Supporting information

Optimized Cartesian coordinates (Å)

(1) Ru(Por)$(CH_3)_2$, C_{2v}, S = 0, Conformation shown in Figure 2(c)

N	0.000000	0.000000	-2.095221
Ru	0.000000	0.000000	-0.067274
N	0.000000	0.000000	2.059777
C	0.000000	2.001751	0.563597
C	0.000000	-2.001751	0.563597
N	-2.054088	-0.000000	-0.053921
N	2.054088	0.000000	-0.053921
C	2.863611	0.000000	1.067360
C	2.880508	0.000000	-1.149795
C	1.116295	0.000000	-2.915979
C	-1.116295	0.000000	-2.915979
C	-2.880508	0.000000	-1.149795
C	-2.863611	0.000000	1.067360
C	-1.106699	-0.000000	2.862315
C	1.106699	0.000000	2.862315
H	3.207664	0.000000	3.150396
C	0.684316	0.000000	4.242562
C	2.426650	0.000000	2.390443
C	4.250655	0.000000	0.649187
C	2.439495	0.000000	-2.472130
C	-0.684316	0.000000	4.242562
C	-2.426650	0.000000	2.390443
C	-4.250655	0.000000	0.649187
C	0.685185	0.000000	-4.284954
H	-3.207664	0.000000	3.150396
C	-2.439495	0.000000	-2.472130
C	-4.261370	-0.000000	-0.712234
C	4.261370	0.000000	-0.712234
C	-0.685185	0.000000	-4.284954
H	3.207824	0.000000	-3.243945
H	-3.207824	0.000000	-3.243945
H	1.348814	0.000000	-5.143346
H	5.121541	0.000000	-1.373608
H	-5.099974	-0.000000	1.324598
H	5.099974	0.000000	1.324598
H	-1.348814	0.000000	-5.143346
H	-1.351416	-0.000000	5.098120
H	-5.121541	0.000000	-1.373608
H	1.351416	0.000000	5.098120
H	0.000000	2.381827	-0.470719
H	0.909149	2.287672	1.096987
H	-0.909149	2.287672	1.096987
H	0.000000	-2.381827	-0.470719
H	-0.909149	-2.287672	1.096987
H	0.909149	-2.287672	1.096987

(2) $Ru(Por)(CH_3)_2$, C_{2v}, S = 1, Conformation shown in Figure 2(b)

N	0.000000	0.000000	-2.052885
Ru	0.000000	0.000000	0.000499
N	0.000000	0.000000	2.042245
C	0.000000	2.247722	0.046259
C	0.000000	-2.247722	0.046259
N	-2.058238	-0.000000	-0.003594
N	2.058238	0.000000	-0.003594
C	2.880243	0.000000	1.101366
C	2.879202	0.000000	-1.110944
C	1.110619	0.000000	-2.873127
C	-1.110619	0.000000	-2.873127
C	-2.879202	0.000000	-1.110944
C	-2.880243	0.000000	1.101366
C	-1.112459	-0.000000	2.864801
C	1.112459	0.000000	2.864801
H	3.207271	0.000000	3.192879
C	0.687282	0.000000	4.231728
C	2.439056	0.000000	2.420630
C	4.265337	0.000000	0.675029
C	2.438448	0.000000	-2.428777
C	-0.687282	0.000000	4.231728
C	-2.439056	0.000000	2.420630
C	-4.265337	0.000000	0.675029
C	0.687199	0.000000	-4.241741
H	-3.207271	0.000000	3.192879
C	-2.438448	0.000000	-2.428777
C	-4.264387	-0.000000	-0.685409
C	4.264387	0.000000	-0.685409
C	-0.687199	0.000000	-4.241741
H	3.206520	0.000000	-3.200861
H	-3.206520	0.000000	-3.200861
H	1.351455	0.000000	-5.100211
H	5.118131	0.000000	-1.354890
H	-5.119815	-0.000000	1.343785
H	5.119815	0.000000	1.343785
H	-1.351455	0.000000	-5.100211
H	-1.350699	-0.000000	5.090757
H	-5.118131	0.000000	-1.354890
H	1.350699	0.000000	5.090757
H	0.000000	2.525525	-1.009107
H	0.915543	2.527641	0.569731
H	-0.915543	2.527641	0.569731
H	0.000000	-2.525525	-1.009107
H	-0.915543	-2.527641	0.569731
H	0.915543	-2.527641	0.569731

(c) $Ru(Por)(CH_3)_2$, C_{2v}, S = 0, conformation shown in Figure 2(a).

N	2.068683	-0.000000	-0.017460
Ru	0.035058	-0.000000	-0.035058
N	-2.060564	-0.000000	-0.042414
C	-0.429677	2.021253	0.429677
H	-1.192590	2.174828	1.192590
H	0.541722	2.413740	0.748839
H	-0.748839	2.413740	-0.541722
C	-0.429677	-2.021253	0.429677
H	-1.192590	-2.174828	1.192590
H	0.541722	-2.413740	0.748839
H	-0.748839	-2.413740	-0.541722
N	0.017460	-0.000000	-2.068683
N	0.042414	-0.000000	2.060564
C	-1.078916	-0.000000	2.859343
C	1.134426	-0.000000	2.877179
C	2.892390	-0.000000	1.100848
C	2.891131	-0.000000	-1.125883
C	1.125883	-0.000000	-2.891131
C	-1.100848	-0.000000	-2.892390
C	-2.877179	-0.000000	-1.134426
C	-2.859343	-0.000000	1.078916
H	-3.171136	-0.000000	3.171136
C	-4.245200	-0.000000	0.664897
C	-2.400289	-0.000000	2.400289
C	-0.664897	-0.000000	4.245200
C	2.459227	-0.000000	2.422187
C	-4.258517	-0.000000	-0.699873
C	-2.422187	-0.000000	-2.459227
C	-0.671048	-0.000000	-4.268865
C	4.268865	-0.000000	0.671048
H	-3.185168	-0.000000	-3.236584
C	2.448085	-0.000000	-2.448085
C	0.694326	-0.000000	-4.266783
C	0.699873	-0.000000	4.258517
C	4.266783	-0.000000	-0.694326
H	3.236584	-0.000000	3.185168
H	3.218327	-0.000000	-3.218327
H	5.125176	-0.000000	1.337400
H	1.360308	-0.000000	5.119060
H	-1.337400	-0.000000	-5.125176
H	-1.340647	-0.000000	5.094374
H	5.123581	-0.000000	-1.360563
H	-5.119060	-0.000000	-1.360308
H	1.360563	-0.000000	-5.123581
H	-5.094374	-0.000000	1.340647

(d) $Ru(Por)(CF_3)_2$, C_{2v}, S = 0, conformation shown in Figure 3(a).

N	-2.132343	0.087227	-0.000000
Ru	-0.118970	0.017192	-0.000000
N	2.007358	-0.079891	-0.000000
C	0.590994	2.017499	-0.000000
C	0.401496	-2.041578	-0.000000
N	-0.107022	0.011853	2.068080
N	-0.107022	0.011853	-2.068080
C	1.014181	-0.034577	-2.873439
C	-1.200168	0.051898	-2.888951
C	-2.956191	0.106561	-1.118380
C	-2.956191	0.106561	1.118380
C	-1.200168	0.051898	2.888951
C	1.014181	-0.034577	2.873439
C	2.803235	-0.114591	1.109986
C	2.803235	-0.114591	-1.109986
H	3.096583	-0.126268	-3.209556
C	4.179053	-0.175907	-0.684648
C	2.334345	-0.092559	-2.431939
C	0.595915	-0.018782	-4.258121
C	-2.521300	0.094621	-2.441105
C	4.179053	-0.175907	0.684648
C	2.334345	-0.092559	2.431939
C	0.595915	-0.018782	4.258121
C	-4.322568	0.138871	-0.684828
H	3.096583	-0.126268	3.209556
C	-2.521300	0.094621	2.441105
C	-0.765178	0.034513	4.269211
C	-0.765178	0.034513	-4.269211
C	-4.322568	0.138871	0.684828
H	-3.296553	0.117066	-3.204528
H	-3.296553	0.117066	3.204528
H	-5.180461	0.158276	-1.348579
H	-1.427014	0.059232	-5.128288
H	1.270007	-0.046434	5.107762
H	1.270007	-0.046434	-5.107762
H	-5.180461	0.158276	1.348579
H	5.033548	-0.214153	1.351153
H	-1.427014	0.059232	5.128288
H	5.033548	-0.214153	-1.351153
F	-0.617326	2.674973	-0.000000
F	1.272371	2.447955	-1.084926
F	1.272371	2.447955	1.084926
F	-0.856523	-2.596499	-0.000000
F	1.044305	-2.528075	1.084885
F	1.044305	-2.528075	-1.084885

(e) $Ru(Por)(CF_3)_2$, C_{2v}, S = 1, conformation shown in Figure 3(b).

N	0.000000	0.000000	-2.035640
Ru	0.000000	0.000000	0.014356
N	0.000000	0.000000	2.109830
C	0.000000	2.190314	0.387609
C	0.000000	-2.190314	0.387609
N	-2.041300	-0.000000	0.012166
N	2.041300	0.000000	0.012166
C	2.857902	0.000000	1.135494
C	2.866115	0.000000	-1.093729
C	1.109953	0.000000	-2.857787
C	-1.109953	0.000000	-2.857787
C	-2.866115	0.000000	-1.093729
C	-2.857902	0.000000	1.135494
C	-1.104282	-0.000000	2.915697
C	1.104282	0.000000	2.915697
H	3.202605	0.000000	3.221942
C	0.681956	0.000000	4.299396
C	2.424107	0.000000	2.460558
C	4.225772	0.000000	0.712540
C	2.429137	0.000000	-2.420011
C	-0.681956	0.000000	4.299396
C	-2.424107	0.000000	2.460558
C	-4.225772	0.000000	0.712540
C	0.681951	0.000000	-4.234917
H	-3.202605	0.000000	3.221942
C	-2.429137	0.000000	-2.420011
C	-4.232240	-0.000000	-0.660610
C	4.232240	0.000000	-0.660610
C	-0.681951	0.000000	-4.234917
H	3.200600	0.000000	-3.187744
H	-3.200600	0.000000	-3.187744
H	1.348820	0.000000	-5.090975
H	5.093604	0.000000	-1.320508
H	-5.081138	-0.000000	1.380387
H	5.081138	0.000000	1.380387
H	-1.348820	0.000000	-5.090975
H	-1.351625	-0.000000	5.153037
H	-5.093604	0.000000	-1.320508
H	1.351625	0.000000	5.153037
F	0.000000	2.876165	-0.802981
F	1.090708	2.636661	1.079281
F	-1.090708	2.636661	1.079281
F	0.000000	-2.876165	-0.802981
F	-1.090708	-2.636661	1.079281
F	1.090708	-2.636661	1.079281

(f) Ru(Por)$(CF_3)_2$, C_{2v}, S = 0, conformation shown in Figure 3(c).

N	2.123336	0.000000	-0.089480
Ru	0.094706	0.000000	-0.094706
N	-2.007285	0.000000	-0.093829
C	-0.325001	2.065433	0.325001
F	-1.241638	2.425444	1.241638
F	0.854797	2.651225	0.689647
F	-0.689647	2.651225	-0.854797
C	-0.325001	-2.065433	0.325001
F	-1.241638	-2.425444	1.241638
F	0.854797	-2.651225	0.689647
F	-0.689647	-2.651225	-0.854797
N	0.089480	0.000000	-2.123336
N	0.093829	0.000000	2.007285
C	-1.024299	0.000000	2.804698
C	1.189521	0.000000	2.817676
C	2.945161	0.000000	1.036387
C	2.952539	0.000000	-1.192580
C	1.192580	0.000000	-2.952539
C	-1.036387	0.000000	-2.945161
C	-2.817676	0.000000	-1.189521
C	-2.804698	0.000000	1.024299
H	-3.117178	0.000000	3.117178
C	-4.186805	0.000000	0.606236
C	-2.346670	0.000000	2.346670
C	-0.606236	0.000000	4.186805
C	2.512398	0.000000	2.355463
C	-4.196515	0.000000	-0.760329
C	-2.355463	0.000000	-2.512398
C	-0.610419	0.000000	-4.319170
C	4.319170	0.000000	0.610419
H	-3.116108	0.000000	-3.291611
C	2.515020	0.000000	-2.515020
C	0.754855	0.000000	-4.324071
C	0.760329	0.000000	4.196515
C	4.324071	0.000000	-0.754855
H	3.291611	0.000000	3.116108
H	3.285008	0.000000	-3.285008
H	5.173425	0.000000	1.279094
H	1.422373	0.000000	5.055457
H	-1.279094	0.000000	-5.173425
H	-1.278357	0.000000	5.038470
H	5.183710	0.000000	-1.416983
H	-5.055457	0.000000	-1.422373
H	1.416983	0.000000	-5.183710
H	-5.038470	0.000000	1.278357

(g) Ru(Por)Ph_2 ,C_{2v}, S = 0, conformation shown in Figure 4(a).

N	2.153063	0.000000	0.054815
Ru	0.057105	0.000000	0.057105
N	-1.980918	0.000000	0.077499
C	0.428710	2.049065	0.428710
C	1.283138	2.732653	1.283138
C	1.295595	4.134096	1.295595
C	0.453324	4.857543	0.453324
C	-0.403183	4.166454	-0.403183
C	-0.423946	2.765155	-0.423946
C	0.428710	-2.049065	0.428710
C	1.283138	-2.732653	1.283138
C	1.295595	-4.134096	1.295595
C	0.453324	-4.857543	0.453324
C	-0.403183	-4.166454	-0.403183
C	-0.423946	-2.765155	-0.423946
N	0.077499	0.000000	-1.980918
N	0.054815	0.000000	2.153063
C	-1.040382	0.000000	2.965566
C	1.169169	0.000000	2.951076
C	2.951076	0.000000	1.169169
C	2.965566	0.000000	-1.040382
C	1.193839	0.000000	-2.800432
C	-1.029820	0.000000	-2.799709
C	-2.799709	0.000000	-1.029820
C	-2.800432	0.000000	1.193839
H	-3.139580	0.000000	3.278901
C	-4.177291	0.000000	0.764511
C	-2.364127	0.000000	2.514063
C	-0.608542	0.000000	4.346900
C	2.492280	0.000000	2.492280
C	-4.177132	0.000000	-0.600463
C	-2.352558	0.000000	-2.352558
C	-0.600463	0.000000	-4.177132
C	4.336961	0.000000	0.755607
H	-3.122856	0.000000	-3.122856
C	2.514063	0.000000	-2.364127
C	0.764511	0.000000	-4.177291
C	0.755607	0.000000	4.336961
C	4.346900	0.000000	-0.608542
H	3.262824	0.000000	3.262824
H	3.278901	0.000000	-3.139580
H	5.187351	0.000000	1.429846
H	1.429846	0.000000	5.187351
H	-1.267078	0.000000	-5.033844
H	-1.271468	0.000000	5.205884
H	5.205884	0.000000	-1.271468
H	-5.033844	0.000000	-1.267078
H	1.431165	0.000000	-5.033526
H	-5.033526	0.000000	1.431165
H	1.955941	2.206649	1.955941
H	1.975193	4.650199	1.975193
H	0.463567	5.947866	0.463567
H	-1.073130	4.707084	-1.073130
H	-1.111556	2.276495	-1.111556

H	1.955941	-2.206649	1.955941
H	1.975193	-4.650199	1.975193
H	0.463567	-5.947866	0.463567
H	-1.073130	-4.707084	-1.073130
H	-1.111556	-2.276495	-1.111556

(h) Ru(Por)Ph_2 [C_{2v}], S=1, conformation CC.

N	2.191615	0.000000	0.120192
Ru	0.107812	0.000000	0.107812
N	-1.938001	0.000000	0.109420
C	0.293269	2.159054	0.293269
C	1.155469	2.847220	1.155469
C	1.181850	4.243469	1.181850
C	0.341124	4.979075	0.341124
C	-0.523265	4.304396	-0.523265
C	-0.549167	2.905434	-0.549167
C	0.293269	-2.159054	0.293269
C	1.155469	-2.847220	1.155469
C	1.181850	-4.243469	1.181850
C	0.341124	-4.979075	0.341124
C	-0.523265	-4.304396	-0.523265
C	-0.549167	-2.905434	-0.549167
N	0.109420	0.000000	-1.938001
N	0.120192	0.000000	2.191615
C	-0.982856	0.000000	2.997948
C	1.228207	0.000000	3.000481
C	3.000481	0.000000	1.228207
C	2.997948	0.000000	-0.982856
C	1.225653	0.000000	-2.748581
C	-0.996086	0.000000	-2.761067
C	-2.761067	0.000000	-0.996086
C	-2.748581	0.000000	1.225653
H	-3.079481	0.000000	3.314221
C	-4.126736	0.000000	0.803371
C	-2.306123	0.000000	2.547212
C	-0.559948	0.000000	4.380060
C	2.552901	0.000000	2.552901
C	-4.135334	0.000000	-0.563536
C	-2.320226	0.000000	-2.320226
C	-0.563536	0.000000	-4.135334
C	4.381670	0.000000	0.805802
H	-3.090492	0.000000	-3.090492
C	2.547212	0.000000	-2.306123
C	0.803371	0.000000	-4.126736
C	0.805802	0.000000	4.381670
C	4.380060	0.000000	-0.559948
H	3.323157	0.000000	3.323157
H	3.314221	0.000000	-3.079481
H	5.236794	0.000000	1.473859
H	1.473859	0.000000	5.236794
H	-1.226086	0.000000	-4.994987
H	-1.228993	0.000000	5.234478
H	5.234478	0.000000	-1.228993
H	-4.994987	0.000000	-1.226086
H	1.474169	0.000000	-4.979945
H	-4.979945	0.000000	1.474169
H	1.824063	2.306918	1.824063
H	1.862900	4.756612	1.862900
H	0.360737	6.069713	0.360737
H	-1.185539	4.864555	-1.185539
H	-1.236902	2.413954	-1.236902

H	1.824063	-2.306918	1.824063
H	1.862900	-4.756612	1.862900
H	0.360737	-6.069713	0.360737
H	-1.185539	-4.864555	-1.185539
H	-1.236902	-2.413954	-1.236902

(i) $Ru(Por)Cl_2$ [C_{2v}], S=1.

N	2.068474	-0.000000	0.000000
Ru	0.000000	-0.000000	0.000000
N	-2.068474	-0.000000	0.000000
Cl	0.000000	2.331404	0.000000
Cl	0.000000	-2.331404	-0.000000
N	0.000000	0.000000	-2.068474
N	-0.000000	-0.000000	2.068474
C	-1.110855	-0.000000	2.876713
C	1.110855	-0.000000	2.876713
C	2.876713	-0.000000	1.110855
C	2.876713	0.000000	-1.110855
C	1.110855	0.000000	-2.876713
C	-1.110855	0.000000	-2.876713
C	-2.876713	0.000000	-1.110855
C	-2.876713	-0.000000	1.110855
H	-3.204376	-0.000000	3.204376
C	-4.254077	-0.000000	0.683779
C	-2.434506	-0.000000	2.434506
C	-0.683779	-0.000000	4.254077
C	2.434506	-0.000000	2.434506
C	-4.254077	0.000000	-0.683779
C	-2.434506	0.000000	-2.434506
C	-0.683779	0.000000	-4.254077
C	4.254077	-0.000000	0.683779
H	-3.204376	0.000000	-3.204376
C	2.434506	0.000000	-2.434506
C	0.683779	0.000000	-4.254077
C	0.683779	-0.000000	4.254077
C	4.254077	0.000000	-0.683779
H	3.204376	-0.000000	3.204376
H	3.204376	0.000000	-3.204376
H	5.109195	-0.000000	1.351589
H	1.351589	-0.000000	5.109195
H	-1.351589	0.000000	-5.109195
H	-1.351589	-0.000000	5.109195
H	5.109195	0.000000	-1.351589
H	-5.109195	0.000000	-1.351589
H	1.351589	0.000000	-5.109195
H	-5.109195	-0.000000	1.351589