C	0.14629587716895	7.81518701591319	3.11495838254978
C	1.37237534036651	8.53777612178467	2.89756791856971
C	2.30997177510473	8.12039276215010	3.89535493362681
C	1.68804220755017	7.12369949476372	4.70103806754233
H	5.22788009295511	6.56026493402266	-0.82611678812179
H	7.09506861100399	5.23612553726683	0.64684256280781
H	6.07120543186485	2.82525309642589	1.30721150447311
H	3.61189943511203	2.62061044690757	0.20227821620595
H	3.08484368646859	4.93535090288591	-1.11357147920547
H	-0.38886546964685	6.24762409770459	4.62692926283300
H	-0.77214630521587	7.92373782559678	2.54467385850831
H	1.53880102209821	9.30397302340124	2.14561062108419
H	3.32027840413809	8.49913744949839	4.01362391588511
H	2.13912593487815	6.60910799240328	5.54516398569017
H	4.17716502459758	5.15496300242721	4.43506297738490
C	4.33270376811700	3.08884477617448	4.01486472868219
N	4.69005104525958	2.00953834041059	4.28978375342515
C	0.92800180001636	3.39924437730630	1.41696126784354
H	1.45422676702054	3.73323722053339	0.51790835235344
H	-0.14762756737983	3.58445151004618	1.28220959065864
H	1.05966660110387	2.30556182902942	1.50677550486137
C	0.76569200332697	3.51571175296784	3.92841922879128
H	1.13845432082620	3.98880246231961	4.84523849624240
H	0.94498685701264	2.42841475514714	4.00359425906341
H	-0.32356748089981	3.66023483699819	3.87496959290706

40

5A-is2

Ru	4.27474433483934	5.26524603349376	1.63849852053176
Ru	1.73581155270510	6.35865668792111	2.56376880278585
O	5.20826207597121	7.98009788848532	2.56491939750593
O	0.89171320900258	6.25416912114995	-0.32461629474927
C	4.76079839659716	6.93961923151155	2.27032481606392
C	1.27088615226900	6.22990519087947	0.78421637517844
C	3.99763577957700	4.44777687334505	3.67315804392600
C	2.79833056172876	4.64000795881684	2.89897481131272
C	1.50338357511228	4.08355991765107	2.78017105692719
C	5.05945086881851	5.54454558149909	-0.44400416543006
C	6.10155075113437	4.94112046717133	0.34744354910564
C	5.63752926446955	3.66443144127237	0.77309363499383
C	4.32657219326008	3.45674803046185	0.22370207219212
C	3.97417120450798	4.61262574672160	-0.53556706094817
C	0.20619520586273	7.01947118664957	4.08465876451726
C	0.19956860393876	7.94566979161161	3.00052151059875

C	1.48880814797385	8.57895549211617	2.94327992443421
C	2.27180484028920	8.07025463159526	4.03150456479502
C	1.49198355934095	7.10556486332096	4.72619631030141
H	4.31797061688272	3.40746228771575	3.81439972295198
H	5.11017227414964	6.51269818685148	-0.93468343151758
H	7.06615197435006	5.38208857557072	0.58287823388627
H	6.18378439297567	2.96508814108291	1.40066338412371
H	3.72074104744198	2.56421531376949	0.35125699847265
H	3.05616131278862	4.75833299506099	-1.09698059011303
H	-0.62303243431087	6.38786032868702	4.39046515090645
H	-0.63316391571360	8.12924103391706	2.32664380278455
H	1.79226541367036	9.34980180013050	2.24058354200502
H	3.28656999347388	8.36442123647683	4.27911950518808
H	1.80860589267947	6.53981073316116	5.59769467535587
C	4.44866232725622	5.29166444554731	4.72574878086628
N	4.83414565091753	5.93945710187873	5.62120819835906
C	0.86558966282968	3.56491806942504	4.06043180855709
H	1.24646847323076	4.07315188996465	4.95453539216716
H	1.07420548493550	2.48465592774890	4.16096326375012
H	-0.22777523717540	3.68144797338798	4.02721998730698
C	0.97941024500777	3.37248526361955	1.55029334727879
H	1.48797400001440	3.68412700384394	0.63315137580961
H	-0.10142768766516	3.53296748593754	1.42644598088926
H	1.13339723486222	2.28511307054814	1.67637623692898

40

5A-is3

Ru	4.44745654329344	5.23824363231208	1.89294845733344
Ru	1.86228462016542	6.35080575912532	2.60386571432479
O	1.40982281542349	6.59274216460599	-0.36812948652209
C	1.61670523241283	6.43507957964817	0.77434798155159
C	3.82071085646523	4.20441325666558	3.74465162532380
C	2.74727500873583	4.54669731288381	2.86619080996063
C	1.43887285708176	4.10695416717437	2.54600456552591
C	0.36914063704049	6.99170898030709	4.17597504696463
C	0.40413124056472	7.98128060528284	3.15112848190379
C	1.72680794490845	8.54858566268273	3.12585082522438
C	2.49032030831493	7.92847578508118	4.16640383790378
C	1.66144075983643	6.96171242702203	4.80662588275761
H	-0.48905375152088	6.38261631133307	4.44572341496760
H	-0.42233131782573	8.25533727179355	2.50116653471791
H	2.06652902315773	9.34518853936726	2.46975184301869
H	3.51962419122327	8.15801057286155	4.42649188495752
H	1.94824638580509	6.32370417123490	5.63826947218195
H	4.14312648981950	4.88202120658555	4.53897684291947
C	4.14578839580328	2.83509183574948	3.98237228291722
N	4.41529835499378	1.71646560390284	4.19120790981272
C	0.98833433850235	3.56011611041252	1.20854087485927
H	1.58252035757973	3.93016972522880	0.36814620509808
H	-0.06726790702745	3.80605777495420	1.02169622173521
H	1.06640845625101	2.45783046649642	1.22617425202980
C	0.64162478062780	3.51464685342002	3.70030736791659
H	0.96741092685297	3.89692558923624	4.67565352977045
H	0.75492371286005	2.41586339087620	3.70405690428369
H	-0.43080006620415	3.72884619205536	3.58096473326930
H	6.85770485396745	4.99313752740348	0.19575561863249
C	6.43296519954306	5.65265804376778	0.94780279609491
C	6.62349996849397	5.54761954811723	2.35929343129454
H	5.26577994802533	7.13813169603023	-0.28721828310715
H	7.23119699297548	4.80589549390812	2.86945300026870
C	5.91467887622956	6.64160618041329	2.97746588330048
H	5.87310659261772	6.85136598693487	4.04269928799670
C	5.28567637737868	7.39673396850249	1.95031070855273

H	4.67944100083222	8.28566869811081	2.09079481528747
C	5.57975556255149	6.78279884370036	0.68964991708028
C	4.12788372976548	3.94577193442654	0.61165815762806
O	4.11917670247776	3.16195813038491	-0.25919634973728

40

5B1-cis

Ru	0.99566447251768	11.63256954705702	10.91631770865962
Ru	0.44982339025285	9.54545589590995	12.73084554067511
O	3.24600502919980	10.95970953257171	12.79235405494582
O	2.39390121354733	7.46895237480175	11.71560485404197
C	-0.57752306647550	10.32962038222843	10.97961816652159
H	-1.54321559225609	10.82435439760785	11.15936952119002
C	-0.58552661014881	8.95351123491985	10.89942900707699
C	-0.98421751894048	7.83220280644205	10.29617811098791
C	-1.63497462588468	7.91364516501228	8.93192743986489
H	-2.63065853363908	7.44024431455233	8.95499286387575
H	-1.03691920325416	7.36203860346048	8.18730562256149
H	-1.74314484447338	8.94984114830686	8.58876231264964
C	-0.82892018319829	6.44881928918534	10.86479684891954
H	-0.16475342457212	5.83651933867145	10.23173666595797
H	-1.80480785818883	5.93589722848064	10.88155555378484
H	-0.42487517654660	6.46153390872402	11.88384263633854
C	-1.07011652665251	10.45429909252125	14.20902443988152
H	-1.80514769617365	11.20643043336343	13.93726822001884
C	-1.24980053719830	9.03707907317684	14.13746337150755
H	-2.14343405575196	8.52118753119816	13.79676396103491
C	-0.04066867153980	8.41320335806016	14.58313657102486
H	0.13009526841313	7.34385951173416	14.67169015031247
C	0.89090481913879	9.45303894045223	14.93822913337964
H	1.89241793645698	9.30945549852605	15.33355118574403
C	0.24806444157190	10.70593185002486	14.70480689267225
H	0.69111240694562	11.68567515647825	14.86232501927249
C	2.21750544053866	10.92895062899081	12.20758692209894
C	1.64958898144942	8.29153217002807	12.06234089213875
H	2.93072118178912	13.69952833267098	9.94269353842876
C	1.91070608219053	13.61663549152995	10.30602563625074
C	1.47292741164194	13.74882135834240	11.65550439328982
H	0.72577076578280	13.21080319300547	8.42846418111782
H	2.11298139299750	13.93487686011866	12.51444191307356
C	0.04213322684264	13.61477000923266	11.69584173150892
H	-0.58427230985066	13.70032053022040	12.57938481976814
C	-0.40400651009054	13.38922339619602	10.36334252732127
H	-1.43287124584463	13.23072286301510	10.05013369856339
C	0.74043661621883	13.35641280272654	9.50511591319983
C	1.83174759592547	10.47709081086592	9.53426303684202
N	2.33537351725910	9.84461093958843	8.67836694349622

40

5B1-trans

Ru	1.31862704131045	11.29376317919862	10.74638880812395
Ru	0.48166193050089	9.48558419139332	12.73025799584258
O	3.14395217044906	11.17679683410959	13.14315963865467
O	2.28159157478501	7.35837048495051	11.56788091928616
C	-0.52652819606793	10.44933408407613	11.09296126647149
H	-1.37905806118368	11.08051034404443	11.37208315582599
C	-0.71045315486016	9.08755823398194	10.95437567875885
C	-1.26558717834660	8.04422195325600	10.33379354720785
C	-2.01329818957559	8.25242589156344	9.03476146946356
H	-3.05055693904601	7.88991578999494	9.12959329294758
H	-1.54827298404609	7.66967161774527	8.22188063541018
H	-2.03713302162578	9.30805681502252	8.73743408886089
C	-1.20788087637726	6.62811458745981	10.83688037193472

H	-0.70310075991637	5.97292580981984	10.10689029212064
H	-2.22725210084010	6.22630115309434	10.96252230470554
H	-0.68294660915509	6.55252583819910	11.79623624414411
C	2.32318480588653	10.03519086509281	9.04421490166210
H	2.44364228328096	8.95594812343490	9.05277570260559
C	1.22583037502516	10.75515643390538	8.49258821946858
H	0.34179055312128	10.31881060075129	8.03614738124381
C	1.46305832889086	12.15229752976869	8.67984588620655
H	0.81298078814778	12.95989363946559	8.35517084202561
C	2.74657878399297	12.30563539161476	9.32270026006283
H	3.23200601989527	13.24609174963778	9.56582941198895
C	3.25837904264313	10.99666412105702	9.55874298929979
H	4.20564825892479	10.76208431340795	10.03805717373436
C	-0.98486609723728	10.40217359152390	14.26329058253729
H	-1.71874472246585	11.16402876397372	14.01675847787530
C	-1.17515328941253	8.98213361024043	14.16753099861299
H	-2.08007455702241	8.47862600980597	13.83894787592808
C	0.03310673271797	8.34331090580183	14.59082320056969
H	0.19790762173139	7.27163687943322	14.65931163735122
C	0.98105915919403	9.37172982357488	14.92900865196306
H	1.99021335493152	9.21737625882846	15.29985067829739
C	0.33721360487967	10.63547336217924	14.73660491706289
H	0.78971431833407	11.61010065428370	14.89790379721676
C	2.24891712429879	11.03613921730228	12.38713241796488
C	1.59796787978490	8.20554802528307	11.98065199443598
C	0.50395238522883	12.93248806588936	11.50758807735024
N	0.01485559922332	13.92071125583296	11.92064121477584

40

5B2-cis1

Ru	0.94989264166344	11.60557179061700	10.78600380060067
Ru	0.45077210078758	9.61857756547289	12.68518484678594
O	3.15509209436625	10.99641242176475	12.76044151654826
C	-0.65178541783121	10.34656786442161	10.97064107127550
H	-1.61181716460235	10.84933718940864	11.14806590988992
C	-0.59806448366506	8.96954587056327	10.90218327677420
C	-1.01362537770672	7.85208195522219	10.29874356042865
C	-1.74715958211935	7.94276426952944	8.97753199875936
H	-2.73134162880237	7.44967100637983	9.04888971575523
H	-1.18633810784196	7.41493480555928	8.18745403393743
H	-1.89681519565442	8.98218341198432	8.65939179434299
C	-0.80560825703042	6.46274673808217	10.83345424094669
H	-0.22565828737411	5.85040159970370	10.12229050566429
H	-1.77805027513076	5.95701283666529	10.96037605601881
H	-0.27984903470977	6.46626766905034	11.79422078872843
C	-1.09299901981388	10.44029812285579	14.19940164132697
H	-1.85388838794232	11.17673885178590	13.95648364212809
C	-1.23263619359517	9.01965196228069	14.09908165808976
H	-2.11316740298032	8.48763814257353	13.74830081358388
C	-0.00352087423123	8.41681039790111	14.511111463294004
H	0.19929920170343	7.35089773100111	14.56193691057013
C	0.90512163375369	9.47166100872390	14.87460087475057
H	1.91598233387348	9.34450855743898	15.25124734910426
C	0.22340649820491	10.71638680380839	14.68027981732227
H	0.63779577188024	11.70396712885057	14.86602575284299
C	2.08981567337557	10.80788070785326	12.27195705745197
C	1.74332568386014	8.24732521071950	12.03727441689717
N	2.53733405210041	7.43476047326622	11.73228298293165
H	2.91894244949059	13.69906912814361	9.85565265324910
C	1.90656151674942	13.62474448116749	10.24233278513011
C	1.51326169546778	13.71467443503317	11.60133561559078
H	0.66942830907455	13.30975072480543	8.37780557737511
H	2.17960437956447	13.85426894565130	12.44848738464398

C	0.08244192741064	13.57928841119413	11.67548835201662
H	-0.51587763613150	13.62501486159535	12.58106623274199
C	-0.40817477391676	13.41228437341623	10.34926803047369
H	-1.44739258139125	13.27955278433223	10.06061735559012
C	0.71315332092991	13.40117137453202	9.45974686030342
C	1.78158460392775	10.50772130881959	9.54543487319725
O	2.31966679428666	9.89620307782489	8.71317161329057

40

5B2-cis2

Ru	1.18929360287910	11.26571333363233	10.79664319412397
Ru	0.61352097341860	9.17850903327517	12.55141202884389
O	2.46536008910983	11.39723486989560	13.54094439706769
C	-0.60796223715009	10.32802860154312	11.12499859062110
H	-1.43907506155422	10.92567231198635	11.51308024326466
C	-0.83565555291383	8.99944938149883	10.88244281323055
C	-1.56083198208544	8.10042798432848	10.20623956918368
C	-2.29434079121508	8.55986271334045	8.96083334397336
H	-3.37592034150198	8.36996121816357	9.06506843374103
H	-1.95686929031596	7.98856005564742	8.07915507698998
H	-2.14205280046075	9.62737377689190	8.76086315433789
C	-1.74406148652688	6.64653235167545	10.54304610314837
H	-1.20581820110749	5.99514045075463	9.83258883669864
H	-2.81009600794568	6.38141092518378	10.45526472108163
H	-1.41899658466071	6.39945764140981	11.55795738446753
C	2.35988543363313	9.94848379095501	9.25985782215000
H	2.40195091342982	8.86418208054349	9.28645190195489
C	1.40141471750121	10.72733222901764	8.55283260719017
H	0.56715347114719	10.34559525169941	7.97138163190214
C	1.70565505362223	12.10672774831113	8.77646975220202
H	1.16955788075260	12.95412148182820	8.35764973438928
C	2.90352850089588	12.17873056016425	9.58179375458460
H	3.40744044135870	13.08824248212792	9.89593980404666
C	3.28872893747760	10.84942500291275	9.89231122634768
H	4.14041370263046	10.55774708472270	10.50123814837022
C	1.76255155308143	10.93473083121882	12.70387476628829
C	0.41627948280987	12.81882631005101	11.43883451236084
O	-0.03473402692570	13.83037637819254	11.79872990904111
H	3.29134642986018	8.87640590167781	13.89260724283592
C	2.48425978246606	8.26844924501617	13.49509465294009
C	2.41718517097701	7.72277828318633	12.16427137949162
H	1.09365681028490	8.09899275922885	15.24379156549657
H	3.17141805880883	7.83784768332764	11.39209610745975
C	1.20546802422034	7.00304988395861	12.05434372839585
H	0.86594220452338	6.47091551954158	11.17201853543999
C	0.50146662800332	7.09695606390062	13.31242800406877
H	-0.43256481061094	6.60852862686619	13.57253500817280
C	1.32548596123787	7.86131791609407	14.20980031417453
C	-0.65688347764591	10.03065819743601	13.81504325834717
N	-1.39626117150899	10.48219303879285	14.61215274157319

40

5B2-trans

Ru	1.19186369592166	11.38189989820170	10.71819712317093
Ru	0.47962870570836	9.59808948915224	12.72429433026914
O	3.11244495613324	11.08936267855981	13.03813156398341
C	-0.61427034087249	10.47316338417238	11.09503758999262
H	-1.50937751751755	11.05987230172183	11.32881304142140
C	-0.67065811892679	9.09810839492848	10.96362834063688
C	-1.19054729062697	8.03588072695452	10.34048717659325
C	-1.98776819734819	8.22175872954772	9.06750304188216
H	-2.99907227486910	7.79626027357371	9.18274385047885
H	-1.51387016547689	7.68247397002794	8.22977021997248

H	-2.08296808165333	9.27919825905429	8.79058909755055
C	-1.04821406170541	6.61756402359854	10.81855851815257
H	-0.57020752202874	5.98901947736495	10.04805189394308
H	-2.04291603508485	6.17777427330639	11.00510206809823
H	-0.45415986266069	6.55189454060270	11.73658253274005
C	2.14251791923028	10.01650556807519	9.06711499400520
H	2.13921012460875	8.93250183339187	9.12649709454960
C	1.13937298309043	10.83226956450552	8.47217688120712
H	0.22781610206702	10.48309002659261	7.99579907241217
C	1.51743509911661	12.20122603110436	8.64993326433487
H	0.97126833089613	13.06803790007340	8.28780472415843
C	2.79907264789273	12.22616368096856	9.31478967245889
H	3.36844677568782	13.11574929224881	9.56855680368932
C	3.16794759800796	10.88188085750549	9.58048844612952
H	4.06910475095659	10.55752321293141	10.09426894537330
C	-1.00686552161795	10.44031625038397	14.28900065298675
H	-1.73673962001907	11.21749703955615	14.08041859327373
C	-1.20618092990058	9.02938058254279	14.12866356852889
H	-2.11068526307011	8.55048686620179	13.76281549356671
C	-0.00537013634667	8.35737539788354	14.51456265917867
H	0.15096811058268	7.28261869443289	14.52395759397207
C	0.95045200702262	9.35857867832741	14.90537625045243
H	1.95816051207809	9.17575875313231	15.26712237406070
C	0.31853115933328	10.63879780981589	14.77038043563016
H	0.77767710690536	11.59973136374423	14.98780887623011
C	2.11919180475505	10.84973740644322	12.43477579877979
C	0.58143697958263	12.93785375184929	11.49998896832368
O	0.22152694376967	13.95383834595475	11.94651299367379
C	1.70894297732293	8.20351556395596	12.00857272709946
N	2.45622564905544	7.36200210761043	11.66491472703807

53

6-1-trans

Ru	2.38493032851636	2.68217035181326	3.90567594293134
Ru	4.87810843618905	2.45439015120148	5.18382910582230
C	4.12693942558399	3.83071710777701	3.64689248323511
C	4.44781926770770	4.67178541180769	4.76084497125388
H	3.63068379133282	4.89492569268810	5.44800643529237
C	4.66245421180556	4.13084488336215	2.29141770840911
C	5.24564024630951	3.19222054912393	1.42033933646330
H	5.35787142936750	2.15883298024798	1.74046785474672
C	5.66265732195479	3.55809271858257	0.13955335063503
H	6.12156271171843	2.80932535545475	-0.50899596732290
C	5.48121867326087	4.86662857404043	-0.32061800848637
H	5.80057017858517	5.14744867645332	-1.32569522938961
C	4.87497312135669	5.80698806192283	0.51859203239423
H	4.71339945199428	6.82966388543439	0.17197775708907
C	4.47985890828476	5.44599845708817	1.80711239943841
H	4.01128055140177	6.19035594388831	2.45314825015608
C	5.53449790336561	5.67549497400310	4.89563204840006
C	5.34076691091831	6.70194724900102	5.84290381645553
H	4.42266435993641	6.70927780873591	6.43542719335367
C	6.29369240871919	7.70445989972237	6.03472560809737
H	6.11412986590140	8.48772011891862	6.77357870320913
C	7.47230254330808	7.70188396167647	5.28386055341755
H	8.22151974590541	8.48180417547286	5.43011445351706
C	7.68520958311495	6.68547545810927	4.34430423910733
H	8.60413467708166	6.67198419579287	3.75506274007089
C	6.73227148813224	5.68515462072054	4.15255847750768
H	6.92328504072436	4.90675396454526	3.41468497925070
C	2.99906508732569	1.10740777510004	4.77880541161870
O	2.87115049320419	0.00365723773912	5.17923115775011
C	1.10476321254156	4.61820760267563	4.07606127233126

H	1.51689501490530	5.60906332288814	3.90464530319236
C	1.01339781493134	3.95632622104216	5.33560302936054
H	1.30240354366645	4.36543834251866	6.29957279992683
C	0.42311304256178	2.66868989044143	5.10741487256149
H	0.21432912170170	1.92401714819203	5.87152570859768
C	0.14730888046825	2.53407945670640	3.71644508351677
H	-0.32296085584835	1.68583549495847	3.22785013256969
C	0.59021001467436	3.74791945952136	3.06940163110992
H	0.51032940958911	3.97106150352573	2.00933692701535
C	6.57479081768965	1.54678486223112	6.33259960045517
H	6.63050346402926	1.63191019385455	7.41472352461460
C	7.12657343977853	2.46916369820313	5.39068193570761
H	7.67742760980252	3.37435004085726	5.62964059076810
C	6.84904636607918	1.96867203965525	4.07483416945834
H	7.15633270044510	2.43431129457307	3.14380788886282
C	6.10987185539028	0.76133072541328	4.20327577276385
H	5.73451828311698	0.14963476348489	3.38719337684126
C	5.92403819058833	0.49999606148338	5.60339332028054
H	5.40195635883929	-0.34985032702379	6.03201887684424
C	4.03548910664789	2.90742422323436	6.77403350015671
O	3.59585985723713	3.16192097472386	7.82125681082335
C	2.68071936610024	1.69900230106972	2.21289590604886
N	2.72001922205694	1.06767546534580	1.21921716176841

53

6-2-cis

Ru	2.73911535151117	2.38320098471811	3.58580627393978
Ru	5.03792391961670	2.46083822426557	5.15640140105618
C	4.30746231172150	3.77464674874696	3.55865398597981
C	4.48727356336333	4.62976242187770	4.69022360837241
H	3.61647146001393	4.79935708738442	5.32230120358156
C	4.90845299451217	4.12031138283726	2.23875549602428
C	5.67700449894797	3.25643190732770	1.43763754723012
H	5.90801799700062	2.25484914888944	1.79493752216761
C	6.14784002459396	3.65852474190738	0.18562560246344
H	6.75279229842312	2.96955330582332	-0.40704339353591
C	5.84515109508780	4.93061888525468	-0.31102748385991
H	6.20968593932913	5.24152423795671	-1.29142852204234
C	5.06695425065520	5.79754839492418	0.46323774789930
H	4.81636548256926	6.79211183407485	0.08900525471623
C	4.61273865740259	5.40134053647179	1.72171823327263
H	4.00979411041559	6.08786977907473	2.31844094704952
C	5.50150822477039	5.69402172951691	4.89629693451363
C	5.19119435958586	6.70147521180386	5.83384612981649
H	4.23819052681433	6.65291639164065	6.36541342382043
C	6.07501677797443	7.75045963637972	6.09506868602550
H	5.80567396496439	8.51473392852910	6.82650572113612
C	7.29989588713942	7.81834492311794	5.42496205562028
H	7.99552723167518	8.63463536187231	5.62695249783496
C	7.62708148300224	6.82498724194578	4.49381827152105
H	8.58167480493933	6.86594255860720	3.96556684234514
C	6.74291653082213	5.77780436327161	4.23340160455061
H	7.02230839388895	5.01985232411863	3.50357434868548
C	3.27268007118403	1.44616873439112	5.31289901154365
O	2.80126610319574	0.62194657872500	6.02745155086369
C	6.54069389405834	1.31469135160924	6.37345324655590
H	6.40730913702265	1.18666878802483	7.44378932829333
C	7.19834002385738	2.42366506897255	5.73135546123079
H	7.67986025448045	3.25832105294496	6.23247964672670
C	7.15815918822690	2.18602941538431	4.31898548305820
H	7.59392752924895	2.82097615151209	3.55366115669376
C	6.45993477175887	0.96414074736325	4.08909989167082
H	6.27410103860218	0.49720837281764	3.12641464187778

C	6.07935703192111	0.42705256088065	5.36262789883698
H	5.52749367541504	-0.49405852252903	5.52778829680162
C	4.38356918682372	3.16790724353615	6.89917767020718
N	4.05581824665957	3.54014182991632	7.96549267685308
H	4.16817652354138	0.54483008917010	1.55180819222298
C	3.17965250877556	0.90648698502649	1.81783937792554
C	2.53805464127533	2.06759061257238	1.29964279760837
H	2.46560339561835	-0.64126541498057	3.28795813888788
H	2.96435292871354	2.77447024227145	0.59442329578497
C	1.25017035540888	2.17043659339999	1.90897497422514
H	0.50774079171343	2.93793792976716	1.70697068899718
C	1.07245133371341	1.03013453880714	2.77747460279013
H	0.18775518142359	0.80640943004607	3.36653015397312
C	2.26743546668621	0.26775830391950	2.72636903933341
C	1.66359398542967	3.52555658577260	4.56309718422266
O	0.88721259450420	4.19674343833941	5.11688265263007

53

6-2-trans

Ru	2.39463392742693	2.70614179267986	3.83118429230558
Ru	4.84194612250509	2.44898355568354	5.12040296928938
C	4.14518789389752	3.83830957379832	3.60748381998518
C	4.43393770628822	4.66421189828431	4.74055972440360
H	3.61135717331425	4.87189277069950	5.42347227574400
C	4.65936926495621	4.13166198959019	2.24383999843885
C	5.22278785674950	3.17557685395856	1.37760515641883
H	5.35051903988008	2.14891178691497	1.71853130988176
C	5.61908420906112	3.51761948021015	0.08394220219665
H	6.06330266820419	2.75672869557121	-0.56068650427351
C	5.44327047501273	4.82242203601103	-0.39002545143729
H	5.74765469122488	5.08645023077445	-1.40414650515901
C	4.86709363763249	5.78157131994761	0.44876568862439
H	4.71519405343089	6.80224338900142	0.09214503229695
C	4.48775675261945	5.44296222168423	1.74855109818310
H	4.04054907350463	6.20063836984154	2.39408366603357
C	5.52401105316531	5.65760690026029	4.90664784288344
C	5.34978775896495	6.63857769354304	5.90562171829315
H	4.44185178152558	6.61878563014287	6.51301132704803
C	6.30998091788834	7.62670324205097	6.13096489054712
H	6.14552135290231	8.37238965210175	6.91115823117067
C	7.47637936926762	7.65915659408334	5.36119759239328
H	8.23035955811746	8.42916781319593	5.53325893305064
C	7.66886210518873	6.69074436191635	4.36844472709820
H	8.57660105122568	6.70507045232658	3.76193825456553
C	6.70916616413280	5.70327704056781	4.14420035798281
H	6.88505660399563	4.96466546624379	3.36322999455667
C	2.69840230838969	1.64630747700299	2.35338324336194
C	3.14324827421043	1.25528382450729	5.01348365023174
O	2.75391620026833	0.95310593195487	1.41601278223789
O	2.81370747209222	0.20796658454264	5.46560987624727
C	1.10071737799117	4.62769255064665	4.03026764523942
H	1.51131414098001	5.61456872707055	3.83546177592933
C	1.05359297234988	3.97310914418202	5.29577322860240
H	1.40359669085919	4.37408121994221	6.24263434465723
C	0.43828078977314	2.69067482125052	5.10733971448024
H	0.26005532817263	1.95234171662683	5.88456163930927
C	0.12034263492175	2.54562041470079	3.73187691343362
H	-0.36428849451307	1.69092425985884	3.26815450497206
C	0.54805249816693	3.74759686546392	3.05166132335167
H	0.42050551393780	3.96147198568093	1.99412535149158
C	6.51294616277088	1.48887288477992	6.31280412649712
H	6.50613000320820	1.50317482256404	7.39904249135960
C	7.07085068521895	2.49565255044807	5.46604312426415

H	7.58273573082510	3.39547474362353	5.79510248082064
C	6.85593172250669	2.09023700346629	4.10432712490124
H	7.19489350036650	2.62505832604706	3.22258227950401
C	6.14958427988674	0.85395510198038	4.11286833784637
H	5.84607998935103	0.27701668702496	3.24360694210808
C	5.92849456793428	0.48658758370137	5.48625231630617
H	5.40943150227713	-0.40103922068173	5.83535167983240
C	4.05642887974837	2.98188709031707	6.87468629033537
N	3.65480500622304	3.25394909221401	7.94663317015722