In Situ Catalyst Modification in Atom Transfer Radical Reactions with Ruthenium Benzylidene Complexes

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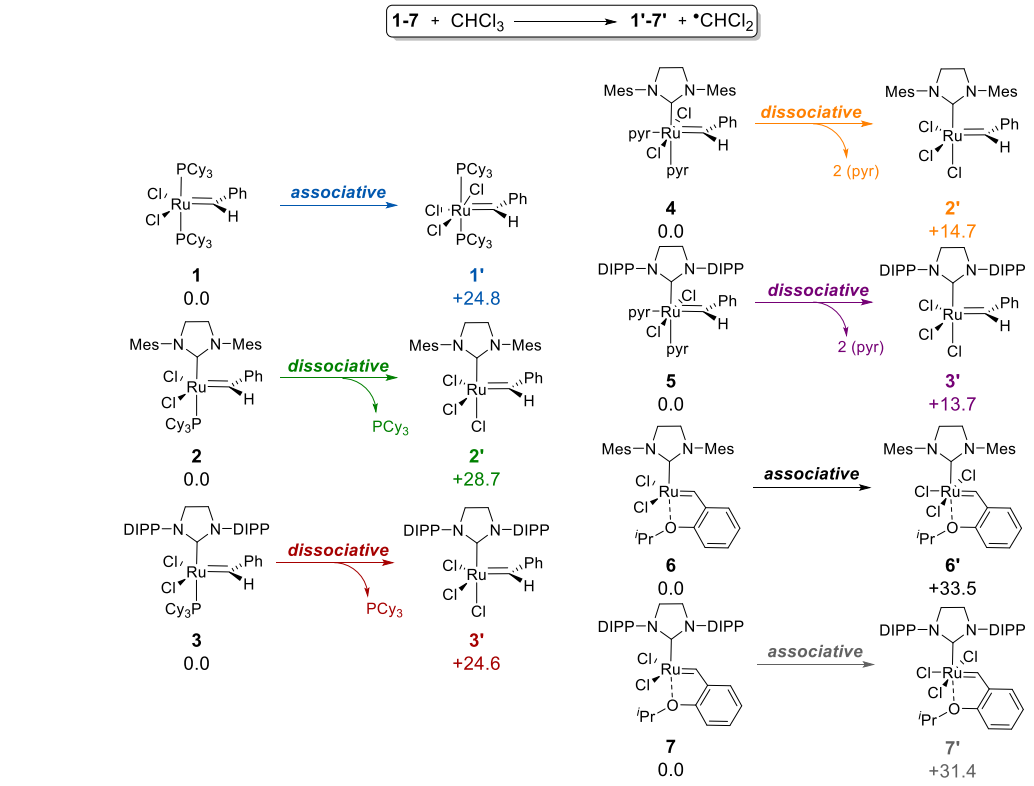
Supporting Information

Computed ΔG_{rxn} (kcal/mol) for ATRA reactions.

Geometry optimizations and frequency calculations were performed at the (U)B3LYP level[1-3] using LANL2DZ for Ru and 6-31G(d) on all other atoms. Thermal corrections were calculated from vibrational frequencies using a standard state of 1 atm and 298.15 K. All frequencies below 100 cm^{-1} were raised to 100 cm^{-1} to correct entropies for the breakdown of the harmonic oscillator approximation as discussed by Truhlar.[4] Subsequent single point energy calculation were performed at the (U)M06-L[5] level using SDD for Ru and 6-311+G(d,p) on all other atoms and including the SMD[6] (chloroform) solvent model. All calculations were performed using Gaussian 09.[7]

(a)



(b)

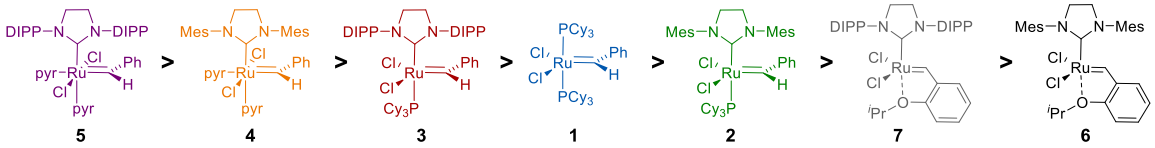


Figure S1. (a) Computed ΔG_{rxn} (kcal/mol) for chlorine atom transfer from CHCl3 to complexes **1**–**7**. (Note: loss of the first pyridine, anti to the benzylidene, from **4** and **5** is exergonic by 4.7 and 5.1 kcal/mol respectively) (b) Computationally predicted order of ATRA activity.

Decomposition study of ruthenium benzylidene complexes.

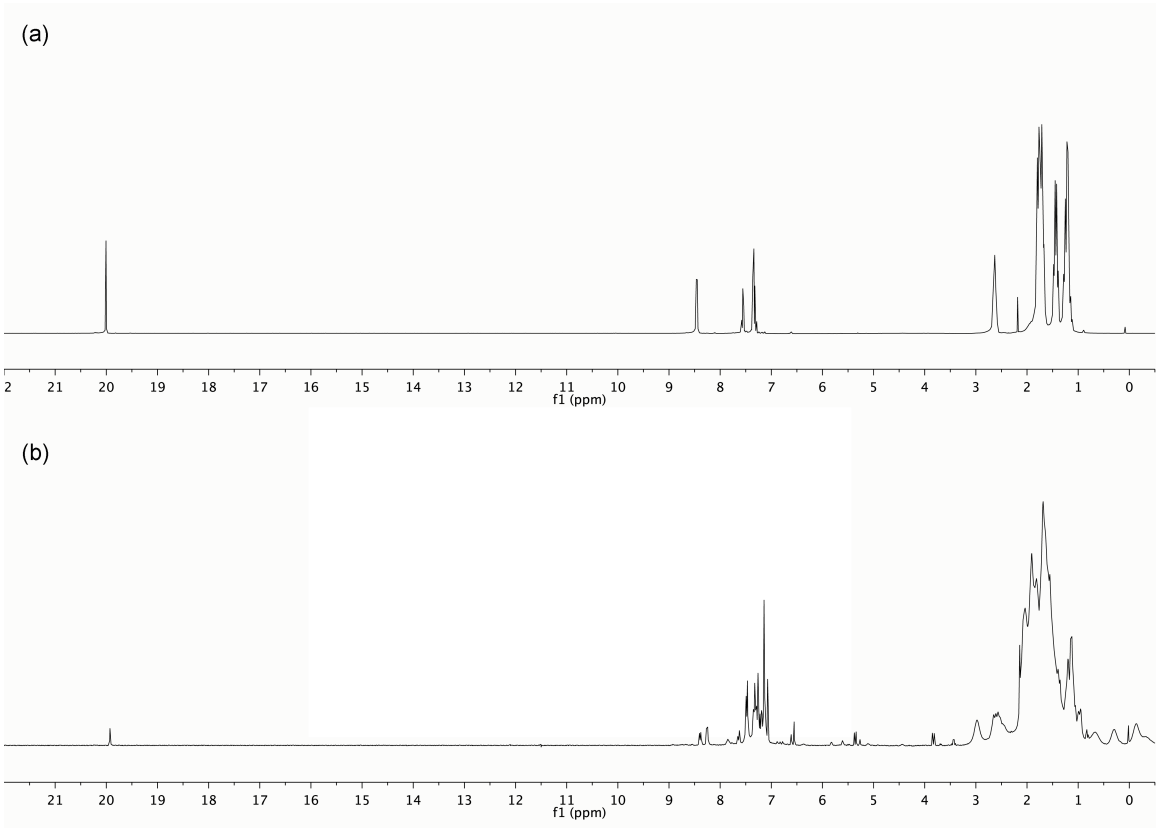


Figure S2. ^{1}H NMR spectra of **1** at (a) 0 min and (b) 200 min after activation in $CDCl_3$ at 65 °C.

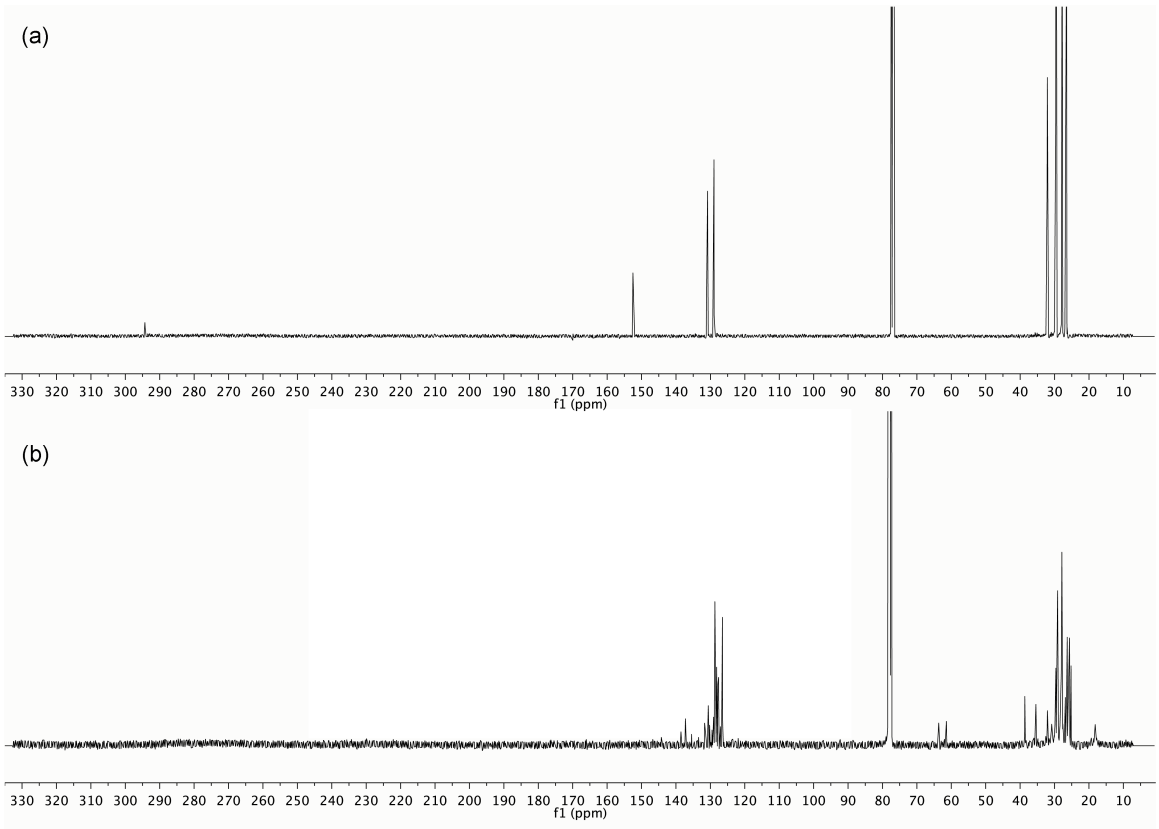


Figure S3. ^{13}C NMR spectra of **1** at (a) 0 min and (b) 200 min after activation in $CDCl_3$ at 65 °C.

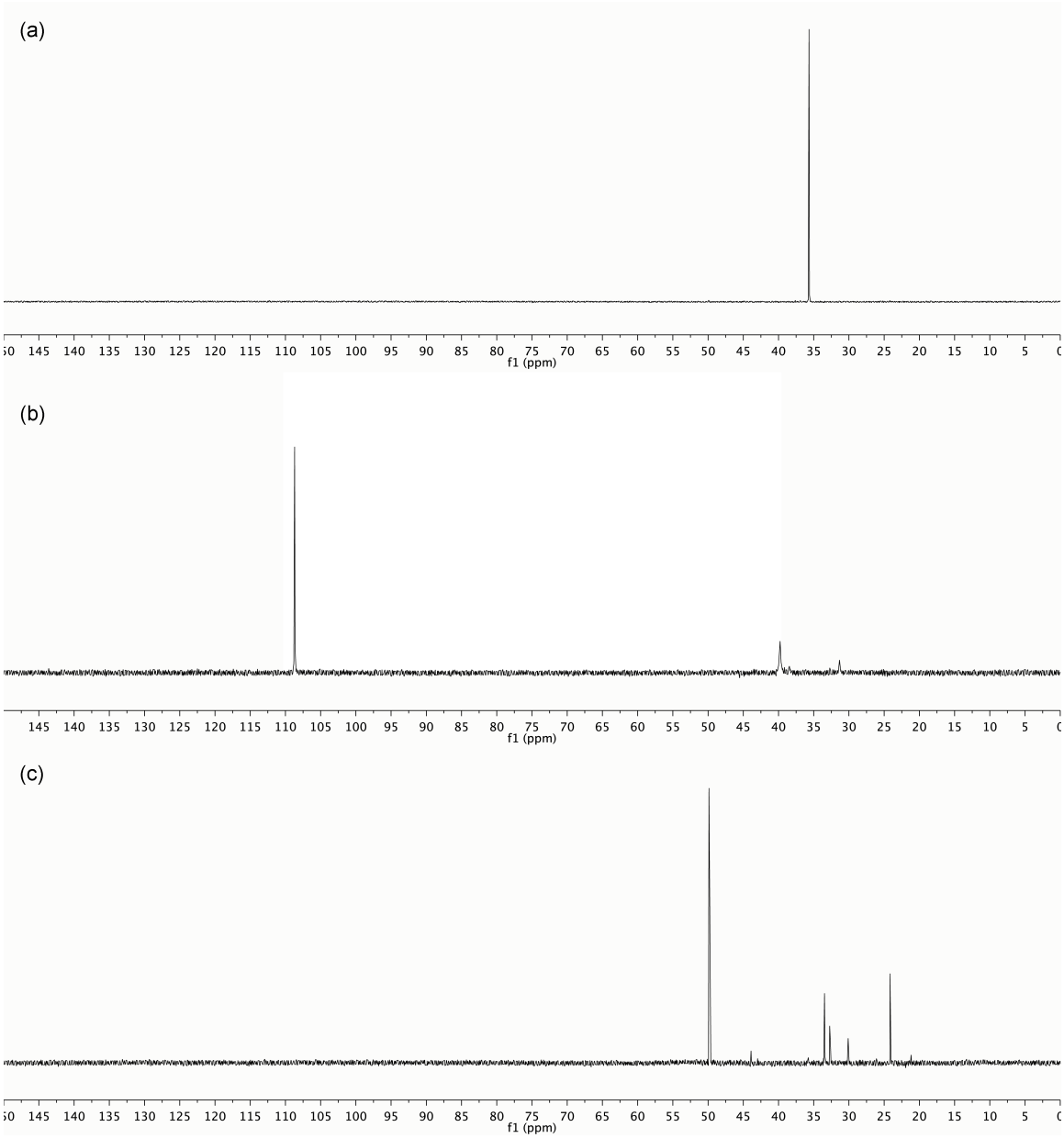


Figure S4. ^{31}P NMR spectra of **1** at (a) 0 min, (b) 200 min after activation in $CDCl_3$ at 65 °C, and (c) bipy added after the activation.

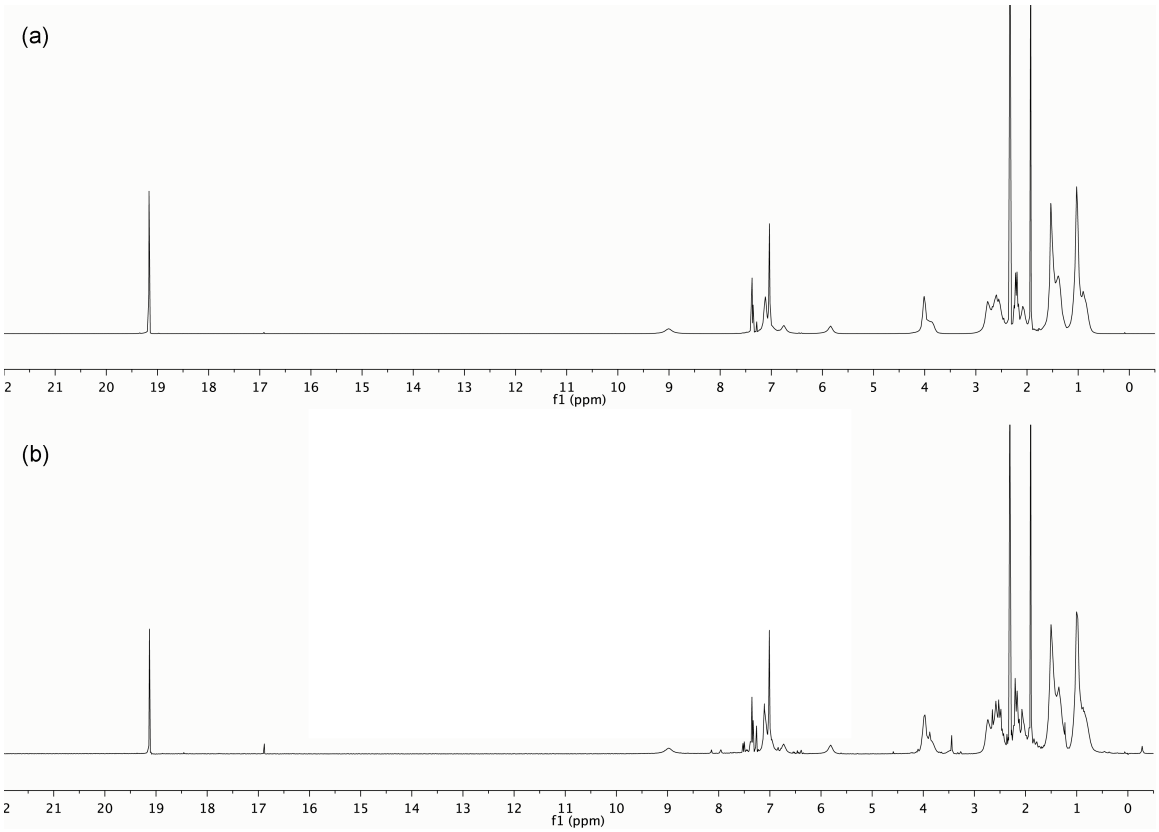


Figure S5. ^{1}H NMR spectra of **2** at (a) 0 min and (b) 270 min after activation in $CDCl_3$ at 65 °C.

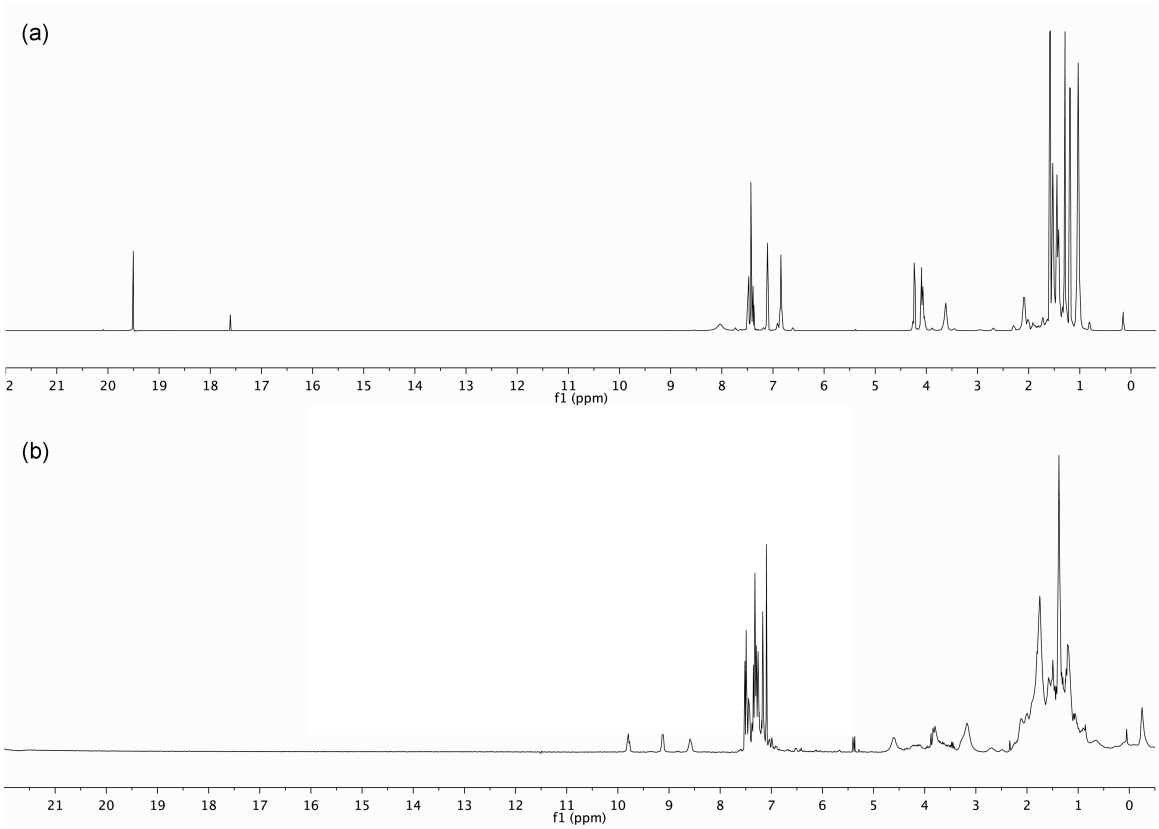


Figure S6. ^{1}H NMR spectra of **3** at (a) 0 min and (b) 60 min after activation in $CDCl_3$ at 65 °C.

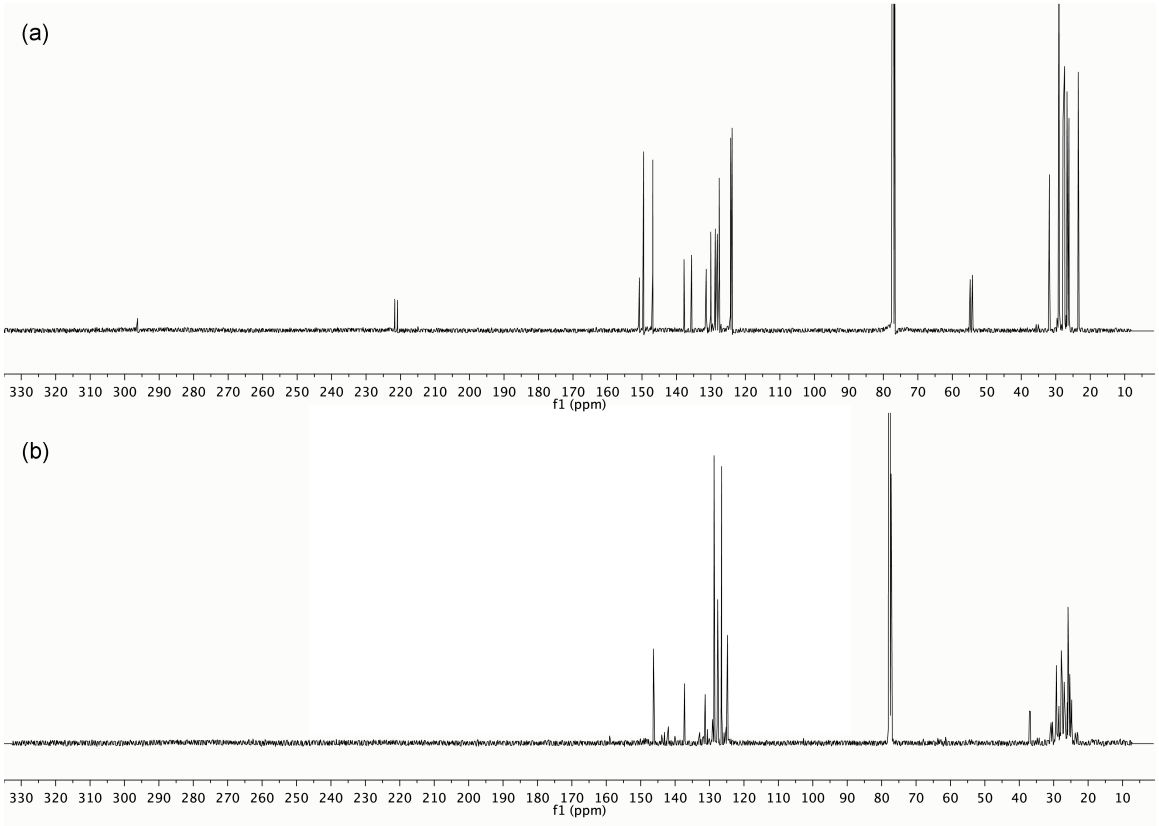


Figure S7. ^{13}C NMR spectra of **3** at (a) 0 min and (b) 60 min after activation in $CDCl_3$ at 65 °C.

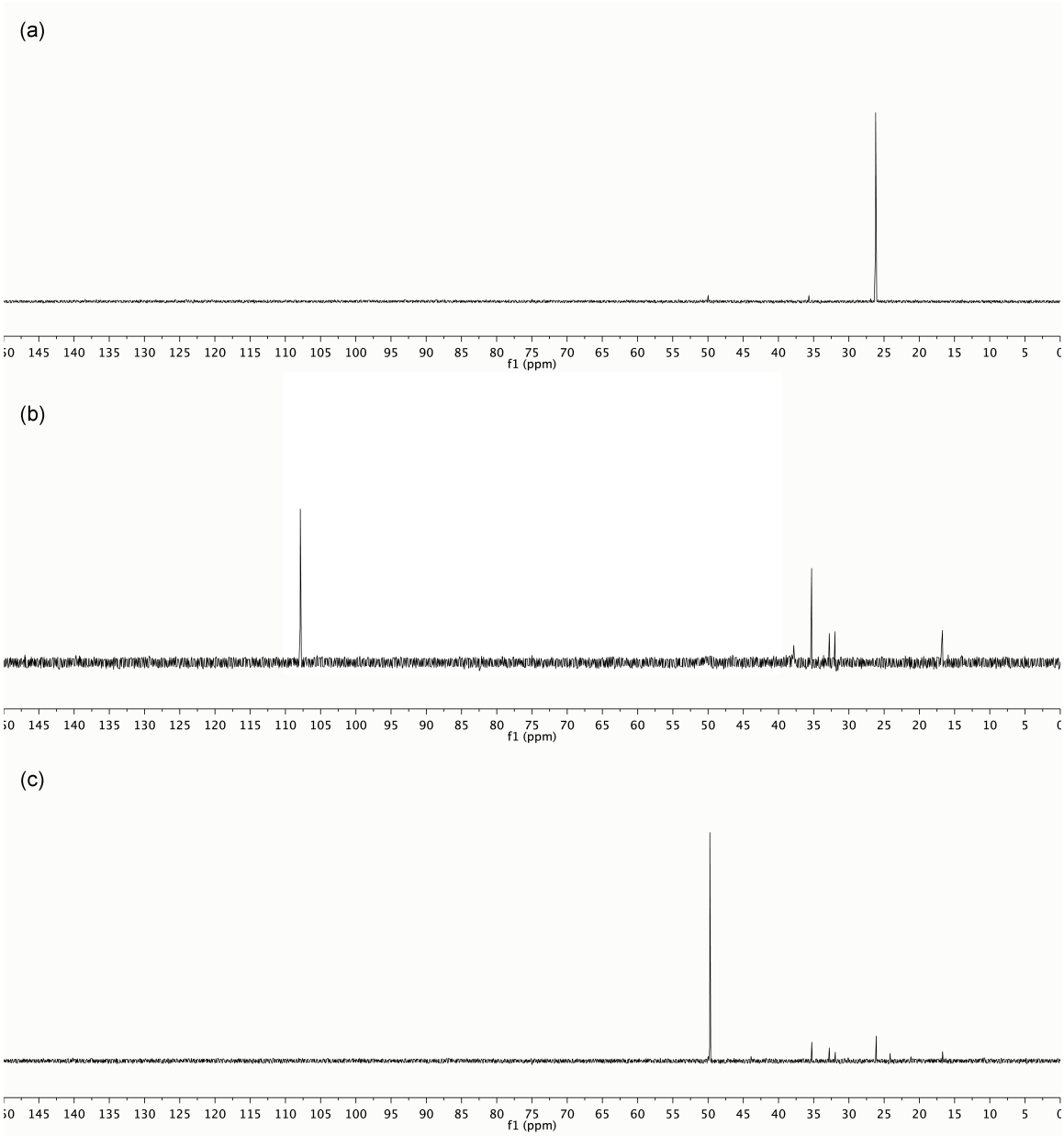


Figure S8. ^{31}P NMR spectra of **3** at (a) 0 min and (b) 60 min after activation in $CDCl_3$ at 65 °C, and (c) bipy added after the activation.

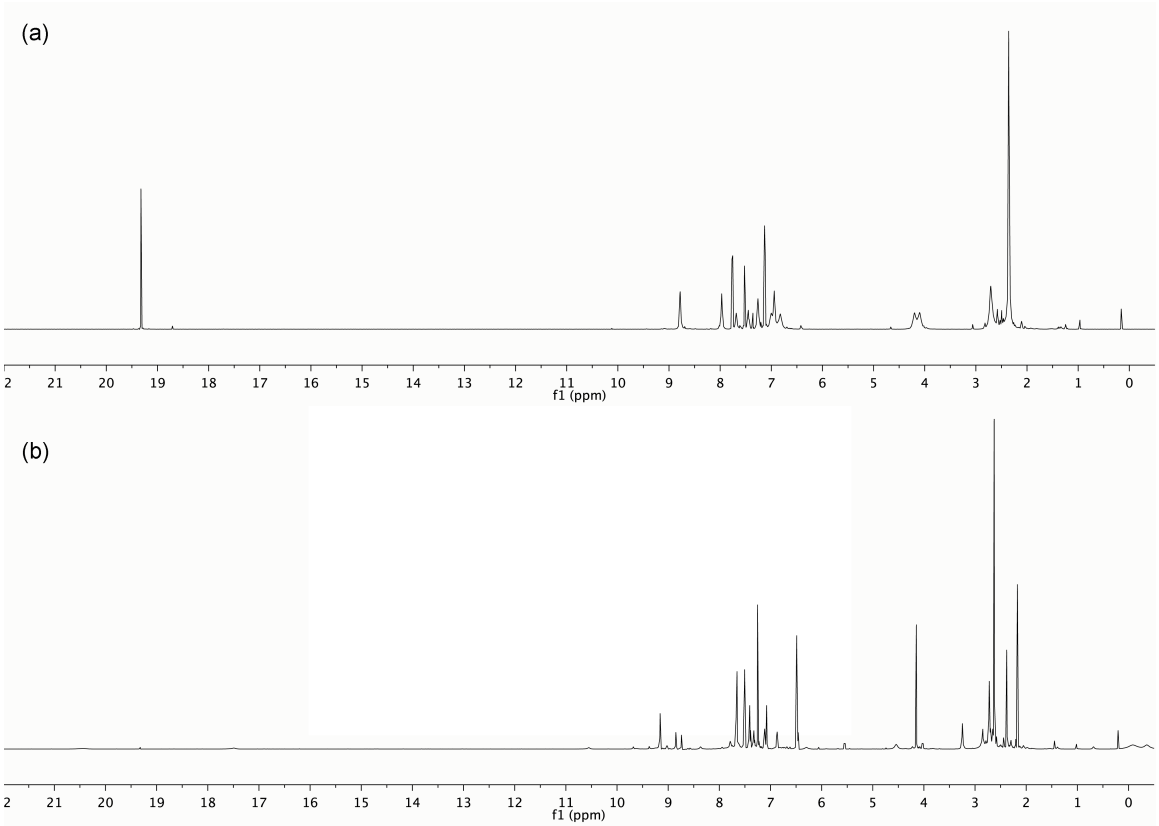


Figure S9. ^{1}H NMR spectra of **4** at (a) 0 min and (b) 270 min after activation in $CDCl_3$ at 65 °C.

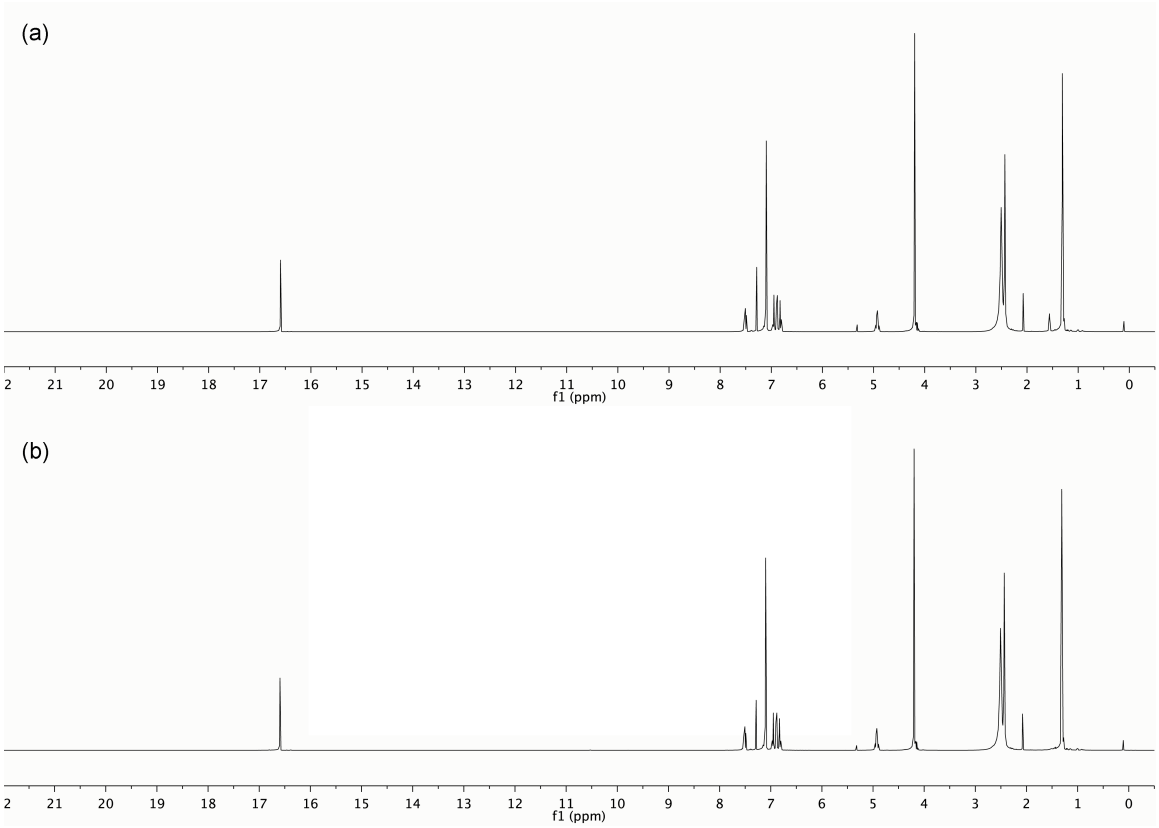


Figure S10. ^{1}H NMR spectra of **5** at (a) 0 min and (b) 270 min after activation in $CDCl_3$ at 65 °C.

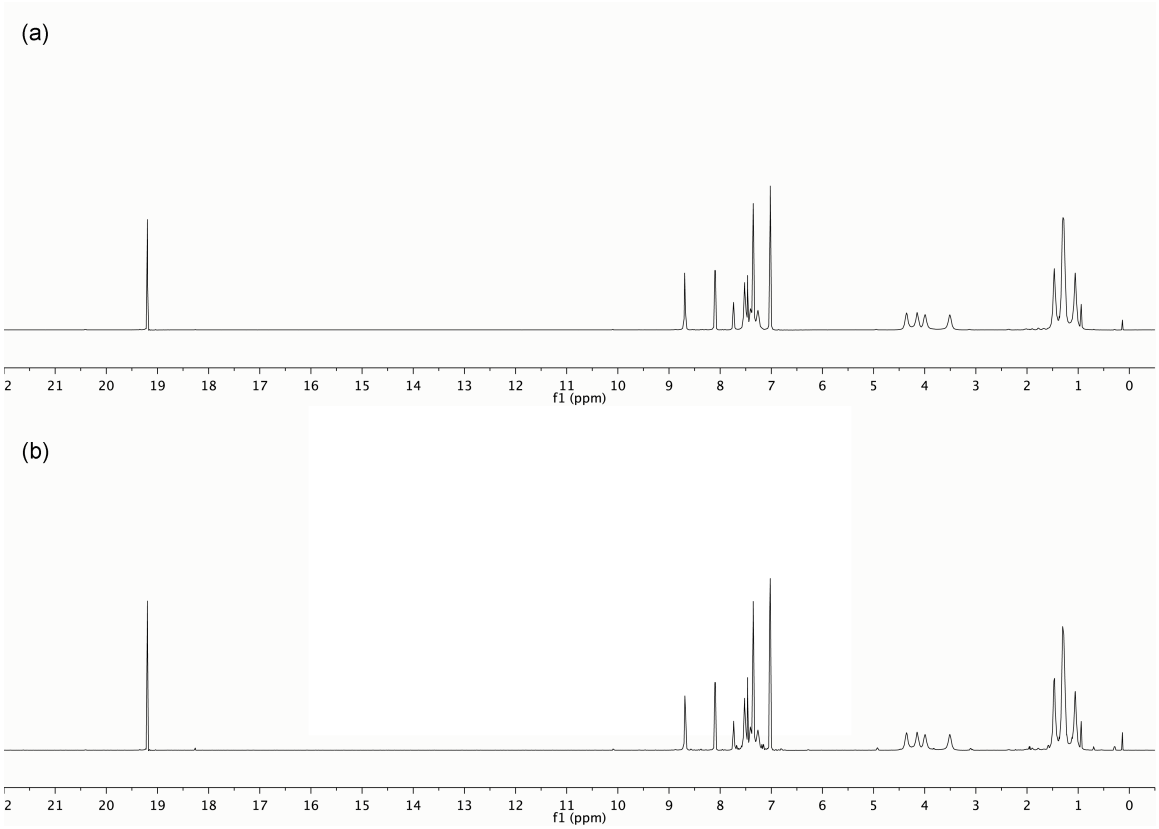


Figure S11. ^{1}H NMR spectra of **6** at (a) 0 min and (b) 270 min after activation in $CDCl_3$ at 65 °C.

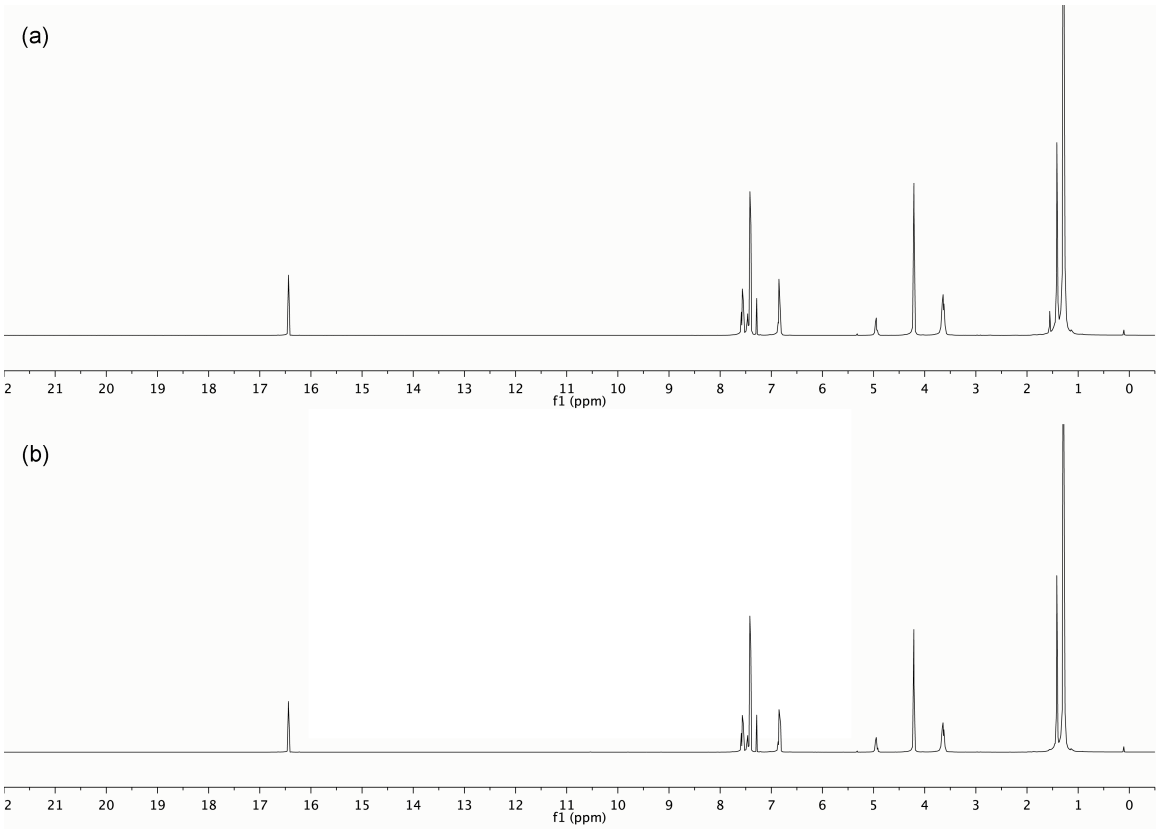


Figure S12. ^{1}H NMR spectra of **7** at (a) 0 min and (b) 270 min after activation in $CDCl_3$ at 65 °C.

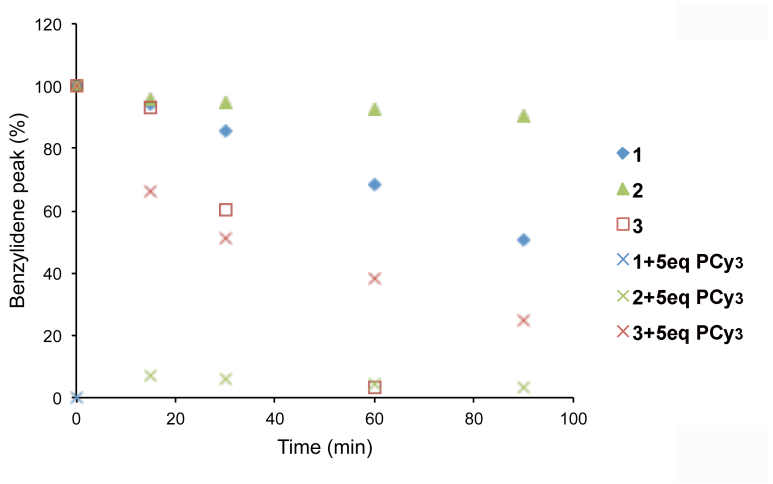


Figure S13. Rate profile of benzylidene ^{1}H NMR resonance decay in $CDCl_3$ with 5 equivalent PCy_3 relative to the catalysts.

X-Ray structure determination.

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON 100 CMOS detector with Mo K_α radiation (λ = 0.71073 Å) from an IμS micro-source for the structure of compound ATRA-activated **1** with bip***y***. The structure was solved by direct methods using SHELXS[8] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[9] using established refinement techniques.[10] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as enhanced rigid bond restraints for anisotropic displacement parameters. The compound crystallizes in the triclinic space group P-1 with one molecule in the asymmetric unit along with 3.3 molecules of dichloromethane. Two of the cyclohexane moieties on the phosphine were disordered over two positions with appropriate restraints. The dichloromethane solvent is located in two cavities. One was modeled as a mixture of three solvent positions and the other over four positions.

Table S1. Crystal data and structure analysis details for ***of*** ATRA-activated 3 with bipy (CCDC 1473173).

Identification code	P15507	
Empirical formula	C41.26 H55.51 Cl8.51 N4 P Ru	
Formula weight	1041.00	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1461(8) Å	a= 95.620(3)°.
	b = 13.3816(11) Å	b= 94.475(3)°.
	c = 18.3452(14) Å	g = 104.537(3)°.
Volume	2385.8(3) $Å^3$	
Z	2	
Density (calculated)	1.449 Mg/m^3	
Absorption coefficient	0.872 mm^{-1}	
F(000)	1069	
Crystal size	0.100 x 0.100 x 0.100 mm^3	
Theta range for data collection	2.244 to 30.603°.	
Index ranges	-14<=h<=11, -19<=k<=18, -26<=l<=26	
Reflections collected	54887	
Independent reflections	14596 [R(int) = 0.0377]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6938	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14596 / 1155 / 719	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.1609	
R indices (all data)	R1 = 0.0807, wR2 = 0.1749	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.869 and -0.896 $e.Å^{-3}$	

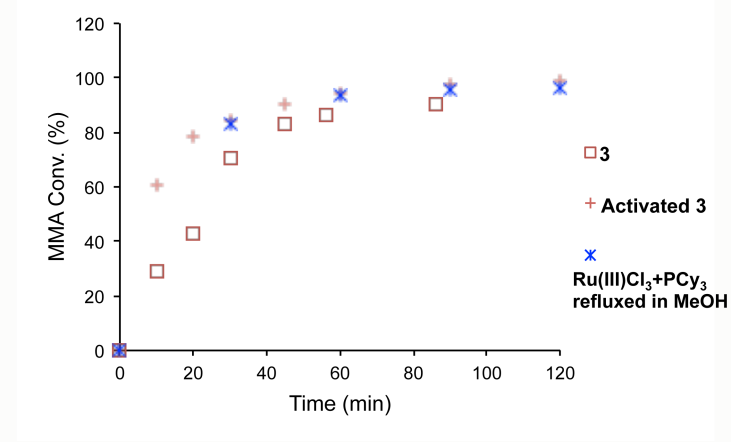


Figure S14. Kinetic study of ATRA of MMA catalyzed by **3**, **activated 3**, and Ru(III)Cl_3 refluxed with PCy_3 (2 equiv).

Coordinates, energies, and thermal corrections of referenced structures in the Figure S1.

1

Ru	0.02417	-0.01668	0.08717
Cl	0.01482	0.85155	2.41646
Cl	0.06511	-0.29116	-2.37566
C	0.00834	-1.73962	0.78195
H	0.16701	-1.74745	1.86951
P	-2.41433	0.44684	0.03002
C	-3.33713	0.14054	1.64609
C	-2.68448	2.29595	-0.26298
C	-3.32512	-0.36352	-1.41825
C	-3.13095	-1.26125	2.25578
C	-4.83674	0.51061	1.63272
H	-2.81494	0.83220	2.31911
C	-2.40185	3.19808	0.95809
C	-1.88012	2.78818	-1.48645
H	-3.75175	2.40067	-0.50090
C	-3.65945	-1.84614	-1.14370
C	-4.56774	0.35750	-1.98845
H	-2.54834	-0.34851	-2.19429
C	-3.72899	-1.33188	3.67184
H	-3.60119	-2.02867	1.62946
H	-2.06279	-1.48522	2.29985
C	-5.43404	0.43265	3.05026
H	-4.99275	1.51654	1.22619
H	-5.38363	-0.18155	0.97850
C	-2.71853	4.66965	0.63433
H	-3.00315	2.88800	1.81915
H	-1.35540	3.09420	1.26742
C	-2.19774	4.25753	-1.80994
H	-0.80689	2.68959	-1.27335
H	-2.06423	2.15894	-2.36362
C	-4.14848	-2.54958	-2.42120
H	-2.78753	-2.37068	-0.74271
H	-4.45000	-1.91091	-0.38414
C	-5.07194	-0.34976	-3.26146
H	-5.37419	0.37665	-1.24346
H	-4.34069	1.39904	-2.23691
C	-5.21569	-0.94851	3.68289
H	-3.17029	-0.64998	4.32855
H	-3.59300	-2.34214	4.07922
H	-4.96162	1.19972	3.68115
H	-6.50462	0.67319	3.01328
C	-1.95387	5.16900	-0.59912
H	-2.48467	5.29359	1.50641
H	-3.79943	4.77631	0.45604
H	-1.59393	4.58573	-2.66581
H	-3.25000	4.33983	-2.12161
C	-5.36812	-1.83595	-3.01956
H	-4.38877	-3.59699	-2.19722
H	-3.33300	-2.56314	-3.15826
H	-5.96756	0.16341	-3.63536
H	-4.30669	-0.25685	-4.04556
H	-5.60731	-0.96211	4.70811
H	-5.78905	-1.69934	3.11850
H	-0.87791	5.18829	-0.37229
H	-2.24137	6.20186	-0.83443
H	-6.21811	-1.92958	-2.32685
H	-5.67428	-2.31919	-3.95627
P	2.48522	0.30175	-0.00409
C	3.39745	-0.66553	-1.34060
C	2.88598	2.09420	-0.45494
C	3.31427	0.07340	1.67935
C	3.13361	-2.18516	-1.31949
C	4.91120	-0.38644	-1.46167
H	2.90119	-0.29249	-2.24579
C	2.55648	2.46100	-1.91873

C	2.22562	3.10112	0.51247
H	3.97458	2.18343	-0.33553
C	3.42274	-1.40707	2.10333
C	4.66331	0.78640	1.92539
H	2.56600	0.53513	2.33700
C	3.71656	-2.85585	-2.57567
H	3.58626	-2.64118	-0.43028
H	2.06036	-2.37260	-1.26857
C	5.49608	-1.06021	-2.71680
H	5.11860	0.68930	-1.49647
H	5.42823	-0.77845	-0.57567
C	2.98236	3.90634	-2.23390
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H	2.45975	2.86023	1.55456
C	3.81796	-1.52249	3.58550
H	2.47662	-1.92894	1.92768
H	4.18435	-1.91365	1.49533
C	5.07656	0.66722	3.40513
H	5.44862	0.34725	1.29644
H	4.60390	1.84705	1.66174
C	5.21682	-2.56959	-2.73258
H	3.17867	-2.48399	-3.45950
H	3.53698	-3.93779	-2.53139
H	5.05276	-0.59843	-3.61119
H	6.57605	-0.86937	-2.76884
C	2.35733	4.91696	-1.26316
H	2.70969	4.15014	-3.26869
H	4.07885	3.98016	-2.17510
H	2.15538	5.23698	0.88026
H	3.73769	4.64821	0.38114
C	5.13932	-0.79463	3.86910
H	3.89858	-2.58079	3.86646
H	3.01864	-1.09010	4.20359
H	6.04670	1.15852	3.55633
H	4.34842	1.21237	4.02280
H	5.59813	-3.01640	-3.65982
H	5.76591	-3.04643	-1.90655
H	1.26807	4.93577	-1.41372
H	2.71985	5.92985	-1.48088
H	5.95573	-1.30825	3.33918
H	5.38173	-0.84348	4.93842
C	-0.17196	-3.09609	0.26306
C	-0.13343	-4.15266	1.20398
C	-0.37850	-3.42540	-1.09548
C	-0.29336	-5.47844	0.80966
H	0.02407	-3.91782	2.25393
C	-0.53459	-4.75203	-1.48601
H	-0.40089	-2.62574	-1.82768
C	-0.49437	-5.78172	-0.53917
H	-0.26066	-6.27272	1.55052
H	-0.68867	-4.98669	-2.53577
H	-0.61856	-6.81514	-0.85226

SCF energy: -3380.488302 hartree
zero-point correction: +1.087415 hartree
enthalpy correction: +1.140713 hartree
free energy correction: +1.000542 hartree
quasiharmonic free energy correction: +1.012707 hartree

1'

Ru	0.06974	-0.14196	0.11899
C	-0.30679	1.67887	0.69224
H	-0.35963	1.66459	1.78286
Cl	0.22302	-2.60519	-0.22972
Cl	0.40898	-0.57998	2.52553
P	2.63619	-0.09692	-0.02800
C	3.30088	-0.43793	-1.76528
C	3.35983	1.61206	0.34562
C	3.52052	-1.21453	1.23446
C	2.81515	-1.74730	-2.42615
C	4.83672	-0.31505	-1.90668
H	2.84087	0.37612	-2.33948
C	3.09318	2.67215	-0.74411
C	2.93782	2.15001	1.72928
H	4.44502	1.44973	0.37496
C	3.57826	-2.70233	0.81771
C	4.92614	-0.75880	1.69876
H	2.84501	-1.14815	2.09540
C	3.22678	-1.78328	-3.90755
H	3.24824	-2.61300	-1.91352
H	1.73285	-1.83830	-2.33523
C	5.25662	-0.36465	-3.38809
H	5.21198	0.61205	-1.45916
H	5.32004	-1.14189	-1.36997
C	3.79836	4.00011	-0.41029
H	3.43992	2.32226	-1.72178
H	2.01598	2.84367	-0.83792
C	3.65674	3.46955	2.05914
H	1.85610	2.32376	1.73278
H	3.12372	1.41237	2.51653
C	4.06808	-3.57908	1.98276
H	2.59696	-3.04315	0.48406
H	4.27384	-2.82053	-0.02449
C	5.42807	-1.64088	2.85893
H	5.64045	-0.82040	0.86661
H	4.92459	0.28101	2.03687
C	4.74387	-1.63176	-4.08603
H	2.71139	-0.97326	-4.44428
H	2.88298	-2.72327	-4.35780
H	4.85588	0.52144	-3.90262
H	6.35032	-0.30006	-3.46161
C	3.41032	4.52999	0.97713
H	3.56272	4.74304	-1.18320
H	4.88761	3.84822	-0.44673
H	3.32200	3.83586	3.03819
H	4.73771	3.28442	2.14905

C	5.44341	-3.12976	2.49134
H	4.10356	-4.62733	1.65925
H	3.33643	-3.52890	2.80161
H	6.43021	-1.30805	3.16046
H	4.77260	-1.48904	3.72881
H	5.00799	-1.61014	-5.15138
H	5.24914	-2.50964	-3.65623
H	2.34565	4.80563	0.97609
H	3.97101	5.44595	1.20434
H	6.19469	-3.30122	1.70558
H	5.75273	-3.73088	3.35629
P	-2.50025	-0.58198	0.11998
C	-2.97689	-2.09095	-0.92101
C	-3.20449	-1.02644	1.81559
C	-3.56908	0.90833	-0.39696
C	-2.47060	-2.10277	-2.38051
C	-4.47179	-2.48625	-0.88209
H	-2.40729	-2.87188	-0.40399
C	-2.68564	-2.37332	2.36841
C	-3.02683	0.10152	2.85747
H	-4.28293	-1.14328	1.64013
C	-3.52335	1.19590	-1.91509
C	-5.04336	0.90498	0.07670
H	-3.07062	1.74704	0.10784
C	-2.67249	-3.49585	-3.00154
H	-3.01463	-1.36285	-2.97991
H	-1.41533	-1.83358	-2.41815
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H	-4.86451	-2.49045	0.14004
H	-5.06534	-1.75600	-1.44835
C	-3.36523	-2.71491	3.70701
H	-2.87923	-3.18271	1.65635
H	-1.60130	-2.32088	2.50178
C	-3.71897	-0.25820	4.18442
H	-1.95917	0.24875	3.04187
H	-3.42797	1.05069	2.48051
C	-4.21175	2.52902	-2.25693
H	-2.49323	1.19397	-2.27895
H	-4.04575	0.39027	-2.44605
C	-5.73412	2.23932	-0.26324
H	-5.58788	0.08582	-0.40827
H	-5.12062	0.73999	1.15439
C	-4.13861	-3.94568	-2.94181
H	-2.04255	-4.21832	-2.46385
H	-2.31984	-3.48562	-4.04090
H	-4.15886	-4.62727	-0.88781
H	-5.74379	-4.13829	-1.48245
C	-3.20097	-1.59186	4.73982
H	-2.94932	-3.65352	4.09473
H	-4.43844	-2.89540	3.53800
H	-3.55759	0.54843	4.91155
H	-4.80686	-0.32518	4.02788
C	-5.66341	2.56090	-1.76084
H	-4.17486	2.68982	-3.34221
H	-3.65048	3.35587	-1.79900
H	-6.77843	2.20387	0.07337
H	-5.25063	3.04753	0.30573
H	-4.24738	-4.96248	-3.34090
H	-4.74623	-3.29030	-3.58413
H	-2.13740	-1.48698	4.99474
H	-3.72785	-1.84761	5.66845
H	-6.25414	1.81885	-2.31839
H	-6.11887	3.53892	-1.96316
Cl	0.02997	0.39138	-2.23108
C	-0.62088	3.01469	0.21542
C	-0.94814	3.98306	1.20285
C	-0.59936	3.43538	-1.13620
C	-1.23925	5.29868	0.86086
H	-0.96696	3.68140	2.24690
C	-0.88536	4.75376	-1.47388
H	-0.35218	2.71234	-1.90225
C	-1.20637	5.68757	-0.48191
H	-1.48722	6.01994	1.63422
H	-0.85833	5.05818	-2.51631
H	-1.42904	6.71565	-0.75504

SCF energy: -3840.703933 hartree
zero-point correction: +1.089891 hartree
enthalpy correction: +1.144698 hartree
free energy correction: +1.001421 hartree
quasiharmonic free energy correction: +1.013029 hartree

2

Ru	-0.08439	-0.35502	0.08573
Cl	0.15607	-0.44132	2.56109
Cl	0.15328	-0.38258	-2.37960
C	-1.78095	0.36466	0.32414
H	-2.09267	0.32429	1.37541
P	1.16771	1.83880	0.14536
C	0.91674	2.87300	1.70410
C	3.02803	1.51144	0.18004
C	0.95544	2.92208	-1.39704
C	-0.55614	3.16315	2.06246
C	1.75776	4.16595	1.79438
H	1.27139	2.17713	2.47508
C	3.57147	0.95855	1.51473
C	3.47746	0.59743	-0.98133
H	3.49454	2.49437	0.02997
C	-0.34045	3.76203	-1.35799
C	2.14203	3.82052	-1.81588
H	0.82324	2.15816	-2.17501
C	-0.66296	3.79903	3.45975
H	-1.00675	3.83877	1.32583
H	-1.12543	2.23111	2.04539
C	1.64524	4.80153	3.19258
H	2.81268	3.97152	1.56881
H	1.40522	4.88958	1.04732
C	5.10866	0.87571	1.46998
H	3.27536	1.59189	2.35688

H	3.14260	-0.03200	1.70871
C	5.01227	0.51534	-1.04293
H	3.06313	-0.40863	-0.83493
H	3.08029	0.94462	-1.94079
C	-0.61876	4.42051	-2.71977
H	-1.19408	3.14461	-1.06817
H	-0.24440	4.55255	-0.60159
C	1.86682	4.49485	-3.17399
H	2.31839	4.59498	-1.05697
H	3.06732	3.24268	-1.89836
C	0.18416	5.07415	3.57556
H	-0.32897	3.06775	4.20943
H	-1.71481	4.01975	3.68437
H	2.09436	4.12286	3.93251
H	2.22999	5.73039	3.22419
C	5.60889	0.03362	0.28783
H	5.48329	0.46284	2.41573
H	5.51863	1.89429	1.39131
H	5.31287	-0.15423	-1.85927
H	5.41885	1.50837	-1.28869
C	0.55844	5.29641	-3.16831
H	-1.53902	5.01599	-2.65985
H	-0.80016	3.63625	-3.46827
H	2.71217	5.14367	-3.43876
H	1.81236	3.71881	-3.95117
H	0.12772	5.48137	4.59339
H	-0.22616	5.84565	2.90640
H	5.31614	-1.01197	0.44849
H	6.70611	0.05477	0.24456
H	0.65839	6.14826	-2.47882
H	0.36708	5.71965	-4.16295
N	-1.77380	-2.97533	0.41402
C	-1.72240	-4.45007	0.50782
H	-2.22005	-4.79214	1.41941
C	-0.22036	-4.73035	0.50525
N	0.35156	-3.41165	0.15962
H	0.07808	-5.47897	-0.23452
C	-3.08298	-2.38714	0.38834
C	1.75978	-3.37473	-0.13971
C	4.49769	-3.61288	-0.73576
C	2.16625	-3.57314	-1.47724
C	2.70026	-3.36428	0.91135
C	4.05744	-3.47236	0.58352
C	3.53517	-3.66778	-1.74775
C	1.16928	-3.73673	-2.59792
C	2.28973	-3.31885	2.36407
H	4.78708	-3.46897	1.39081
H	3.85302	-3.81563	-2.77753
C	5.97072	-3.70829	-1.05781
C	-5.73961	-1.48880	0.34345
C	-3.74037	-2.12432	1.60481
C	-3.74130	-2.23728	-0.84954
C	-5.06286	-1.78581	-0.84454
C	-5.06288	-1.66729	1.55282
C	-3.05846	-2.33034	2.93655
C	-3.04411	-2.54373	-2.15294
H	-5.57454	-1.65749	-1.79595
H	-5.57760	-1.45353	2.48741
C	-7.15716	-0.96807	0.31090
H	0.41729	-4.50018	-2.36236
H	0.63942	-2.79925	-2.79308
H	1.94518	-4.30566	2.70451
H	1.48927	-2.59823	2.54923
H	6.52690	-4.19713	-0.25049
H	6.41024	-2.71159	-1.19648
H	6.14314	-4.27205	-1.98076
H	-2.70251	-3.58584	-2.19940
H	-2.16133	-1.91056	-2.29615
H	-3.68690	-1.95411	3.74993
H	-2.09044	-1.81968	2.98115
H	-7.62840	-1.02157	1.29773
H	-7.77783	-1.53486	-0.39282
H	-7.17831	0.08097	-0.01206
C	-0.56440	-2.40793	0.17295
H	-3.72138	-2.38196	-2.99692
H	-2.87410	-3.39480	3.13642
H	3.14312	-3.04674	2.99327
H	1.67765	-4.04320	-3.51733
H	0.14757	-5.05203	1.48594
H	-2.24031	-4.89681	-0.34971
C	-2.79814	1.04042	-0.48720
C	-3.87239	1.63430	0.21695
C	-2.79077	1.15271	-1.89492
C	-4.88419	2.32278	-0.44801
H	-3.90181	1.55050	1.29995
C	-3.81309	1.82584	-2.55794
H	-1.97165	0.71056	-2.44918
C	-4.85943	2.41687	-1.84148
H	-5.68997	2.78267	0.11829
H	-3.79103	1.89710	-3.64229
H	-5.64854	2.94901	-2.36682

SCF energy: -3258.735255 hartree
zero-point correction: +1.024009 hartree
enthalpy correction: +1.081328 hartree
free energy correction: +0.932045 hartree
quasiharmonic free energy correction: +0.945234 hartree

2'

Ru	-0.38550	0.87045	-0.56329
Cl	-0.36005	-0.11178	-2.75908
Cl	-0.56247	1.55157	1.71604
C	1.48206	0.98032	-0.68315
H	1.94027	0.21582	-1.31503
N	0.33671	-2.10810	0.38688
C	-0.27432	-3.37420	0.85810
H	-0.02214	-4.19030	0.17483
C	-1.77513	-3.04723	0.86908
N	-1.80314	-1.63873	0.42131

H	-2.22316	-3.13158	1.86387
C	1.77151	-2.04479	0.29660
C	-3.05863	-0.92651	0.38475
C	-5.50672	0.44266	0.32825
C	-3.55548	-0.35107	1.57159
C	-3.82443	-0.93053	-0.80127
C	-5.03045	-0.22380	-0.80502
C	-4.76878	0.34156	1.50958
C	-2.88036	-0.52480	2.91220
C	-3.41712	-1.72104	-2.02130
H	-5.61750	-0.20471	-1.72026
H	-5.14495	0.81151	2.41574
C	-6.78448	1.24570	0.27616
C	4.57560	-2.06773	0.18767
C	2.41150	-2.54882	-0.85271
C	2.50870	-1.58978	1.40827
C	3.90457	-1.60270	1.32327
C	3.81110	-2.53524	-0.88570
C	1.63537	-3.09746	-2.02634
C	1.83341	-1.10233	2.66732
H	4.48081	-1.24255	2.17267
H	4.31379	-2.90946	-1.77476
C	6.08592	-2.09820	0.13972
H	-3.31914	-1.37829	3.44956
H	-1.80565	-0.68461	2.82519
H	-3.31979	-2.78972	-1.78729
H	-2.46316	-1.38380	-2.43389
H	-7.48953	0.83285	-0.45332
H	-6.57975	2.28296	-0.01940
H	-7.28012	1.27647	1.25227
H	1.13825	-1.84927	3.07127
H	1.25549	-0.18873	2.49213
H	2.31143	-3.33645	-2.85251
H	0.89306	-2.38045	-2.38994
H	6.45423	-2.12669	-0.89082
H	6.47962	-2.98573	0.65265
H	6.52028	-1.22199	0.63343
C	-0.57739	-1.14435	0.15972
H	2.57682	-0.89188	3.44186
H	1.10519	-4.02275	-1.76413
H	-4.17654	-1.62641	-2.80301
H	-3.02552	0.36229	3.53481
H	-2.35218	-3.67034	0.17864
H	0.11661	-3.62657	1.84915
C	2.41756	1.95716	-0.19205
C	3.79403	1.70720	-0.43575
C	2.05474	3.15599	0.47018
C	4.76730	2.60252	-0.01418
H	4.07865	0.79561	-0.95307
C	3.03628	4.05292	0.87728
H	1.00875	3.37249	0.63594
C	4.38743	3.77824	0.64405
H	5.81701	2.39702	-0.20386
H	2.74776	4.97366	1.37571
H	5.14672	4.48588	0.96710
Cl	-0.87050	3.02854	-1.39789

SCF energy: -2671.640816 hartree
zero-point correction: +0.536635 hartree
enthalpy correction: +0.575207 hartree
free energy correction: +0.462567 hartree
quasiharmonic free energy correction: +0.472883 hartree

3

Ru	0.01785	-0.03515	0.04172
Cl	0.00272	0.41866	2.48191
Cl	0.01347	-0.06268	-2.42405
C	0.15414	-1.84509	0.43615
H	0.39347	-2.00604	1.49332
P	-2.51013	0.07658	0.08914
C	-3.29599	-0.44189	1.72551
C	-3.07224	1.87463	-0.06960
C	-3.40458	-0.76888	-1.35920
C	-2.89527	-1.84841	2.21924
C	-4.82478	-0.24512	1.82939
H	-2.80983	0.25678	2.41876
C	-2.80376	2.75812	1.16665
C	-2.49460	2.56379	-1.32499
H	-4.16245	1.82069	-0.19268
C	-3.64072	-2.27731	-1.12110
C	-4.71796	-0.12509	-1.86250
H	-2.65637	-0.67309	-2.15831
C	-3.38919	-2.08144	3.65792
H	-3.31640	-2.62305	1.56769
H	-1.80800	-1.94956	2.18835
C	-5.31918	-0.49163	3.26735
H	-5.11523	0.76352	1.51364
H	-5.33543	-0.94398	1.15335
C	-3.45732	4.14032	0.98407
H	-3.19369	2.29716	2.07940
H	-1.72273	2.86984	1.31294
C	-3.14690	3.94169	-1.53187
H	-1.41098	2.68648	-1.20379
H	-2.62670	1.94517	-2.21870
C	-4.12344	-2.97635	-2.40359
H	-2.73208	-2.76169	-0.75763
H	-4.40586	-2.40987	-0.34463
C	-5.21989	-0.82285	-3.14125
H	-5.49200	-0.19498	-1.08610
H	-4.58383	0.93796	-2.07973
C	-4.90571	-1.87776	3.78049
H	-2.86915	-1.38420	4.33018
H	-3.11418	-3.09369	3.98239
H	-4.89831	0.28021	3.92836
H	-6.41048	-0.37684	3.30757
C	-2.98216	4.84037	-0.29727
H	-3.24328	4.76726	1.85944
H	-4.55056	4.01631	0.95031
H	-2.71131	4.42779	-2.41432

H	-4.21772	3.80509	-1.74765
C	-5.40708	-2.33227	-2.94239
H	-4.28419	-4.04351	-2.20270
H	-3.33368	-2.91595	-3.16586
H	-6.16104	-0.35945	-3.46536
H	-4.49239	-0.65094	-3.94790
H	-5.22781	-2.00861	4.82174
H	-5.42444	-2.65033	3.19280
H	-1.92159	5.09981	-0.18779
H	-3.52627	5.78379	-0.43836
H	-6.22625	-2.50583	-2.22831
H	-5.70924	-2.80613	-3.88532
N	3.14325	-0.27602	0.21595
C	4.38087	0.51603	0.39606
H	4.61861	0.59594	1.46365
C	3.97847	1.84950	-0.20346
N	2.50161	1.79221	-0.10415
H	4.27620	1.93347	-1.25498
C	3.26203	-1.70984	0.28955
C	1.79282	3.04691	-0.23407
C	0.73163	5.62307	-0.47480
C	1.55760	3.58667	-1.52527
C	1.55021	3.81404	0.93697
C	1.00417	5.09483	0.78265
C	1.01031	4.87431	-1.61190
C	1.96510	2.88730	-2.82070
C	1.95114	3.36169	2.34086
H	0.81085	5.69681	1.66475
H	0.82313	5.30375	-2.59109
C	3.73900	-4.45263	0.42103
C	3.33179	-2.33810	1.55634
C	3.47874	-2.43242	-0.91048
C	3.70051	-3.81124	-0.81323
C	3.56647	-3.71894	1.59003
C	3.23892	-1.56766	2.87295
C	3.56653	-1.75431	-2.27782
H	3.85534	-4.39005	-1.71832
H	3.62424	-4.22415	2.54974
H	2.15338	1.83462	-2.59526
H	2.09380	2.27948	2.32321
H	3.08614	-0.77553	-2.20254
H	2.86107	-0.56476	2.65543
C	2.04776	0.51169	0.03434
H	4.36972	2.70978	0.34032
H	5.22155	0.04425	-0.11405
C	3.27599	4.03246	2.76985
H	3.57762	3.67457	3.76158
H	4.09870	3.82742	2.07612
H	3.16273	5.12199	2.82692
C	0.87204	3.64721	3.40148
H	0.73330	4.72204	3.57091
H	-0.08460	3.20296	3.12027
H	1.17284	3.20246	4.35666
H	0.32009	6.62492	-0.56826
H	3.91654	-5.52384	0.47170
C	3.25506	3.52072	-3.39138
H	4.07711	3.53068	-2.66769
H	3.58872	2.96816	-4.27789
H	3.07622	4.55985	-3.69347
C	0.86554	2.92168	-3.89876
H	-0.07028	2.50441	-3.52282
H	0.68477	3.93964	-4.26523
H	1.17598	2.31563	-4.75730
C	2.83670	-2.51890	-3.39570
H	2.84819	-1.92206	-4.31464
H	3.31957	-3.47737	-3.62221
H	1.79512	-2.70824	-3.13223
C	5.04354	-1.54527	-2.68216
H	5.60470	-0.96447	-1.94197
H	5.55469	-2.50903	-2.79601
H	5.10517	-1.01691	-3.64117
C	4.63584	-1.44326	3.52261
H	5.01893	-2.42806	3.81689
H	5.37190	-0.99804	2.84420
H	4.58389	-0.82173	4.42453
C	2.25891	-2.19401	3.88243
H	2.57688	-3.19520	4.19740
H	2.20503	-1.56689	4.77930
H	1.24737	-2.25669	3.47385
C	-0.03844	-3.12680	-0.24798
C	0.05530	-4.29004	0.55283
C	-0.33125	-3.29459	-1.61928
C	-0.13573	-5.56003	0.01455
H	0.28396	-4.18456	1.60958
C	-0.51314	-4.56603	-2.15631
H	-0.40962	-2.41305	-2.24450
C	-0.41926	-5.70213	-1.34527
H	-0.06152	-6.43617	0.65332
H	-0.73383	-4.67316	-3.21515
H	-0.56809	-6.69092	-1.77175

SCF energy: -3494.626490 hartree
zero-point correction: +1.197933 hartree
enthalpy correction: +1.261943 hartree
free energy correction: +1.099527 hartree
quasiharmonic free energy correction: +1.114330 hartree

3’

Ru	0.05590	-1.01516	-0.94000
Cl	0.74643	0.51426	-2.62863
Cl	-0.43891	-2.30366	1.01718
C	-1.71453	-0.51283	-1.29035
H	-1.82873	0.50440	-1.67116
N	-0.16805	1.36752	1.17523
C	0.65081	2.18383	2.10369
H	0.75441	3.20007	1.70702
C	1.97492	1.42219	2.12474
N	1.86119	0.56277	0.92466
H	2.07784	0.79218	3.01533

C	-1.55396	1.73333	0.99471
C	3.04024	-0.08504	0.37881
C	5.33748	-1.27998	-0.65531
C	3.47696	-1.32122	0.91360
C	3.79994	0.60645	-0.60196
C	4.93774	-0.02805	-1.11177
C	4.62410	-1.90562	0.35859
C	2.83116	-1.98798	2.12470
C	3.49798	2.03704	-1.04736
H	5.52418	0.46918	-1.87719
H	4.96620	-2.86274	0.73844
C	-4.20479	2.56979	0.77571
C	-1.88396	2.74603	0.05919
C	-2.52767	1.17456	1.85667
C	-3.85293	1.60603	1.71439
C	-3.22627	3.13650	-0.03535
C	-0.84561	3.48072	-0.78841
C	-2.18769	0.18879	2.97177
H	-4.61858	1.18546	2.35869
H	-3.50432	3.90930	-0.74559
H	1.83396	-1.56317	2.25984
H	2.44369	2.24211	-0.84055
H	-1.17675	-0.18763	2.79698
H	0.09965	2.93391	-0.72721
C	0.58446	0.48313	0.48691
H	2.84804	2.07125	2.05506
H	0.17194	2.24074	3.08273
C	-2.21523	0.89644	4.34489
H	-1.91544	0.20001	5.13677
H	-1.54249	1.76142	4.38301
H	-3.22321	1.25819	4.58108
C	-3.12104	-1.03558	2.99349
H	-2.77154	-1.75085	3.74633
H	-4.15027	-0.76168	3.25472
H	-3.12746	-1.54540	2.02760
C	3.66311	-1.69517	3.39400
H	3.79846	-0.62055	3.56356
H	3.17166	-2.12005	4.27751
H	4.66209	-2.14112	3.31880
C	2.64903	-3.50778	1.95712
H	2.11206	-3.74602	1.03594
H	3.61017	-4.03561	1.95101
H	2.06506	-3.90247	2.79589
C	4.36025	3.04113	-0.24688
H	4.22730	2.94926	0.83652
H	5.42506	2.88430	-0.45577
H	4.11079	4.07059	-0.53124
C	3.72134	2.27826	-2.55217
H	4.78675	2.26951	-2.81140
H	3.20587	1.53025	-3.15704
H	3.33329	3.26614	-2.82652
C	-0.61699	4.90742	-0.23969
H	0.18303	5.40708	-0.79843
H	-1.52461	5.51432	-0.34012
H	-0.34231	4.90609	0.82119
C	-1.22117	3.55330	-2.28083
H	-2.13549	4.13592	-2.44319
H	-0.41644	4.04383	-2.83956
H	-1.35484	2.55842	-2.71285
H	6.21939	-1.75625	-1.07536
H	-5.23913	2.89188	0.68685
C	-2.94805	-1.25352	-1.25965
C	-4.13797	-0.53493	-1.54915
C	-3.04284	-2.64403	-1.00427
C	-5.37123	-1.17202	-1.56203
H	-4.07363	0.53043	-1.75059
C	-4.28148	-3.27557	-1.03122
H	-2.14140	-3.20763	-0.80887
C	-5.44310	-2.54569	-1.30326
H	-6.27396	-0.60856	-1.78008
H	-4.34304	-4.34355	-0.84388
H	-6.40628	-3.04921	-1.32149
Cl	0.14245	-2.91228	-2.35161

SCF energy: -2907.538298 hartree
zero-point correction: +0.710312 hartree
enthalpy correction: +0.755353 hartree
free energy correction: +0.631344 hartree
quasiharmonic free energy correction: +0.641692 hartree

4

Ru	-0.02145	0.45802	-0.11273
Cl	-0.37367	0.20904	-2.58869
Cl	0.07301	0.64496	2.37872
C	1.81323	0.46988	-0.53492
H	2.05369	-0.00515	-1.49118
N	0.90938	-2.48006	0.27998
C	0.50015	-3.87585	0.53112
H	0.75527	-4.50509	-0.33015
C	-1.00449	-3.74778	0.74426
N	-1.26871	-2.34715	0.35603
H	-1.29740	-3.90760	1.78830
C	2.31932	-2.29066	0.07466
C	-2.65875	-2.00181	0.21846
C	-5.42235	-1.56713	-0.03445
C	-3.41490	-1.67843	1.36076
C	-3.27816	-2.19076	-1.03341
C	-4.65309	-1.95472	-1.13512
C	-4.78679	-1.45313	1.20453
C	-2.79740	-1.60238	2.73655
C	-2.50459	-2.66389	-2.24014
H	-5.13490	-2.08783	-2.10169
H	-5.37316	-1.18479	2.08114
C	-6.89595	-1.26868	-0.18075
C	5.10251	-2.19515	-0.29158
C	2.85586	-2.49079	-1.21407
C	3.15876	-2.10225	1.19139
C	4.53931	-2.04803	0.97957
C	4.24469	-2.42732	-1.37077

C	1.97176	-2.75876	-2.40906
C	2.60023	-1.97685	2.58693
H	5.19156	-1.88632	1.83519
H	4.66462	-2.56906	-2.36459
C	6.59567	-2.08552	-0.49184
H	-2.62943	-2.60613	3.15193
H	-1.83713	-1.08001	2.73104
H	-2.00139	-3.62095	-2.04913
H	-1.73632	-1.94060	-2.53084
H	-7.33432	-1.80909	-1.02664
H	-7.06217	-0.19697	-0.35564
H	-7.45383	-1.53962	0.72247
H	2.13663	-2.91544	2.92067
H	1.83406	-1.19810	2.64547
H	2.57683	-2.87023	-3.31423
H	1.25296	-1.94844	-2.57668
H	6.91128	-2.55098	-1.43147
H	7.14776	-2.56174	0.32634
H	6.90727	-1.03296	-0.52266
C	-0.13731	-1.61205	0.15161
H	3.39679	-1.73668	3.29796
H	1.39165	-3.68265	-2.28838
H	-3.17771	-2.81140	-3.09066
H	-3.46705	-1.08111	3.42831
H	-1.58796	-4.43041	0.11943
H	1.02429	-4.27306	1.40517
N	0.04266	2.74233	-0.31646
C	-0.00536	3.55001	0.75835
C	0.14732	3.31228	-1.53183
C	0.04514	4.93892	0.66136
H	-0.08014	3.04737	1.71648
C	0.20407	4.69227	-1.71352
H	0.17269	2.62320	-2.36933
C	0.15208	5.52612	-0.59782
H	0.00270	5.53960	1.56470
H	0.28831	5.09499	-2.71810
H	0.19523	6.60650	-0.70703
N	-2.41694	1.17968	0.03524
C	-3.14991	1.33562	-1.07965
C	-2.89336	1.70998	1.17548
C	-4.36065	2.02905	-1.10197
H	-2.72842	0.89922	-1.97856
C	-4.09296	2.41619	1.24479
H	-2.27336	1.55907	2.05368
C	-4.84233	2.58598	0.08103
H	-4.90467	2.12824	-2.03651
H	-4.42296	2.82511	2.19522
H	-5.77829	3.13875	0.09647
C	2.97182	1.21670	-0.04549
C	3.04302	1.84690	1.21696
C	4.09341	1.32554	-0.90223
C	4.18297	2.55032	1.59639
H	2.20244	1.75220	1.89387
C	5.22579	2.04345	-0.52745
H	4.05983	0.83703	-1.87238
C	5.27376	2.65717	0.72743
H	4.22302	3.02079	2.57565
H	6.06935	2.12411	-1.20839
H	6.15742	3.21504	1.02767

SCF energy: -2708.098977 hartree
zero-point correction: +0.718332 hartree
enthalpy correction: +0.765626 hartree
free energy correction: +0.636907 hartree
quasiharmonic free energy correction: +0.647800 hartree

5

Ru	0.04428	0.77857	-0.15548
Cl	-0.08636	0.56014	-2.65072
Cl	-0.09219	0.92796	2.31101
C	1.90806	0.76386	-0.38648
H	2.25124	0.24830	-1.28664
N	0.85378	-2.22613	-0.14463
C	0.32590	-3.60569	-0.22626
H	0.26299	-3.92184	-1.27496
C	-1.03841	-3.44126	0.40436
N	-1.29690	-2.00057	0.18327
H	-1.01913	-3.65631	1.47877
C	2.29003	-2.10733	-0.16422
C	-2.67734	-1.58644	0.27477
C	-5.41113	-1.03904	0.44048
C	-3.29014	-1.48997	1.54840
C	-3.43915	-1.48307	-0.91757
C	-4.80280	-1.18698	-0.80207
C	-4.66193	-1.20638	1.59884
C	-2.55948	-1.77581	2.86179
C	-2.85439	-1.77249	-2.30067
H	-5.40206	-1.08717	-1.70131
H	-5.15083	-1.12482	2.56507
C	5.08032	-2.18703	-0.16674
C	2.97851	-2.26820	-1.39181
C	2.98738	-2.02146	1.06710
C	4.38727	-2.05092	1.03174
C	4.37849	-2.30057	-1.36269
C	2.26309	-2.44011	-2.73132
C	2.27505	-1.97080	2.41764
H	4.94242	-1.97519	1.96124
H	4.92538	-2.42166	-2.29332
H	-1.48441	-1.77273	2.66154
H	-1.78161	-1.57352	-2.26752
H	1.25952	-1.60410	2.25515
H	1.20321	-2.21584	-2.58165
C	-0.14277	-1.29014	-0.02554
H	-1.81629	-4.04922	-0.05877
H	0.97503	-4.30037	0.30904
N	0.18384	3.05667	-0.31888
C	-0.12546	3.86245	0.71288
C	0.58640	3.62627	-1.47016
C	-0.04787	5.25101	0.63351

H	-0.42980	3.35816	1.62374
C	0.69131	5.00612	-1.63051
H	0.80685	2.93822	-2.27937
C	0.36864	5.83844	-0.55999
H	-0.30970	5.85187	1.49897
H	1.02165	5.41000	-2.58244
H	0.44107	6.91873	-0.65314
N	-2.32451	1.62907	-0.25347
C	-2.76866	2.16266	-1.40525
C	-3.03456	1.87181	0.85905
C	-3.92344	2.93893	-1.48904
H	-2.15785	1.95436	-2.27766
C	-4.20196	2.63577	0.86843
H	-2.63056	1.44938	1.77092
C	-4.65851	3.18186	-0.32907
H	-4.23054	3.34380	-2.44873
H	-4.73326	2.79395	1.80204
H	-5.56302	3.78398	-0.35826
C	3.00659	1.52523	0.20653
C	2.90897	2.26922	1.40493
C	4.24842	1.52876	-0.47281
C	4.00249	2.98098	1.89052
H	1.97471	2.25331	1.95267
C	5.33770	2.24810	0.01038
H	4.34622	0.95069	-1.38760
C	5.21667	2.97804	1.19570
H	3.91049	3.54115	2.81759
H	6.27969	2.23825	-0.53182
H	6.06490	3.54010	1.57873
C	-3.07020	-3.25444	-2.68278
H	-2.61134	-3.94589	-1.96872
H	-4.14011	-3.49256	-2.72977
H	-2.63623	-3.45812	-3.66920
C	-3.43027	-0.88412	-3.41766
H	-4.47284	-1.13548	-3.65021
H	-3.38068	0.17466	-3.15589
H	-2.84641	-1.02772	-4.33300
C	-2.96921	-3.16385	3.40755
H	-2.38173	-3.41382	4.29936
H	-4.02806	-3.16923	3.69354
H	-2.82937	-3.96355	2.67262
C	-2.80398	-0.71670	3.95289
H	-3.85885	-0.66444	4.24747
H	-2.22829	-0.97601	4.84917
H	-2.47298	0.27164	3.62917
C	2.39841	-3.89173	-3.24169
H	1.82138	-4.02765	-4.16425
H	3.44498	-4.13327	-3.46436
H	2.04415	-4.62441	-2.50802
C	2.76711	-1.45998	-3.80806
H	3.82545	-1.62122	-4.04624
H	2.19489	-1.60135	-4.73204
H	2.62648	-0.42201	-3.49611
C	2.18925	-3.38278	3.03832
H	1.66242	-4.09227	2.39045
H	3.19077	-3.78960	3.22520
H	1.65696	-3.34571	3.99652
C	2.93033	-1.00450	3.42020
H	2.28812	-0.90594	4.30210
H	3.90824	-1.36437	3.76383
H	3.05801	-0.00880	2.98925
H	6.16710	-2.21333	-0.16740
H	-6.47309	-0.81507	0.50452

SCF energy: -2943.994551 hartree
zero-point correction: +0.892033 hartree
enthalpy correction: +0.946140 hartree
free energy correction: +0.804311 hartree
quasiharmonic free energy correction: +0.816288 hartree

6

Ru	-0.17343	0.49572	-0.03775
Cl	-0.59782	0.72902	2.32756
Cl	-0.53020	0.60262	-2.42304
O	-0.13982	2.85897	-0.09872
N	-1.39953	-2.18234	0.00970
N	0.77292	-2.44677	0.05514
C	-0.21166	-1.51223	0.01338
C	-2.71881	-1.60816	-0.01902
C	-1.25415	-3.64736	0.03680
H	-1.70069	-4.08967	-0.86076
H	-1.76509	-4.06384	0.91168
C	0.26863	-3.83386	0.09412
H	0.60134	-4.33098	1.01214
H	0.65979	-4.40262	-0.75614
C	-3.39154	-1.35967	1.19631
C	2.19320	-2.25348	0.07573
C	2.89733	-2.22526	-1.14249
C	-3.36652	-1.41539	-1.25824
C	1.63477	0.86034	-0.04249
C	2.85525	-2.15234	1.31346
C	1.15425	3.28108	-0.16157
C	2.09997	2.22536	-0.12828
C	4.28800	-2.07913	-1.09592
H	4.84155	-2.04406	-2.03195
C	-1.24598	3.81225	-0.00812
H	-1.04159	4.59815	-0.74463
C	-4.64135	-0.84041	-1.25521
H	-5.13378	-0.66386	-2.20936
C	-4.66585	-0.78491	1.14146
H	-5.17768	-0.56529	2.07625
C	1.57119	4.60879	-0.26336
H	0.85716	5.42260	-0.28843
C	3.89267	3.86631	-0.29568
H	4.95104	4.10313	-0.34712
C	4.24708	-2.00808	1.30513
H	4.76850	-1.91653	2.25564
C	3.47019	2.54527	-0.19409
H	4.19189	1.73277	-0.16778

C	-5.30048	-0.50035	-0.07056
C	2.93936	4.88837	-0.33170
H	3.25854	5.92407	-0.41176
C	4.98141	-1.97228	0.11480
C	-2.50761	3.06646	-0.41927
H	-2.38180	2.60358	-1.40140
H	-3.34275	3.77517	-0.46171
H	-2.75672	2.28862	0.31039
C	-1.32503	4.38598	1.40415
H	-1.49795	3.57757	2.12014
H	-2.15294	5.10202	1.46328
H	-0.40465	4.90481	1.68812
H	2.41657	0.10420	0.00359
C	2.09266	-2.14938	2.61738
H	1.39359	-1.30641	2.67220
H	1.50378	-3.06592	2.74922
H	2.78164	-2.07696	3.46433
C	2.17732	-2.30060	-2.46805
H	1.60008	-3.22864	-2.56764
H	1.47372	-1.46854	-2.59034
H	2.89228	-2.26798	-3.29572
C	6.48777	-1.84963	0.13680
H	6.96518	-2.83841	0.16457
H	6.86172	-1.33493	-0.75472
H	6.83272	-1.29865	1.01821
C	-2.82939	-1.77984	2.53350
H	-3.18910	-1.12253	3.32995
H	-3.16039	-2.80083	2.77493
H	-1.74101	-1.75057	2.55648
C	-2.77700	-1.89369	-2.56372
H	-3.09792	-2.92671	-2.76382
H	-3.12553	-1.27606	-3.39611
H	-1.68853	-1.85768	-2.56859
C	-6.68558	0.10404	-0.09994
H	-7.45840	-0.67585	-0.13493
H	-6.87675	0.71113	0.79111
H	-6.82642	0.73902	-0.98113

SCF energy: -2404.619383 hartree
zero-point correction: +0.624574 hartree
enthalpy correction: +0.666369 hartree
free energy correction: +0.547906 hartree
quasiharmonic free energy correction: +0.559194 hartree

6'

Ru	-0.20222	0.54829	0.31554
Cl	-0.43908	0.20871	2.69178
Cl	0.15802	1.03850	-2.07664
O	1.02473	3.16724	0.38747
N	-1.80875	-1.85307	-0.45140
N	0.31684	-2.40911	-0.39108
C	-0.56353	-1.39208	-0.19671
C	-3.11567	-1.24733	-0.31453
C	-1.81322	-3.25887	-0.91047
H	-2.17995	-3.30758	-1.94054
H	-2.48521	-3.84908	-0.28155
C	-0.34846	-3.67217	-0.77893
H	-0.18504	-4.43072	-0.00572
H	0.07814	-4.04440	-1.71470
C	-3.80331	-1.40274	0.90285
C	1.73833	-2.50020	-0.18885
C	2.60082	-2.34381	-1.29024
C	-3.73332	-0.68271	-1.44556
C	1.69379	0.48733	0.51867
C	2.22292	-2.88983	1.07825
C	2.28625	2.86678	0.05557
C	2.65570	1.49784	0.24629
C	3.97285	-2.53411	-1.08159
H	4.64852	-2.40515	-1.92425
C	0.54217	4.55209	0.39024
H	1.40950	5.19481	0.57370
C	-5.04183	-0.21262	-1.30797
H	-5.52445	0.23945	-2.17166
C	-5.10944	-0.91019	0.98473
H	-5.64615	-1.01282	1.92536
C	3.25498	3.78512	-0.37842
H	2.99170	4.81440	-0.58432
C	4.97156	2.05160	-0.29371
H	6.00814	1.75583	-0.41984
C	3.60242	-3.06504	1.22998
H	3.98684	-3.35212	2.20625
C	4.02137	1.13461	0.11937
H	4.29531	0.10071	0.30689
C	-5.74057	-0.29882	-0.10078
C	4.57208	3.37019	-0.55673
H	5.30563	4.09670	-0.89659
C	4.49430	-2.89299	0.16489
C	-0.08498	4.86373	-0.96349
H	0.64208	4.75269	-1.77463
H	-0.45531	5.89553	-0.96883
H	-0.91781	4.18213	-1.15438
C	-0.41273	4.67840	1.56977
H	-1.26640	4.00839	1.45085
H	-0.77326	5.71180	1.63047
H	0.09816	4.43414	2.50659
H	2.10604	-0.41370	0.97150
C	1.30118	-3.09204	2.25821
H	0.79188	-2.16411	2.54372
H	0.52076	-3.83307	2.04600
H	1.86538	-3.44859	3.12497
C	2.08497	-1.98882	-2.66308
H	1.43918	-2.77977	-3.06733
H	1.49851	-1.06406	-2.64746
H	2.91712	-1.85995	-3.36161
C	5.97532	-3.13156	0.34976
H	6.22011	-4.19623	0.23781
H	6.56593	-2.58286	-0.39110
H	6.31033	-2.82690	1.34712
C	-3.18334	-2.07879	2.10202

H	-3.94212	-2.26125	2.86912
H	-2.73253	-3.04665	1.84763
H	-2.39545	-1.45942	2.54297
C	-3.02705	-0.55940	-2.77273
H	-2.68096	-1.52974	-3.15256
H	-3.70213	-0.13785	-3.52355
H	-2.14949	0.09036	-2.69600
C	-7.13661	0.26363	0.02791
H	-7.68830	0.19066	-0.91579
H	-7.71127	-0.25835	0.80061
H	-7.10553	1.32551	0.30543
Cl	-2.20580	1.89754	0.13432

SCF energy: -2864.819012 hartree
zero-point correction: +0.625441 hartree
enthalpy correction: +0.669345 hartree
free energy correction: +0.544939 hartree
quasiharmonic free energy correction: +0.557332 hartree

7

Ru	-0.22069	0.87634	0.00483
Cl	0.58149	1.28353	-2.21930
Cl	-0.36298	1.14254	2.39230
O	-1.20014	3.05305	-0.14488
N	1.90473	-1.14506	0.40451
N	-0.04321	-2.16091	0.43683
C	0.55855	-0.95288	0.23300
C	2.98884	-0.22421	0.13684
C	2.21081	-2.48131	0.95125
H	2.40880	-2.40762	2.02698
H	3.09002	-2.90866	0.46680
C	0.92685	-3.25061	0.66004
H	1.00254	-3.87712	-0.23878
H	0.60685	-3.88213	1.49235
C	3.58899	-0.24165	-1.15000
C	-1.40943	-2.54865	0.20562
C	-1.87082	-2.31117	2.73263
H	-0.89593	-1.81856	2.68902
C	3.21530	-1.25630	-2.23047
H	2.22072	-1.64614	-1.99672
C	-2.29288	-2.64386	1.30483
C	3.51609	0.57539	1.18021
C	-1.98845	0.49897	-0.36168
C	-1.80658	-2.91633	-1.10188
C	-2.83420	-1.32319	3.41576
H	-3.83691	-1.74927	3.54369
H	-2.91471	-0.39529	2.84353
H	-2.45492	-1.06473	4.41061
C	-2.54012	2.91003	-0.35001
C	-2.96210	1.56131	-0.46475
C	-3.59976	-3.08444	1.05772
H	-4.29894	-3.16078	1.88517
C	-0.56768	4.37193	-0.18530
H	-1.19342	5.03849	0.41965
C	4.56939	1.44821	0.87128
H	4.97713	2.08176	1.65252
C	4.64257	0.64509	-1.39532
H	5.10417	0.66141	-2.37733
C	-3.46336	3.95346	-0.43265
H	-3.15255	4.98752	-0.34981
C	-5.25633	2.33228	-0.74481
H	-6.30978	2.11844	-0.89757
C	-3.12627	-3.34672	-1.29037
H	-3.45698	-3.62511	-2.28706
C	-4.33162	1.29695	-0.66520
H	-4.65052	0.26118	-0.75037
C	5.11560	1.50073	-0.40530
H	5.92983	2.18748	-0.62246
C	-4.81491	3.65366	-0.62674
H	-5.52870	4.47074	-0.68817
C	-4.01821	-3.42768	-0.22466
H	-5.03741	-3.76643	-0.39255
C	3.15125	-0.66815	-3.65156
H	2.47867	0.19008	-3.69059
H	2.78018	-1.43080	-4.34700
H	4.14067	-0.36159	-4.01169
C	0.78922	4.22501	0.48652
H	0.67718	3.81356	1.49291
H	1.26594	5.20941	0.55441
H	1.44052	3.56671	-0.09768
C	-0.47144	4.86326	-1.62697
H	0.12616	4.16064	-2.21451
H	0.00769	5.84893	-1.64637
H	-1.45638	4.95391	-2.09462
H	-2.37785	-0.50615	-0.51130
C	4.21453	-2.43678	-2.21588
H	3.91454	-3.20183	-2.94234
H	5.21997	-2.09328	-2.48717
H	4.29046	-2.91493	-1.23333
C	-1.72812	-3.59701	3.57480
H	-1.02312	-4.30703	3.12580
H	-1.36854	-3.35427	4.58169
H	-2.69039	-4.11334	3.67871
C	-0.86484	-2.86948	-2.30287
H	0.09917	-2.47897	-1.96553
C	-0.62421	-4.28241	-2.87446
H	-1.54805	-4.71288	-3.27860
H	0.10772	-4.24322	-3.68971
H	-0.24656	-4.97211	-2.11026
C	-1.36727	-1.91293	-3.40187
H	-1.44135	-0.88684	-3.03075
H	-0.66408	-1.90777	-4.24256
H	-2.34622	-2.22133	-3.78826
C	3.07792	0.44043	2.63676
H	2.09646	-0.03902	2.65845
C	4.08204	-0.44876	3.40620
H	5.06863	0.02826	3.45270
H	3.73796	-0.60996	4.43507
H	4.21696	-1.42883	2.93519

C	2.92579	1.78907	3.36221
H	2.24965	2.45511	2.82200
H	2.50069	1.62444	4.35833
H	3.88949	2.29546	3.49617

SCF energy: -2640.514715 hartree
zero-point correction: +0.798495 hartree
enthalpy correction: +0.846703 hartree
free energy correction: +0.717986 hartree
quasiharmonic free energy correction: +0.728044 hartree

7'

Ru	0.16142	-0.81929	0.43263
Cl	0.56323	-1.33080	-1.93742
Cl	-0.10523	-0.35634	2.78145
O	1.88814	-3.01680	0.70513
N	-2.03240	1.05123	-0.40375
N	-0.12096	2.14126	-0.33318
C	-0.70665	0.92386	-0.14733
C	-3.15443	0.12827	-0.41096
C	-2.41277	2.46254	-0.64029
H	-2.92535	2.85111	0.24670
H	-3.09266	2.52968	-1.49064
C	-1.07211	3.13291	-0.88313
H	-0.86554	3.28659	-1.94800
H	-0.96352	4.08841	-0.36710
C	-3.54981	-0.43531	-1.64584
C	1.23561	2.60760	-0.17244
C	0.65780	3.30376	2.25780
H	-0.19594	2.64548	2.07778
C	-2.77576	-0.24689	-2.94792
H	-1.80343	0.19166	-2.70982
C	1.60700	3.19219	1.06551
C	-3.93596	-0.01409	0.75718
C	1.98968	-0.27777	0.56634
C	2.10602	2.61618	-1.28906
C	1.29999	2.84455	3.58020
H	2.12059	3.50321	3.88925
H	1.67542	1.82093	3.50620
H	0.54849	2.86022	4.37710
C	3.06539	-2.50464	0.31772
C	3.14643	-1.07814	0.36159
C	2.89672	3.72759	1.17536
H	3.20758	4.17221	2.11556
C	1.70888	-4.46302	0.88830
H	2.69610	-4.87941	1.11241
C	-5.11168	-0.76916	0.66637
H	-5.72396	-0.90172	1.55322
C	-4.73461	-1.17994	-1.67233
H	-5.05481	-1.63090	-2.60665
C	4.19942	-3.24749	-0.04297
H	4.15319	-4.32465	-0.13677
C	5.52277	-1.19948	-0.18015
H	6.47564	-0.71355	-0.36375
C	3.38219	3.17160	-1.11673
H	4.06900	3.18684	-1.95763
C	4.40577	-0.45692	0.16081
H	4.46063	0.62547	0.23392
C	-5.51008	-1.35047	-0.53126
H	-6.42687	-1.93267	-0.57669
C	5.40233	-2.59224	-0.29548
H	6.26864	-3.18491	-0.57757
C	3.78107	3.71429	0.10037
H	4.77475	4.14179	0.20753
C	-2.49245	-1.58718	-3.65206
H	-1.98163	-2.27733	-2.97748
H	-1.84397	-1.41939	-4.51973
H	-3.41410	-2.05870	-4.01416
C	0.81875	-4.64575	2.11020
H	1.27601	-4.18611	2.99211
H	0.69331	-5.71752	2.30324
H	-0.16237	-4.19533	1.94823
C	1.14940	-5.06093	-0.39696
H	0.18614	-4.60202	-0.63351
H	1.01194	-6.14114	-0.27072
H	1.82648	-4.89412	-1.24119
H	2.19635	0.73385	0.91272
C	-3.51925	0.71045	-3.90435
H	-2.93864	0.85864	-4.82290
H	-4.49676	0.30299	-4.18909
H	-3.69623	1.69603	-3.45633
C	0.13445	4.75009	2.40138
H	-0.36432	5.10595	1.49254
H	-0.58410	4.81328	3.22677
H	0.95514	5.44483	2.61706
C	1.70956	2.10713	-2.67332
H	0.77509	1.54761	-2.58078
C	1.48654	3.29151	-3.64036
H	2.41968	3.84381	-3.80495
H	1.13853	2.92577	-4.61332
H	0.74769	4.00743	-3.26243
C	2.74422	1.13410	-3.26919
H	2.91371	0.28191	-2.60778
H	2.37061	0.74038	-4.22066
H	3.70242	1.62882	-3.46994
C	-3.58290	0.62176	2.09852
H	-2.57472	1.04035	2.02955
C	-4.56006	1.76405	2.45160
H	-5.58083	1.38356	2.57691
H	-4.26419	2.24050	3.39395
H	-4.59540	2.53873	1.67614
C	-3.55255	-0.41857	3.23507
H	-2.88920	-1.24933	2.98528
H	-3.18195	0.04670	4.15533
H	-4.55329	-0.81633	3.44286
Cl	-1.53429	-2.55889	0.37574

SCF energy: -3100.716636 hartree
zero-point correction: +0.798636 hartree

enthalpy correction: +0.849384 hartree
free energy correction: +0.712629 hartree
quasiharmonic free energy correction: +0.725046 hartree

$CHCl_2$ radical

C	-0.01215	0.69636	0.00000
H	0.48595	1.65778	0.00000
Cl	-0.01215	-0.17164	1.48494
Cl	-0.01215	-0.17164	-1.48494

SCF energy: -959.054220 hartree
zero-point correction: +0.015796 hartree
enthalpy correction: +0.020390 hartree
free energy correction: +-0.011498 hartree
quasiharmonic free energy correction: +-0.011498 hartree

$CHCl_3$

C	0.00000	0.00000	0.45448
H	0.00000	0.00000	1.54004
Cl	0.00000	1.70503	-0.08367
Cl	-1.47660	-0.85252	-0.08367
Cl	1.47660	-0.85252	-0.08367

SCF energy: -1419.312384 hartree
zero-point correction: +0.019955 hartree
enthalpy correction: +0.025369 hartree
free energy correction: +-0.008233 hartree
quasiharmonic free energy correction: +-0.008233 hartree

PCy_3

P	-0.22986	-0.06738	-1.04452
C	0.54858	1.56777	-0.46764
C	-1.83682	-0.12733	-0.03922
C	0.76007	-1.50840	-0.30565
C	1.95365	-1.88536	-1.21375
C	2.59805	-3.21202	-0.77537
C	3.01565	-3.18038	0.70242
C	1.83607	-2.79568	1.60764
C	1.20285	-1.46140	1.17007
C	1.97639	1.72593	-1.03460
C	2.51111	3.15416	-0.83623
C	2.46073	3.57291	0.64037
C	1.04799	3.40484	1.21894
C	0.51783	1.97122	1.02271
C	-2.73471	1.07575	-0.40891
C	-4.09528	1.03081	0.30819
C	-4.83466	-0.28570	0.03635
C	-3.95933	-1.49016	0.40668
C	-2.59797	-1.44522	-0.30853
H	-0.07577	2.29933	-1.00589
H	-1.61569	-0.07521	1.03749
H	0.04020	-2.33632	-0.40030
H	1.62209	-1.95270	-2.25695
H	2.71285	-1.09226	-1.17954
H	3.46465	-3.43597	-1.41124
H	1.87799	-4.02958	-0.93005
H	3.82420	-2.44561	0.83390
H	3.42627	-4.15273	1.00385
H	2.16369	-2.73012	2.65366
H	1.07396	-3.58826	1.56802
H	1.94554	-0.66345	1.30259
H	0.35689	-1.21607	1.82431
H	2.65077	1.02349	-0.52555
H	1.99317	1.46142	-2.09945
H	1.90507	3.85180	-1.43304
H	3.53783	3.22658	-1.21834
H	2.79856	4.61096	0.75541
H	3.16224	2.95034	1.21585
H	0.36713	4.11254	0.72257
H	1.04041	3.66245	2.28633
H	-0.49954	1.89974	1.42443
H	1.13379	1.28200	1.61240
H	-2.23157	2.02085	-0.17359
H	-2.89977	1.07461	-1.49668
H	-4.70798	1.88589	-0.00631
H	-3.93839	1.14162	1.39160
H	-5.09435	-0.34121	-1.03126
H	-5.78133	-0.31494	0.59121
H	-4.47509	-2.42799	0.16194
H	-3.79649	-1.49855	1.49481
H	-2.75371	-1.55354	-1.39217
H	-2.00096	-2.30886	0.00696

SCF energy: -1047.272340 hartree
zero-point correction: +0.485699 hartree
enthalpy correction: +0.506201 hartree
free energy correction: +0.437505 hartree
quasiharmonic free energy correction: +0.441040 hartree

Pyridine

C	-1.14254	-0.72167	-0.00022
C	-1.19865	0.67327	-0.00012
C	0.00025	1.38544	0.00010
C	1.19889	0.67286	0.00022
C	1.14228	-0.72207	0.00012
N	-0.00026	-1.42094	-0.00010
H	0.00042	2.47232	0.00016
H	-2.05996	-1.30854	-0.00037
H	-2.15767	1.18295	-0.00023

H	2.15812	1.18216	0.00036
H	2.05949	-1.30927	0.00019

SCF energy: -248.319038 hartree
zero-point correction: +0.089105 hartree
enthalpy correction: +0.094316 hartree
free energy correction: +0.061705 hartree
quasiharmonic free energy correction: +0.061705 hartree

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