Electronic Supporting Information

Proton-responsive naphthyridinone-based Ru^{II} complexes and their reactivity with water and alcohols

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I. Characterization of ligand and Ru complexes

Ligand L-H

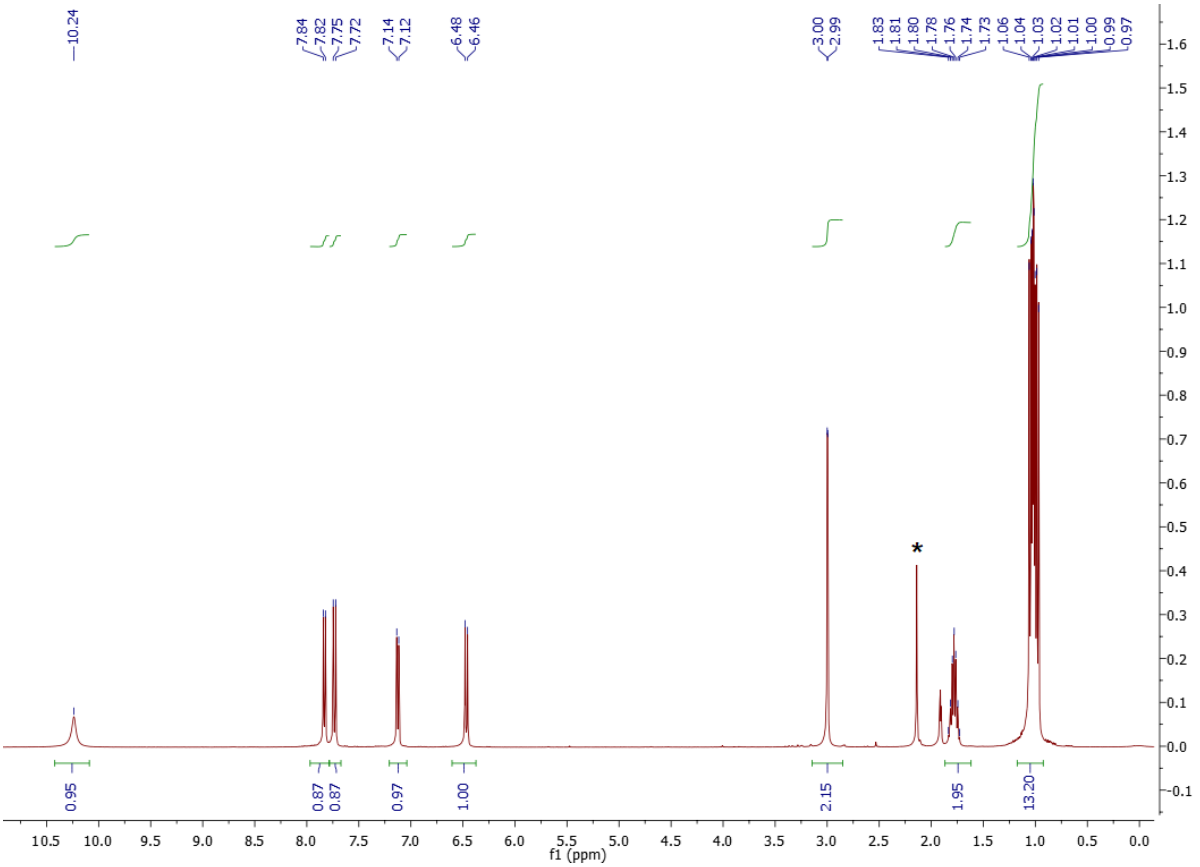


Figure S1. ^{1}H NMR spectrum of **L-H** in CD_3CN at 20 °C. The peak marked with an asterisk is from residual solvent (H_2O).

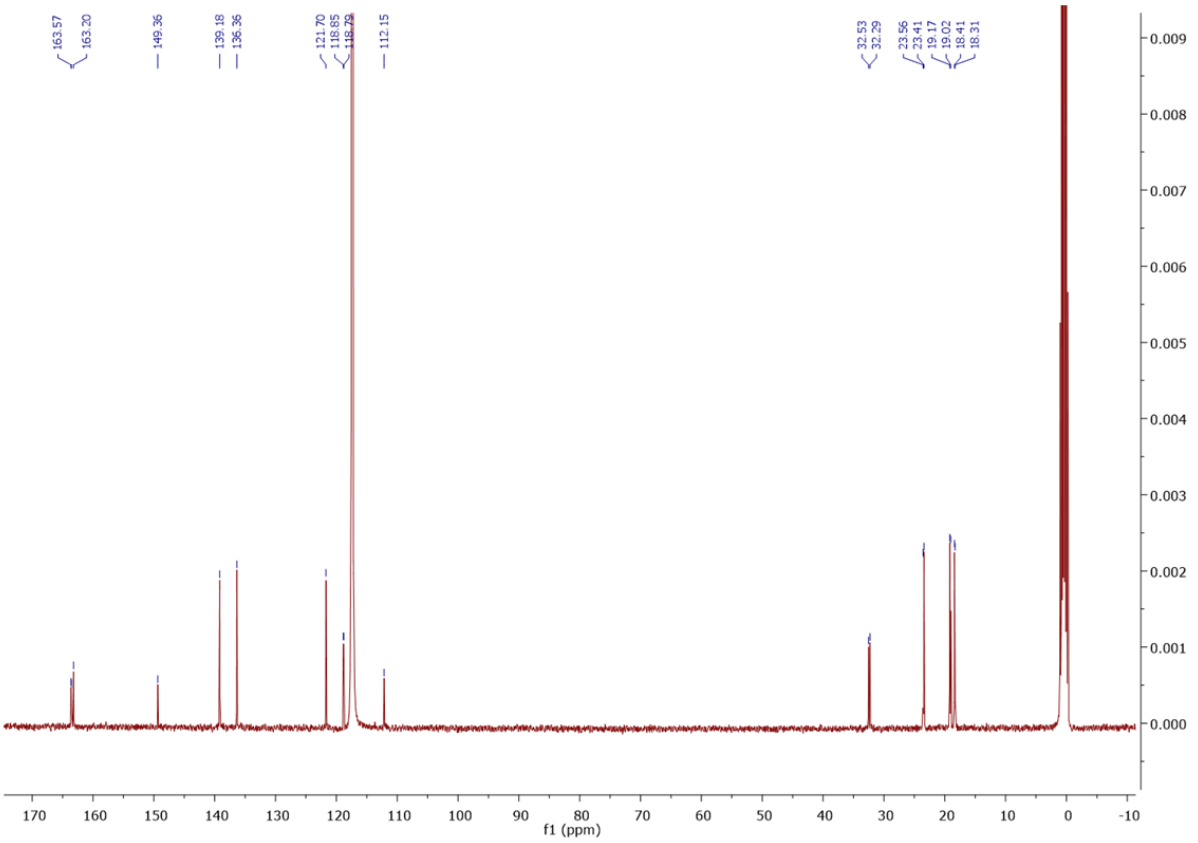


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **L-H** in CD_3CN at 20 °C.

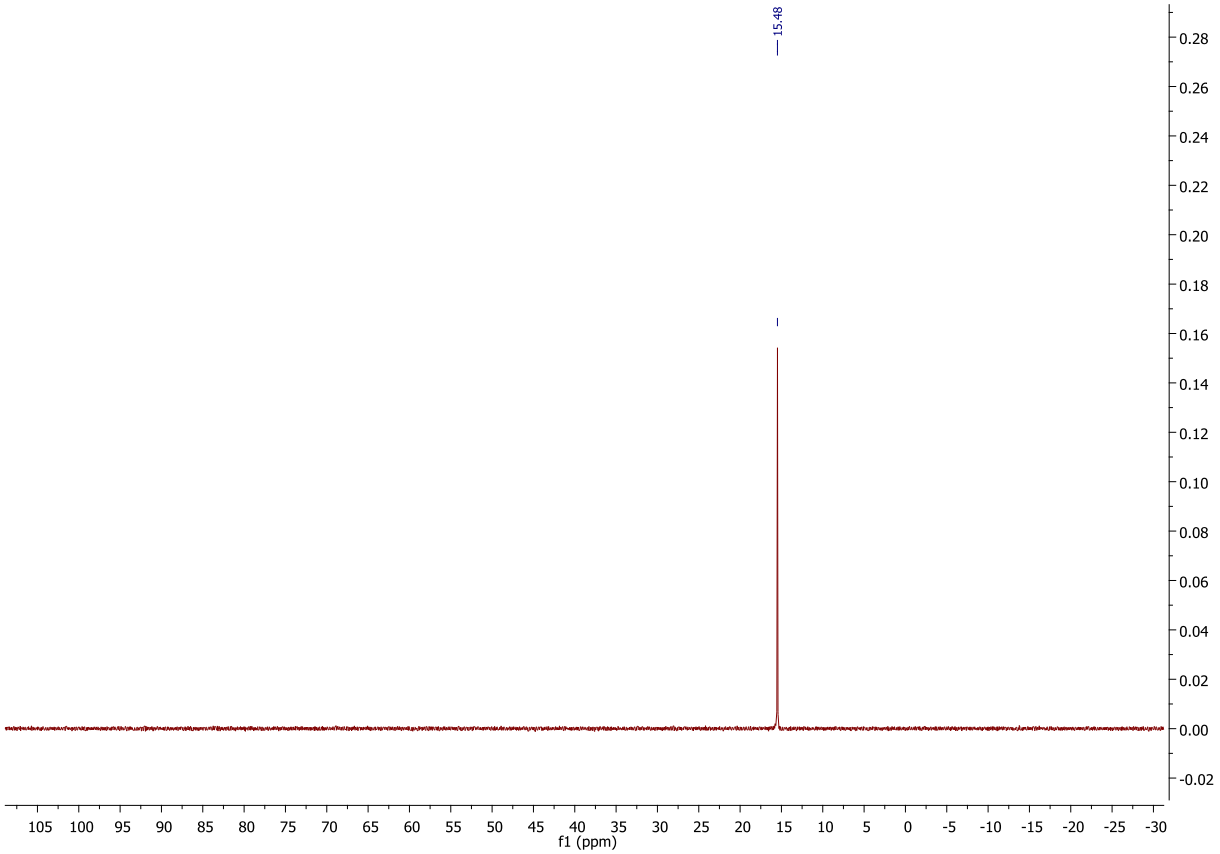


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of **L-H** in CD_3CN at 20 °C.

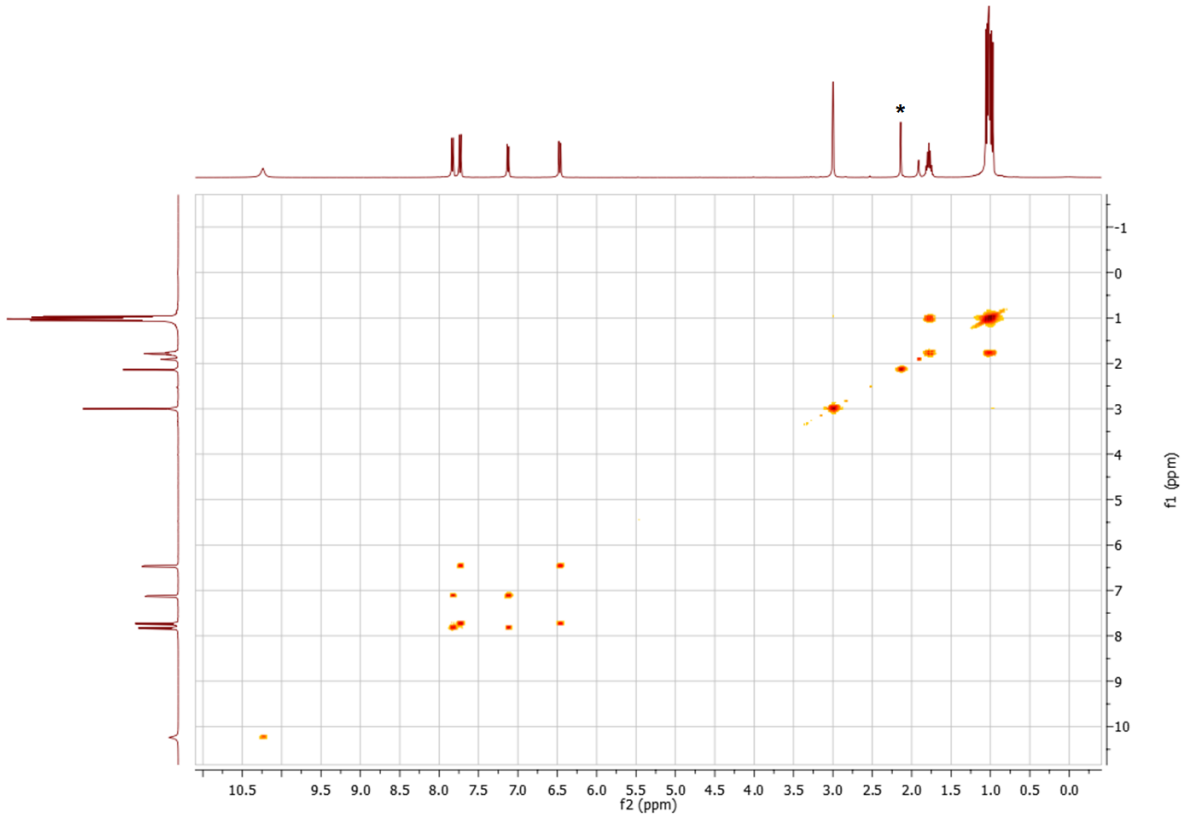


Figure S4. ^{1}H-^{1}H COSY NMR spectrum of **L-H** in CD_3CN at 20 °C. Peak marked with an asterisk is from residual water.

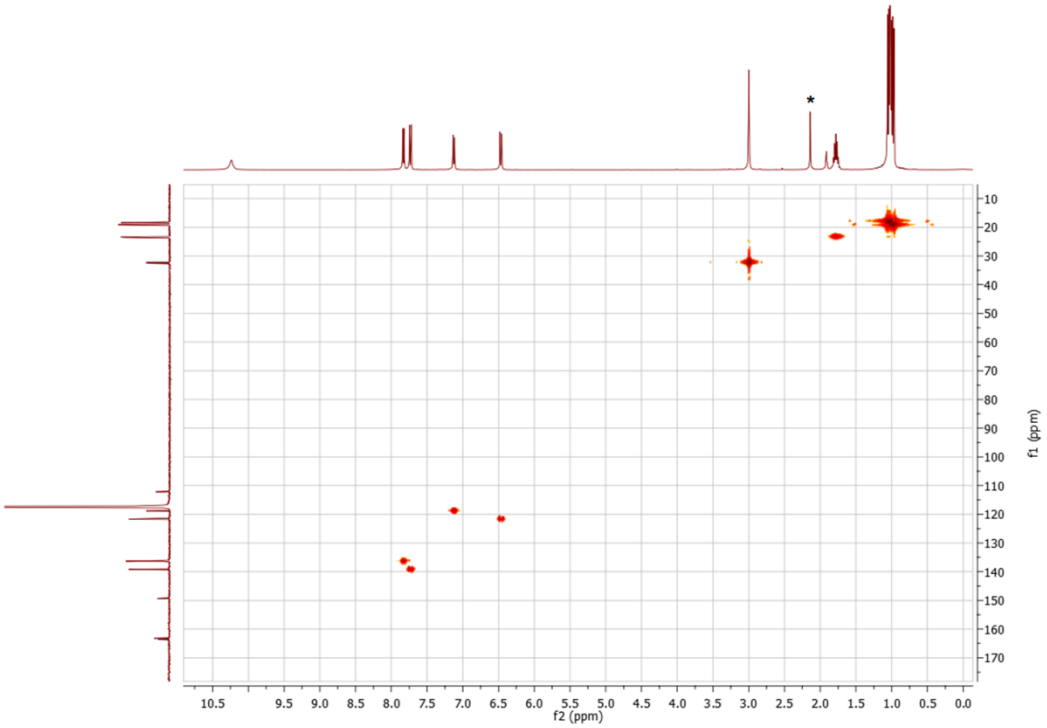


Figure S5. ^{1}H-^{13}C HMQC NMR spectrum of **L-H** in CD_3CN at 20 °C. The peak marked with an asterisk is from residual water.

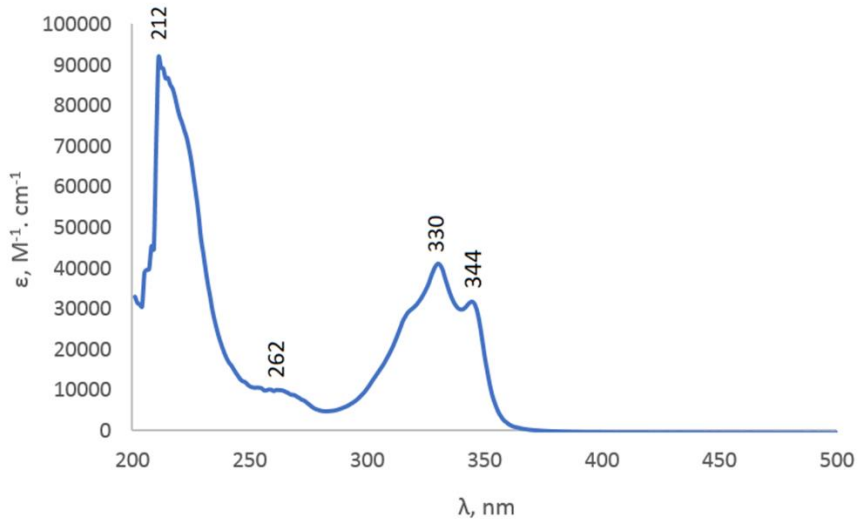


Figure S6. UV-vis absorbance spectrum of **L-H** in CD_3OD (24 µM).

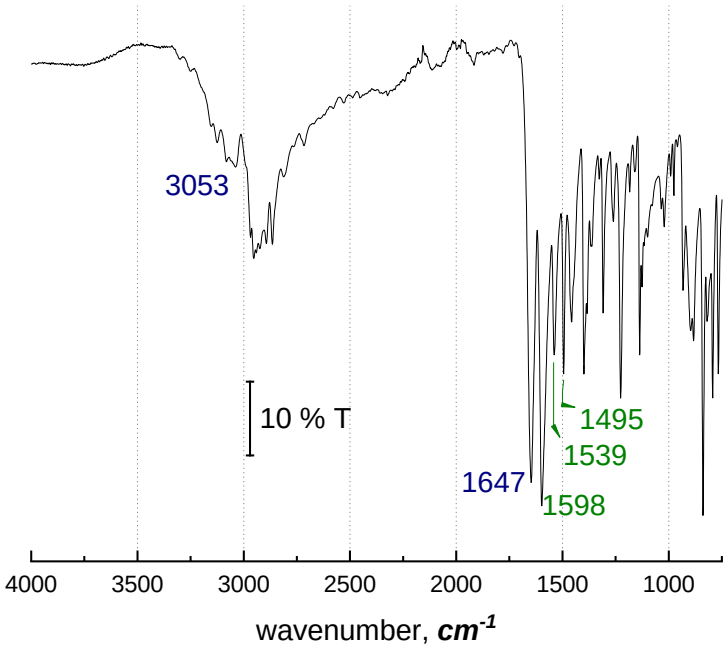


Figure S7. ATR FT-IR spectrum of **L-H** (solid).

[Ru(L-H)Cl$_2$], 1

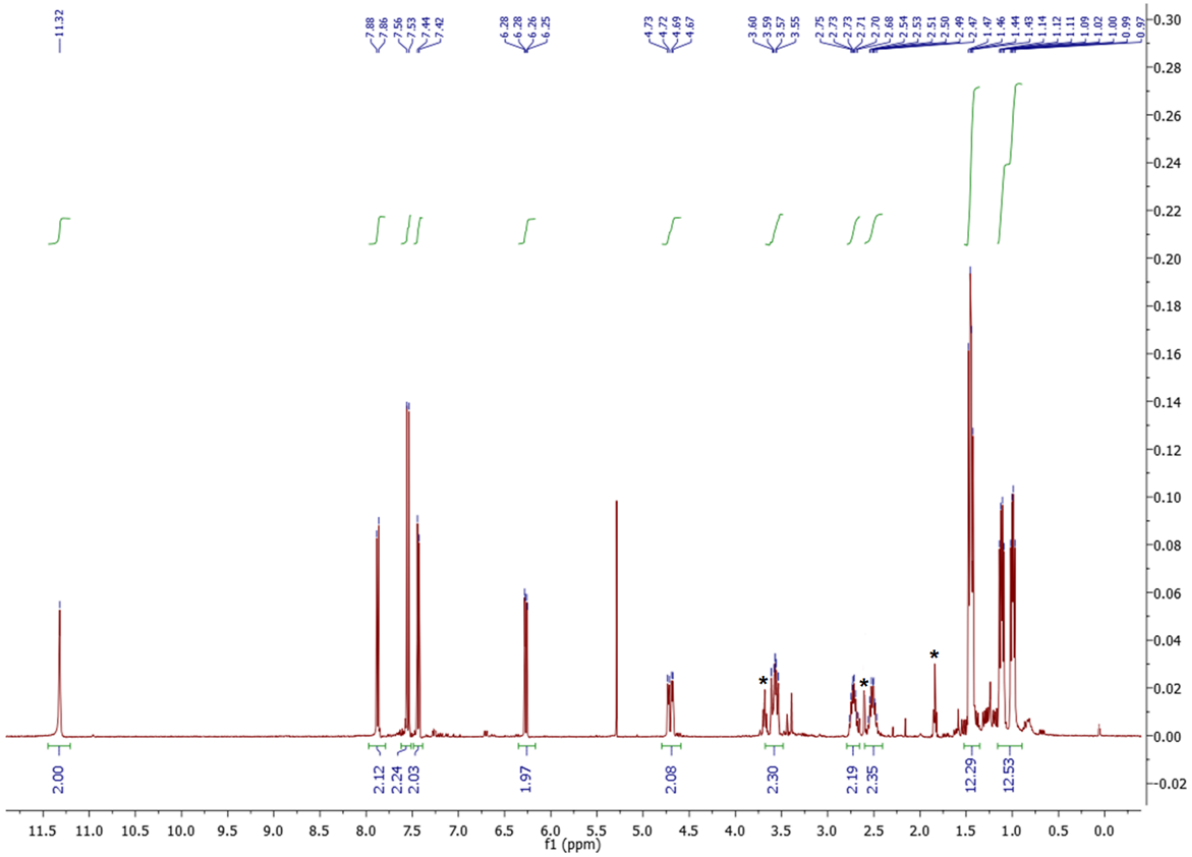


Figure S8. ^{1}H NMR spectrum of **1** in CD_2Cl_2 at 20 °C. Peaks marked with an asterisk are from residual solvent, THF and DMSO.

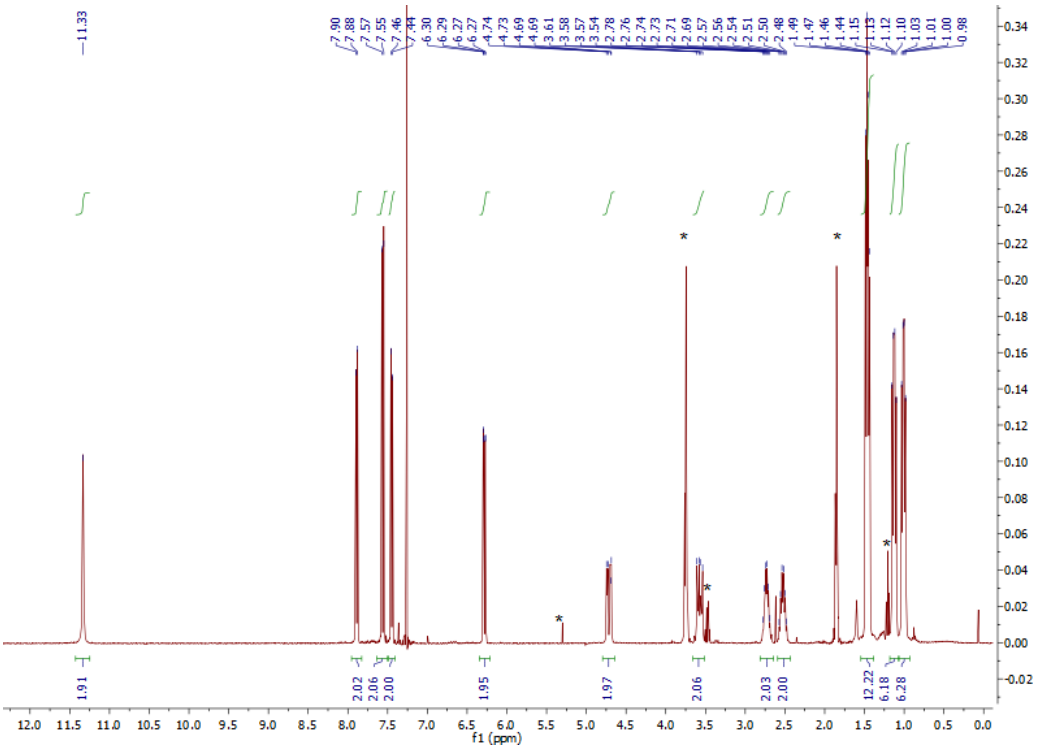


Figure S9. ^{1}H NMR spectrum of **1** in $CDCl_3$ at 20 °C. Peaks marked with an asterisk are from residual solvents (THF, diethyl ether and CH_2Cl_2).

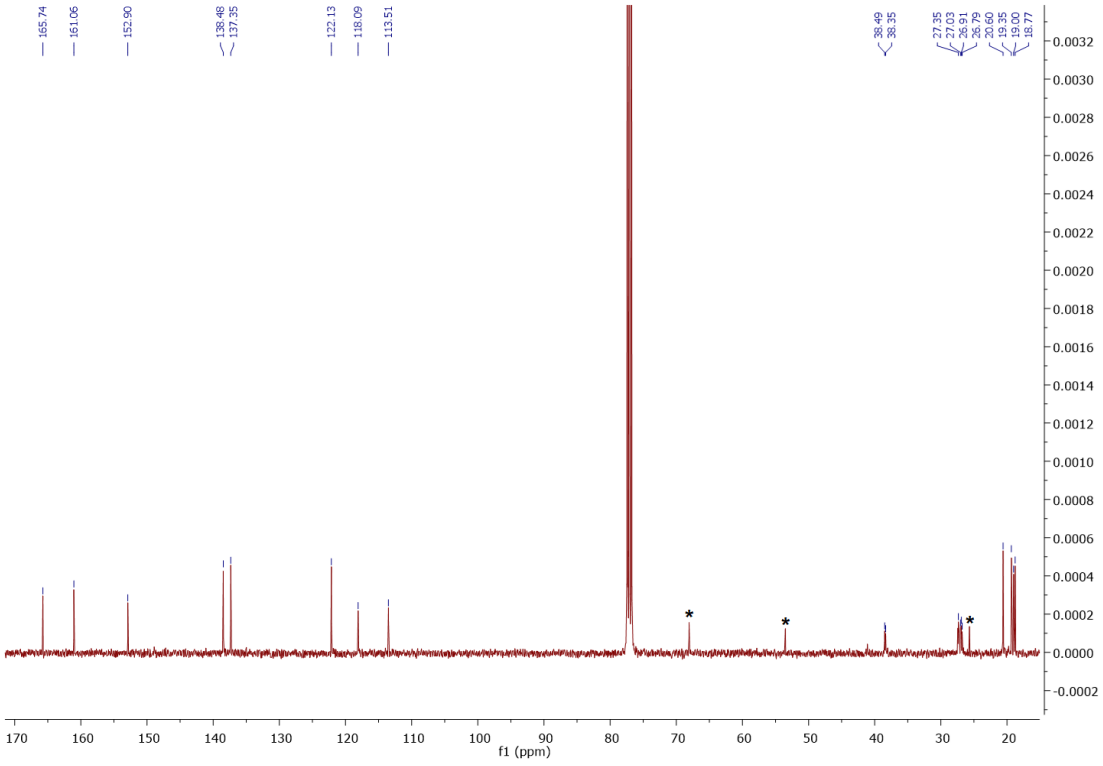


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$ at 20 °C. Peaks marked with an asterisk are from residual solvents (THF and Et_2O).

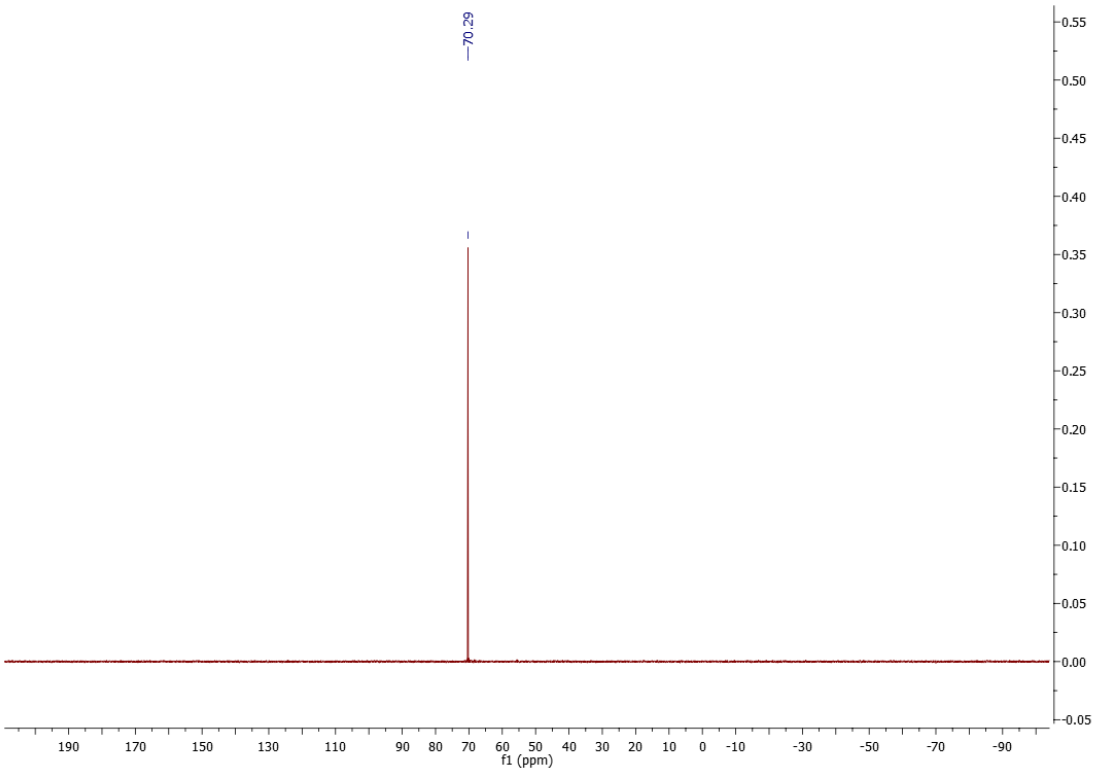


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$ at 20 °C.

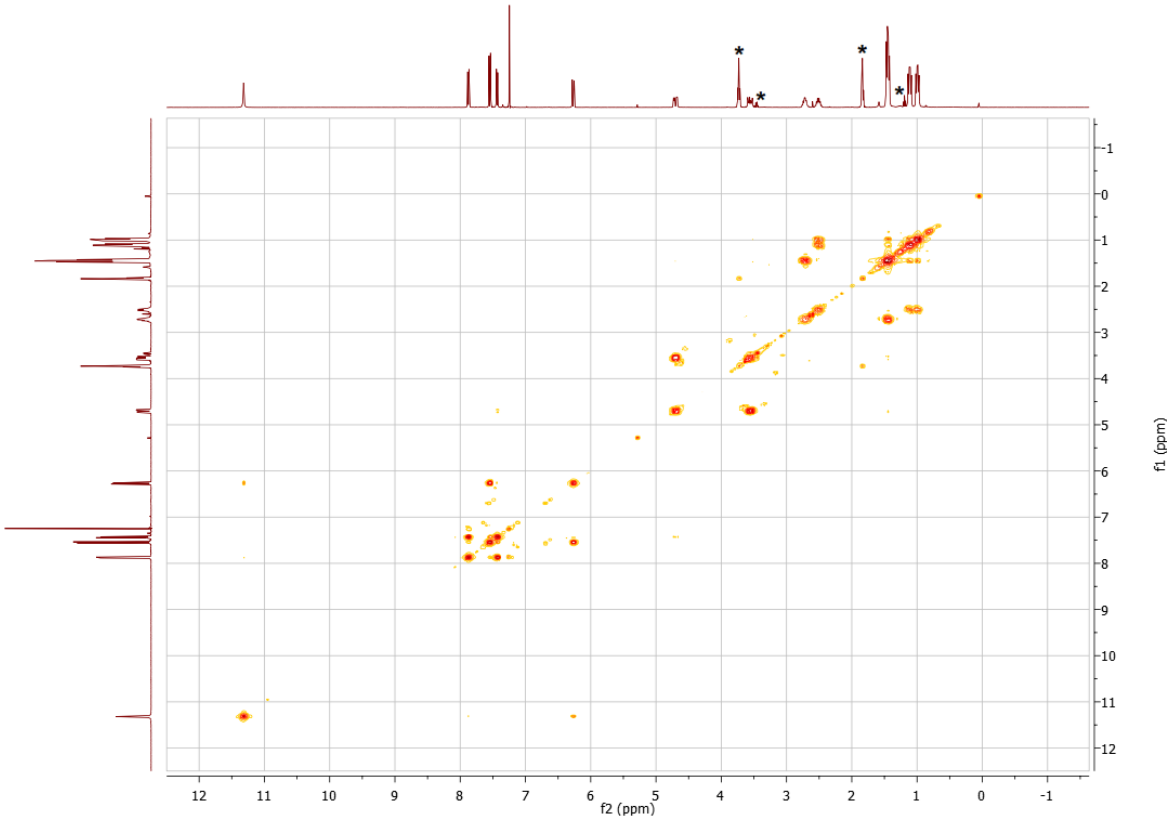


Figure S12. ^{1}H-^{1}H COSY spectrum of **1** in $CDCl_3$ at 20 °C. Peaks marked with an asterisk are from residual solvents (THF and Et_2O).

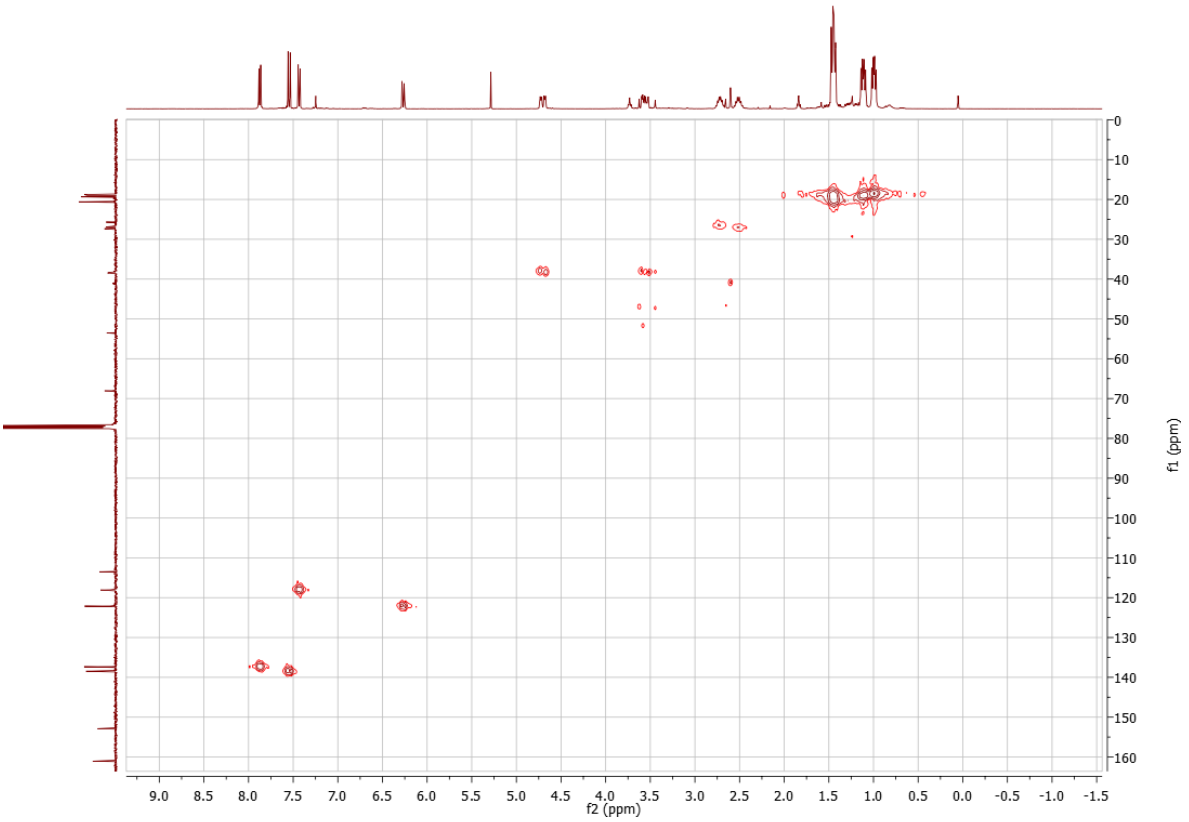


Figure S13. ^{1}H-^{13}C HMQC NMR spectrum of **1** in $CDCl_3$ at 20 °C.

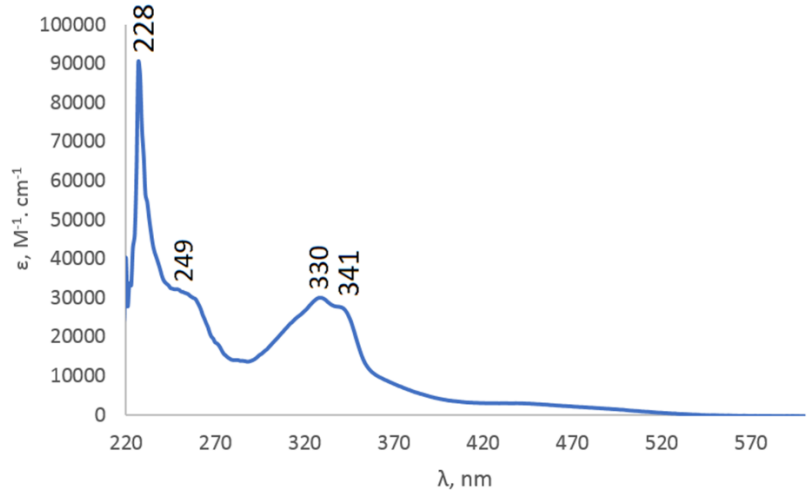


Figure S14. UV-vis absorbance spectrum of complex **1** in MeCN (5 µM).

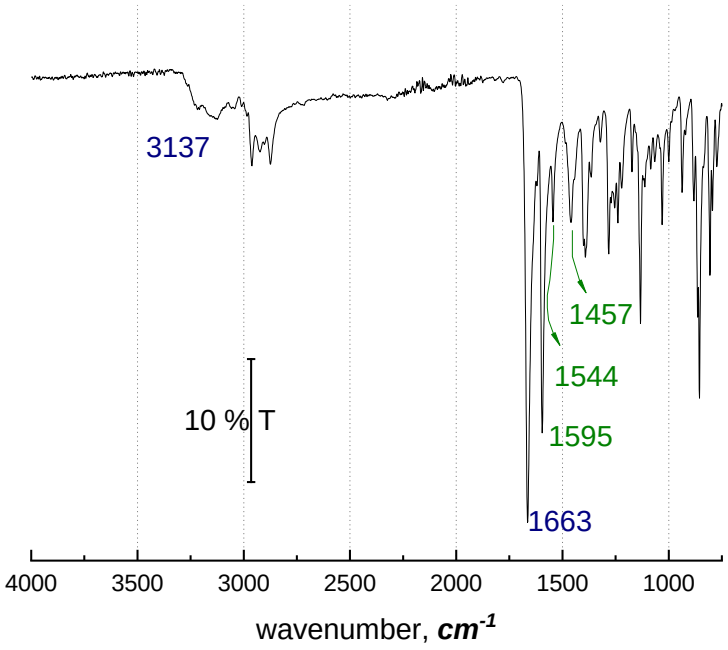


Figure S15. ATR FT-IR spectrum of **1** (solid).

$[Ru_2(L)_2(L\text{-}H)_2]$, 2

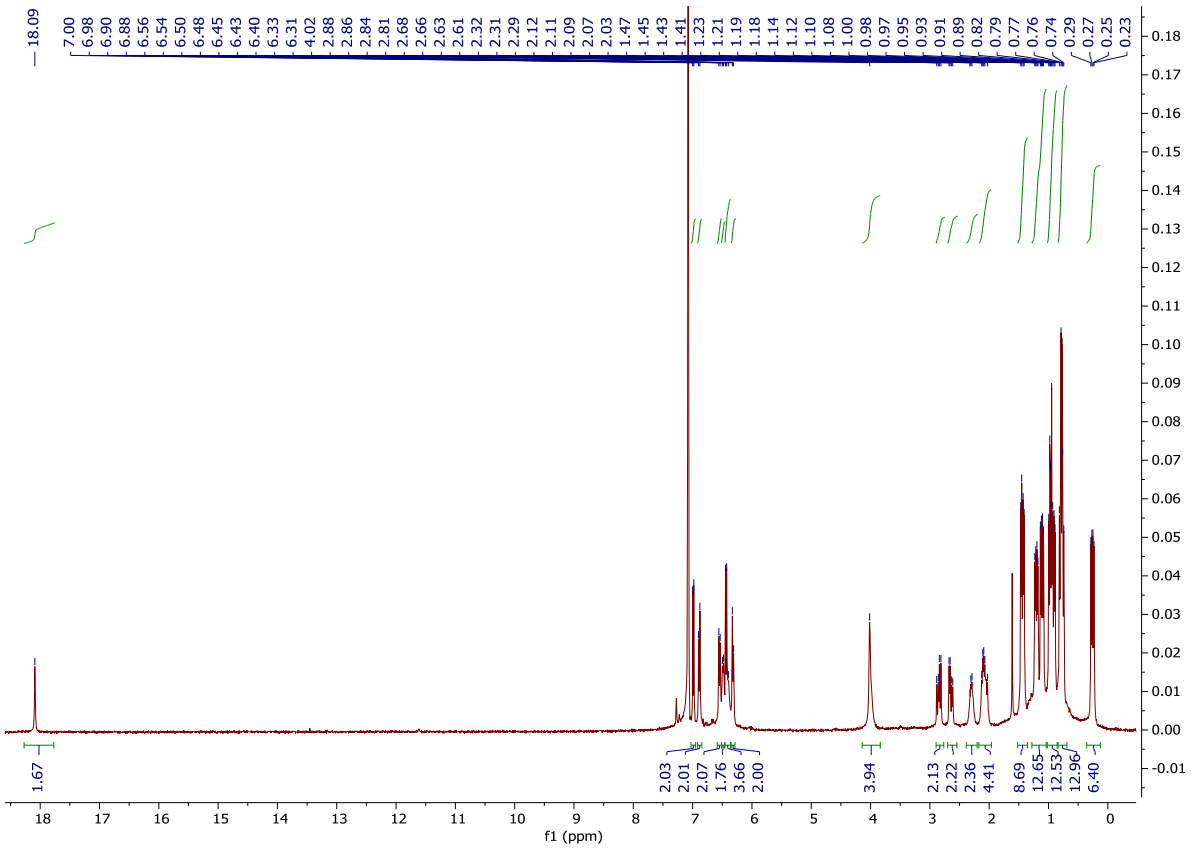


Figure S16. ^{1}H NMR spectrum of **2** in C_6D_6 at 20 °C. The peak marked with an asterisk is from residual DMSO.

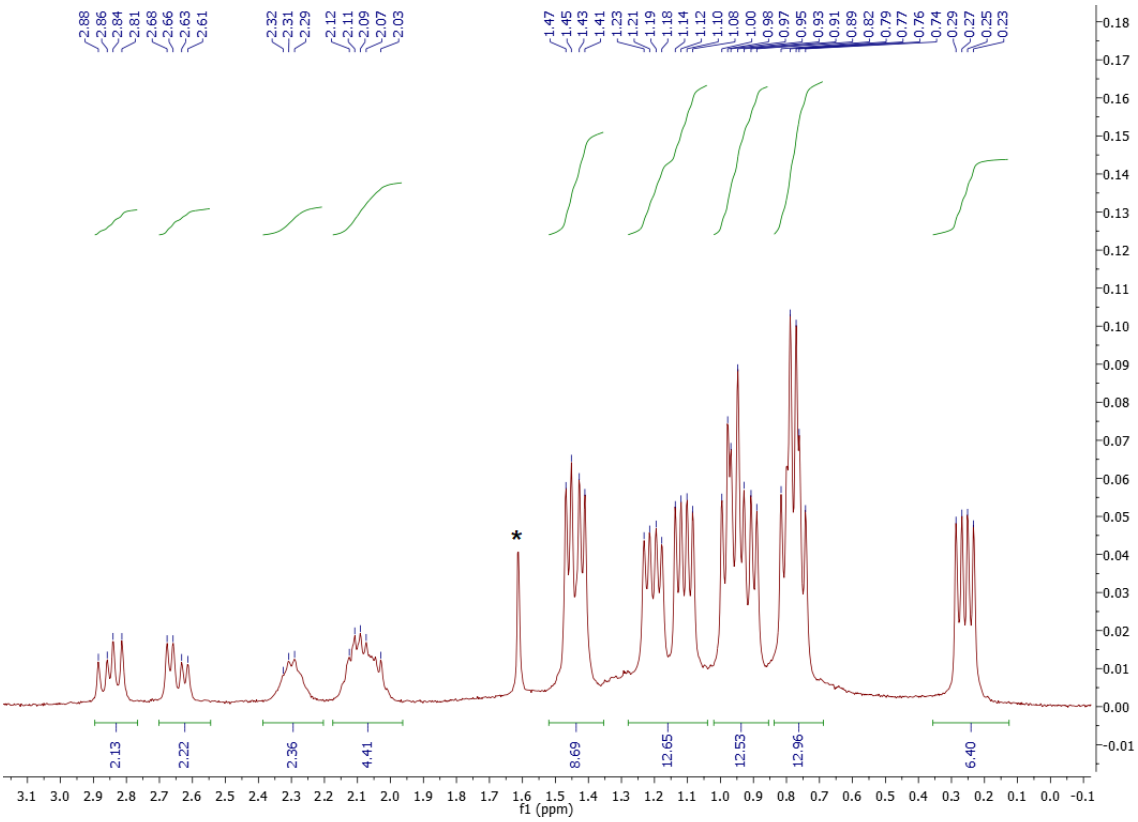


Figure S17. Expanded ^{1}H NMR spectrum of **2** in C_6D_6 at 20 °C (0.0 – 3.1 ppm). The peak marked with an asterisk is from residual DMSO.

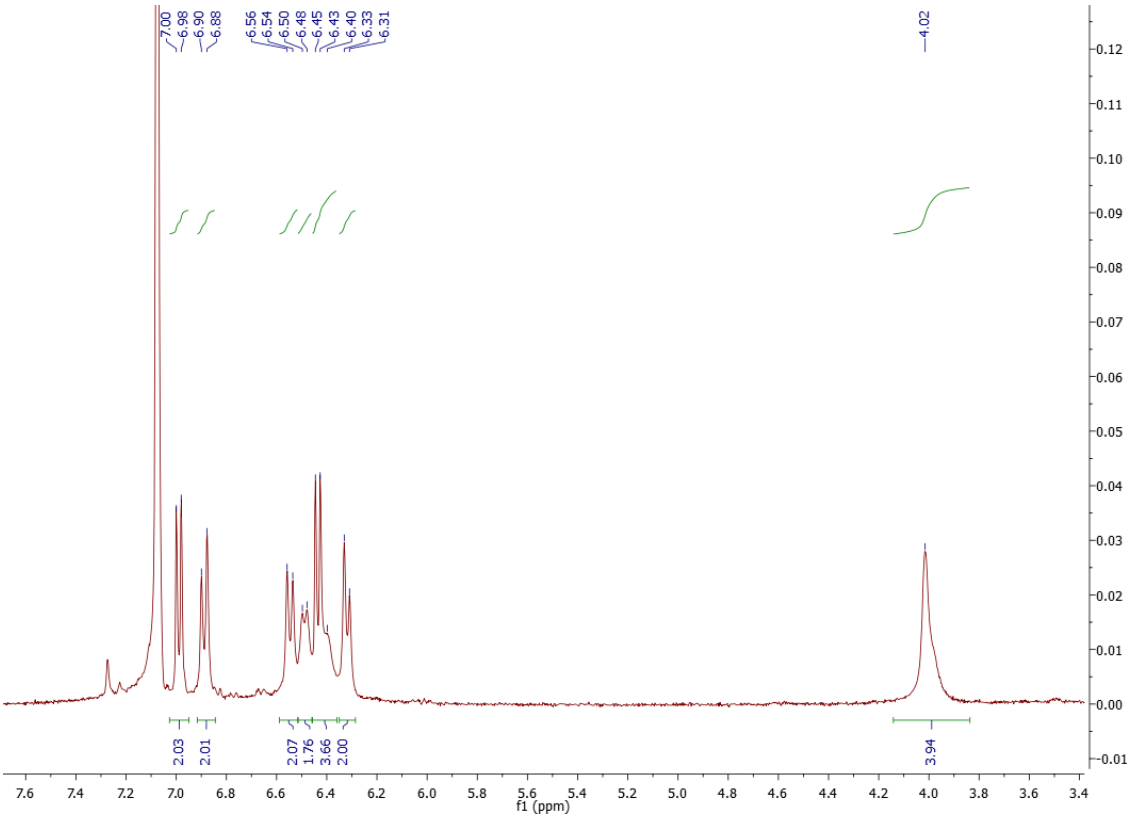


Figure S18. Expanded ^{1}H NMR spectrum of **2** in C_6D_6 at 20 °C (3.4 – 7.6 ppm).

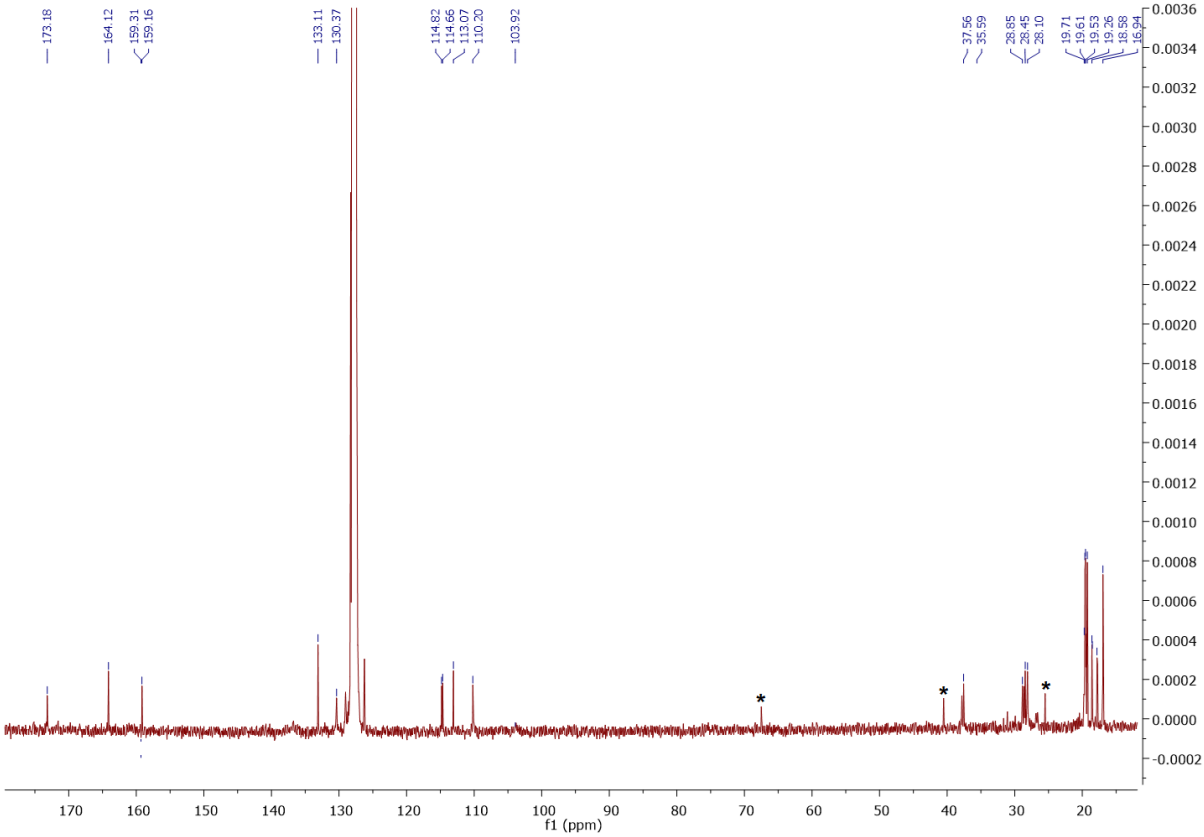


Figure S19. $^{13}C\{^{1}H\}$ spectrum of **2** in CD_3CN at 20 °C. Peaks marked with an asterisk are from residual DMSO and THF. Some aromatic peaks could not be detected due to overlap with the solvent signal.

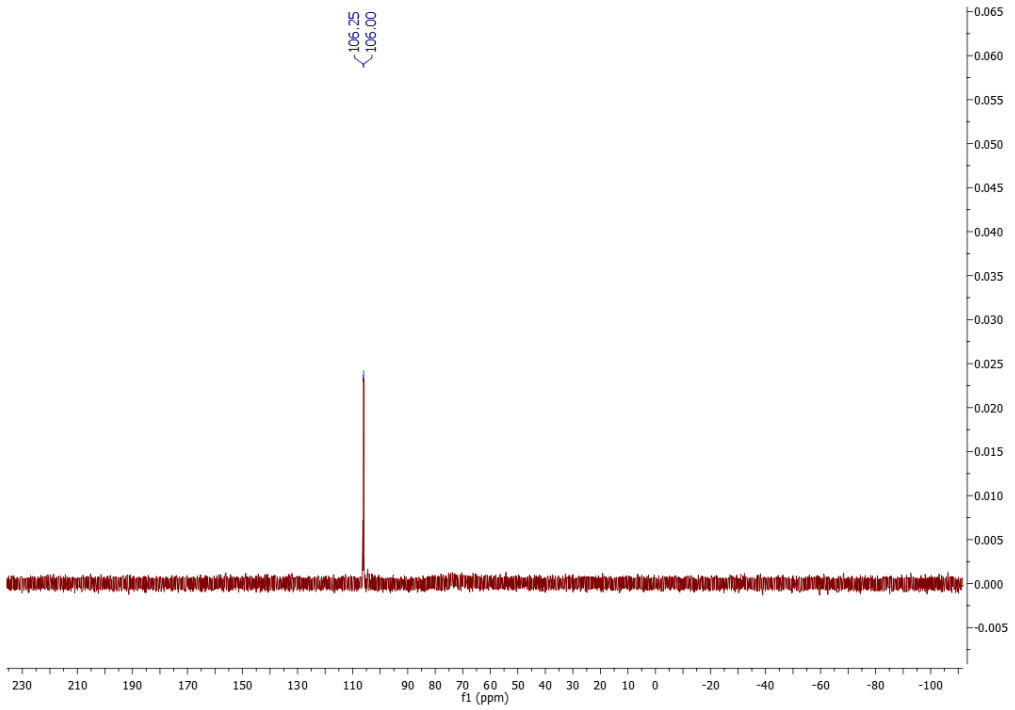


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in CD_3CN at 20 °C.

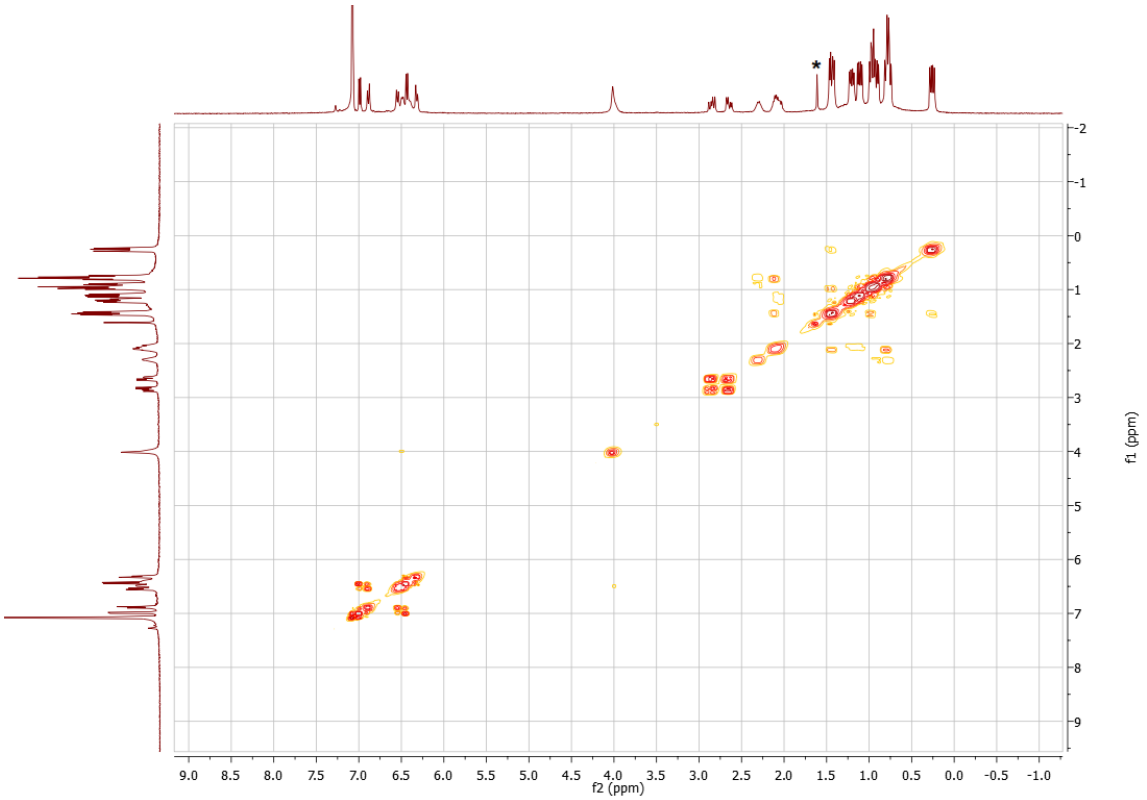


Figure S21. ^{1}H-^{1}H COSY NMR spectrum of **2** in C_6D_6 at 20 °C. Peak marked with an asterisk is from residual DMSO.

Figure S22. ^{1}H-^{13}C HMQC NMR spectrum of **2** in C_6D_6 at 20 °C. The peak marked with an asterisk is from residual DMSO.

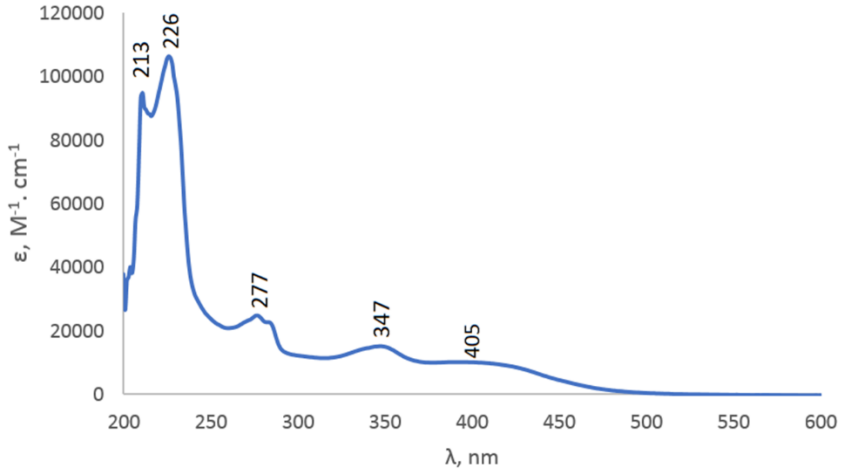


Figure S23. UV-vis absorbance spectrum of complex **2** in C_6D_6 (5 µM).

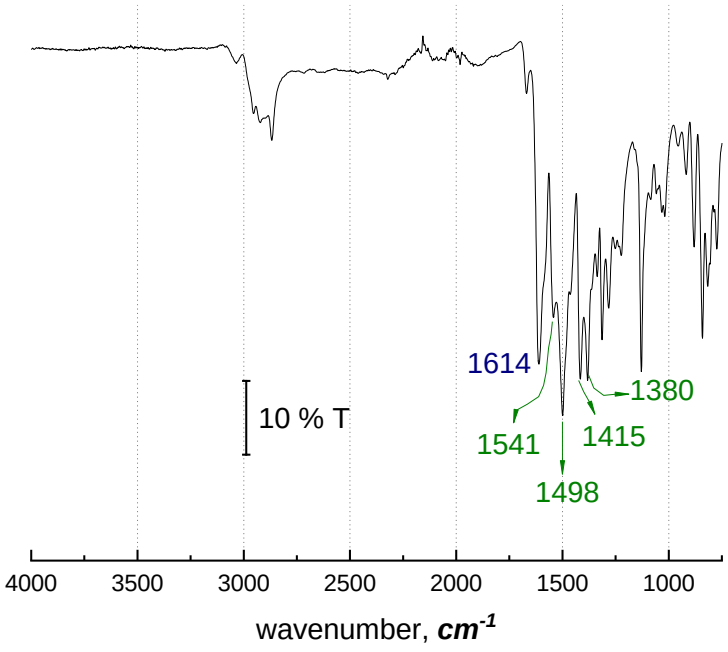


Figure S24. ATR FT-IR spectrum of **2** (solid).

$[Ru(L)_2(H_2O)_2]$, 3

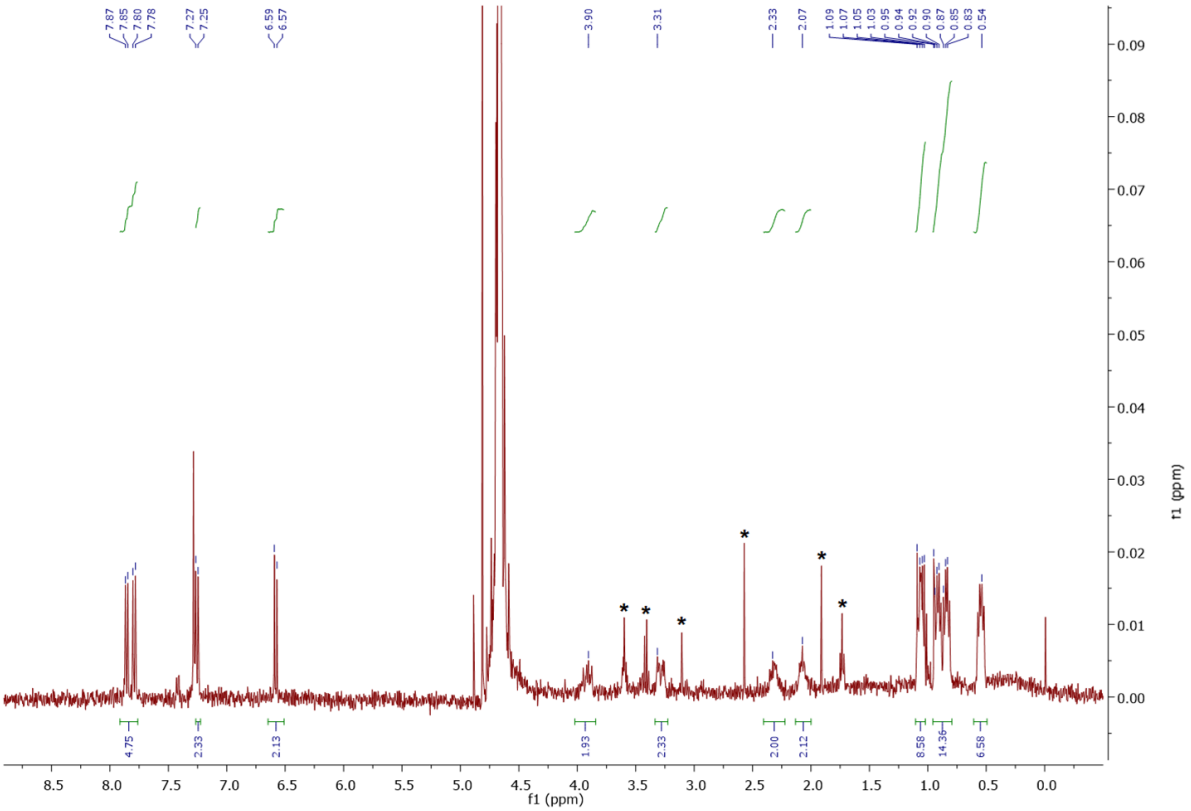


Figure S25. ^{1}H NMR spectrum of **3** in D_2O at 20 °C. Peaks marked with an asterisk are from THF and an unidentified impurity.

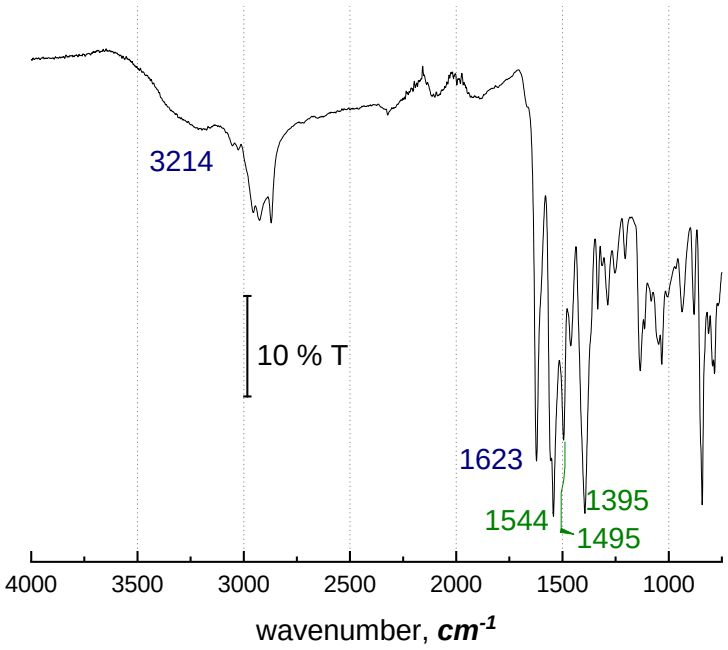


Figure S26. ATR FT-IR spectrum of **3** (solid).

[Ru(L)$_2$(MeOH)$_2$], 4

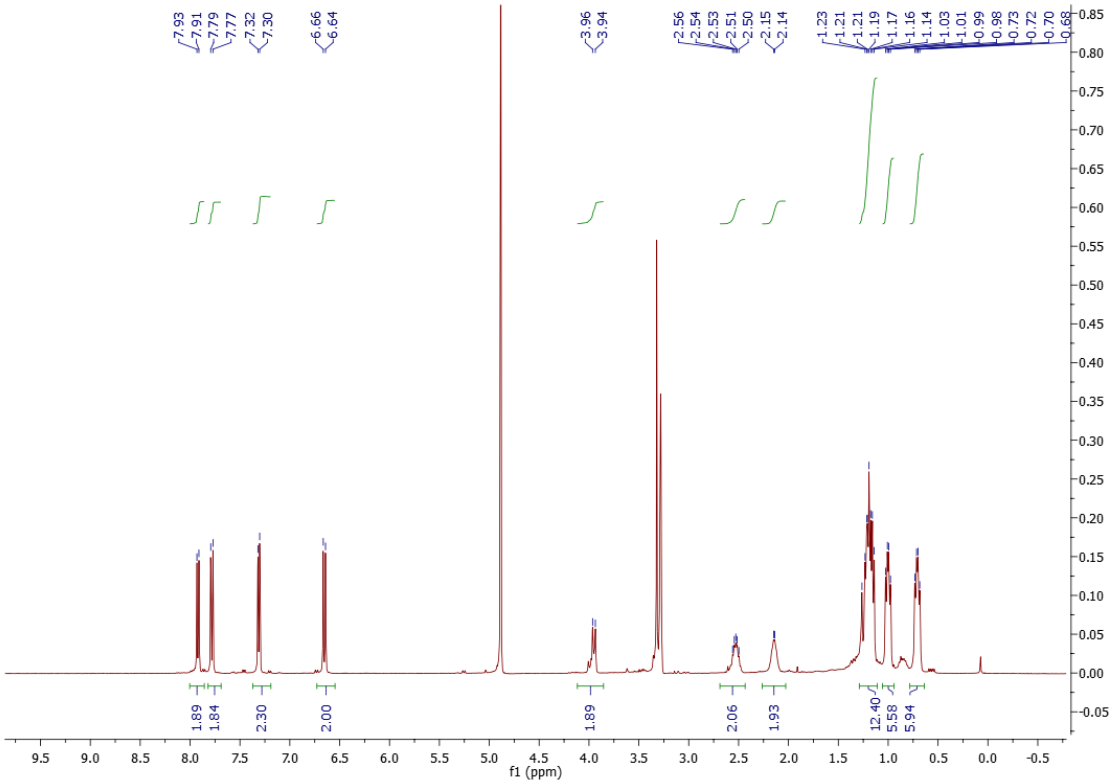


Figure S27. ^{1}H NMR spectrum of **4** in CD_3OD at 20 °C.

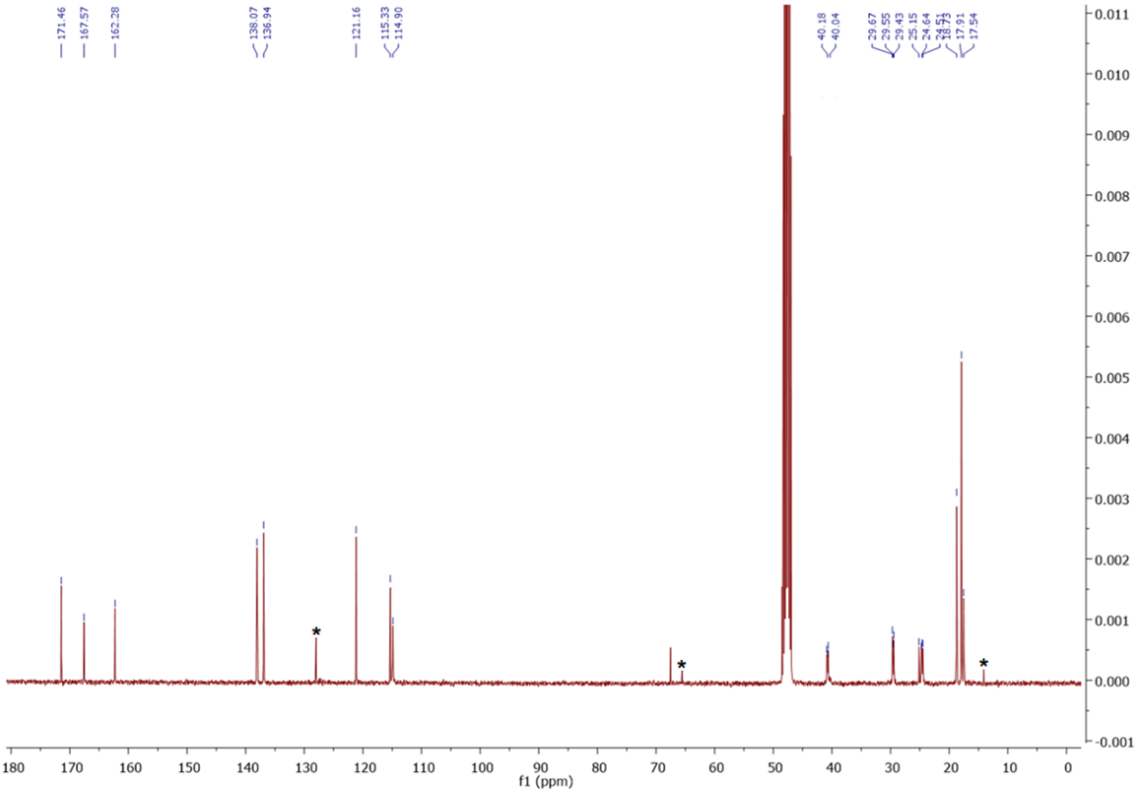


Figure S28. $^{13}C\{^{1}H\}$ spectrum of **4** in CD_3CN at 20 °C. Peaks marked with an asterisk are from residual solvents.

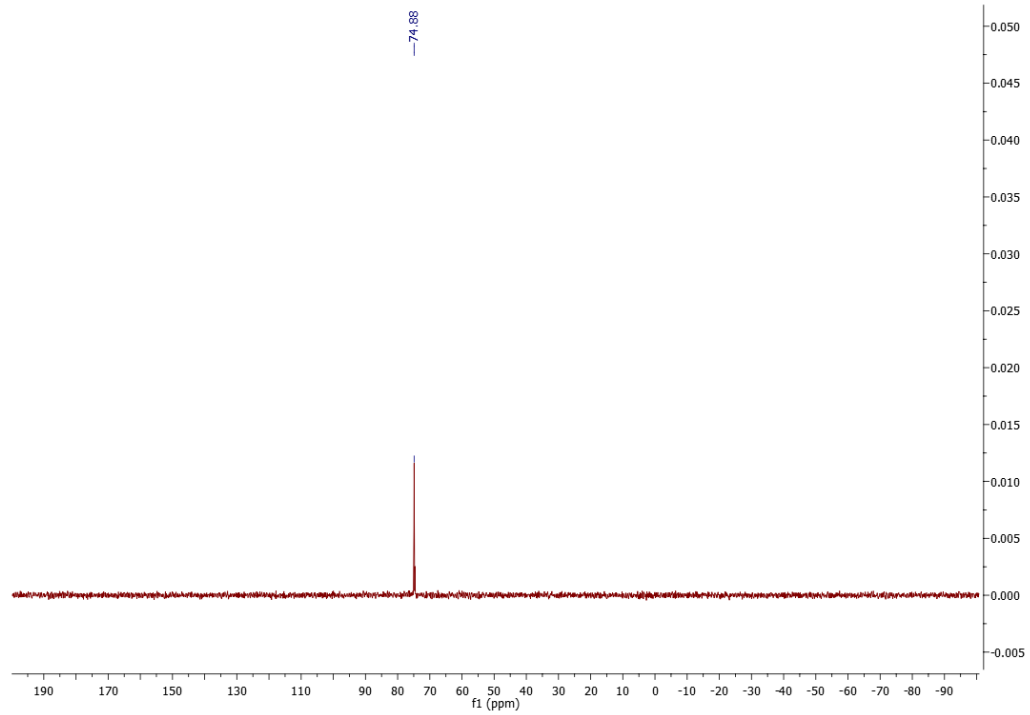


Figure S29. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in CD_3CN at 20 °C.

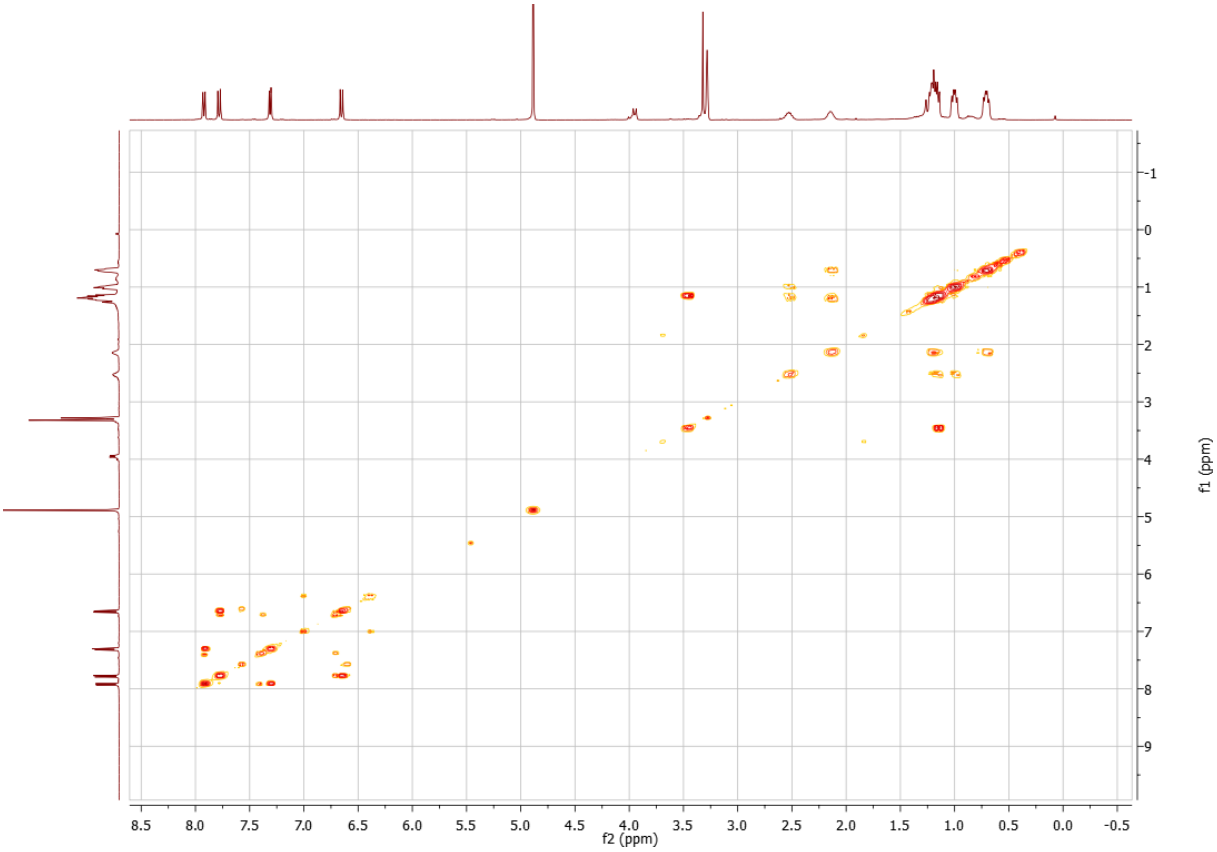


Figure S30. ^{1}H-^{1}H COSY NMR spectrum of **4** in CD_3OD at 20 °C.

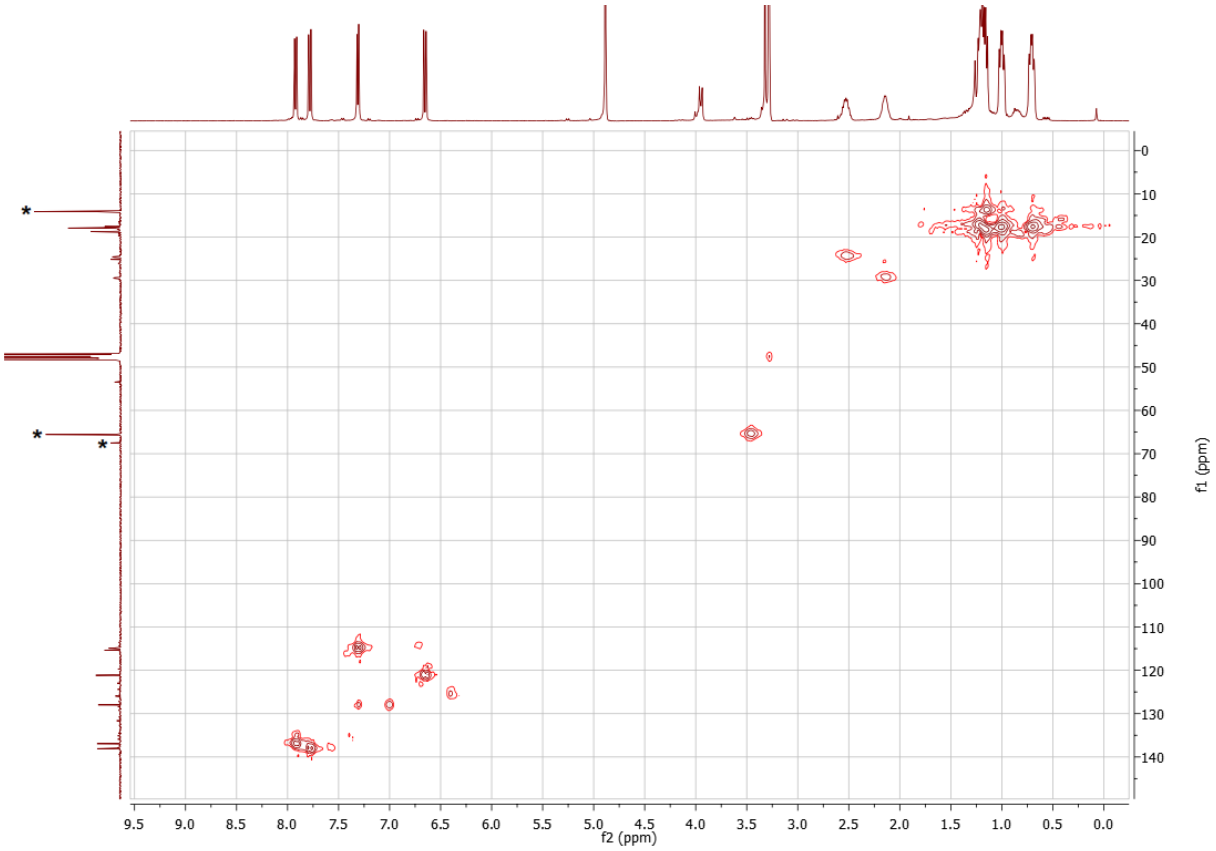


Figure S31. ^{1}H-^{13}C HMQC NMR spectrum of **4** in CD_3OD at 20 °C. Peaks marked with an asterisk are from residual THF and Et_2O.

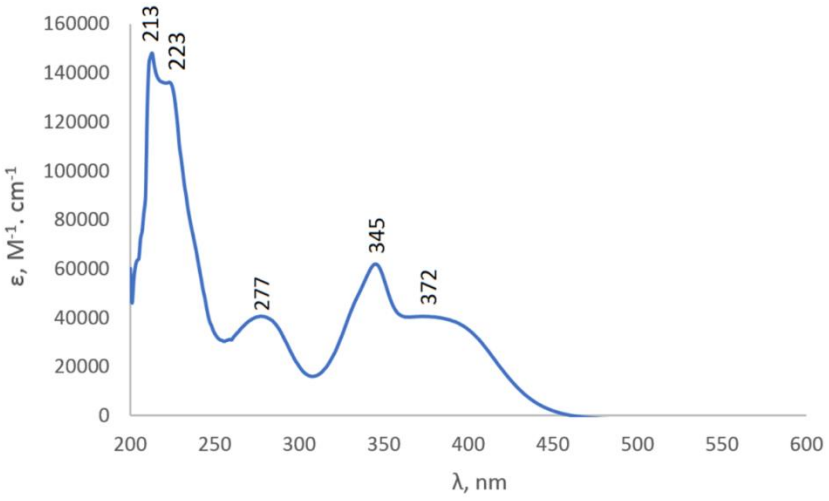


Figure S32. UV-vis absorbance spectrum of **4** in methanol (24 µM).

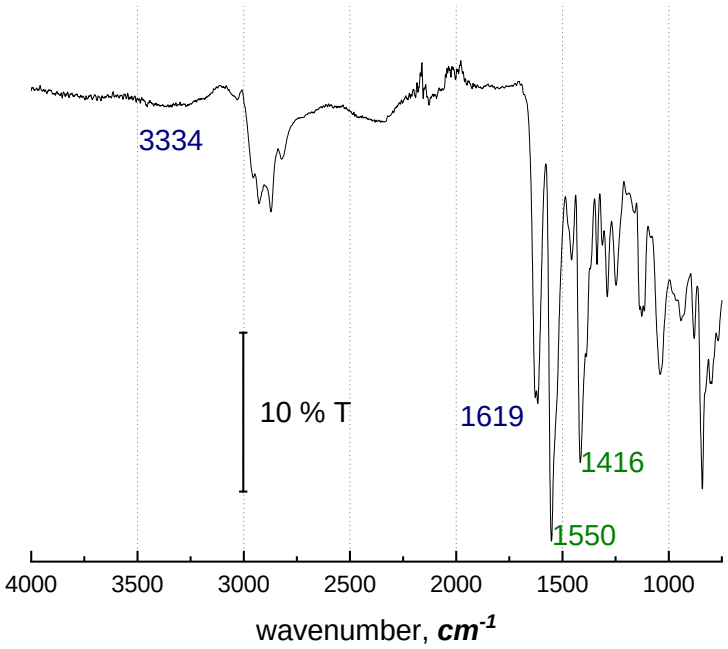


Figure S33. ATR FT-IR spectrum of **4** (solid).

II. Reactivity with alcohols.

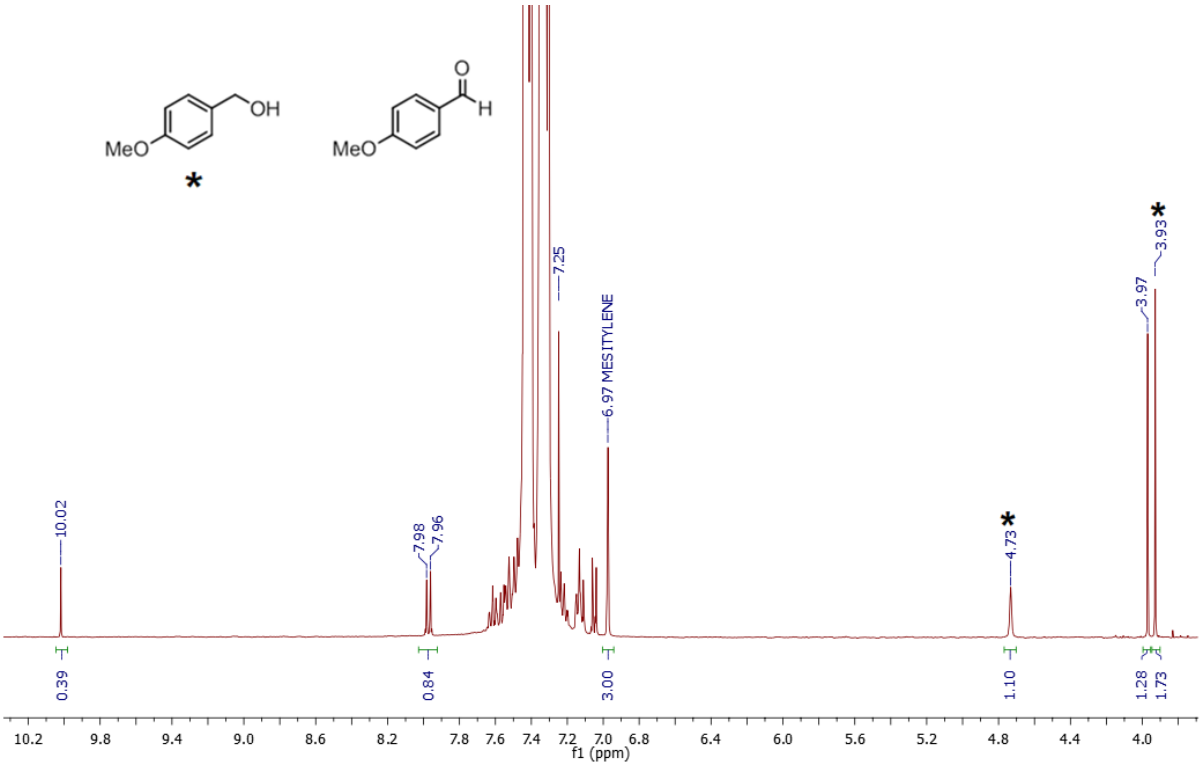


Figure S34. ^{1}H NMR spectrum of the reaction mixture of 3 mL of toluene, 0.22 mmol *para*-anisyl alcohol, 0.22 mmol mesitylene, and 5 mol% of **3**; open system under inert atmosphere, after 16 h at 160 °C ($CDCl_3$, 20 °C, 400 MHz). MeO peaks integration was used to determine yield and conversion.

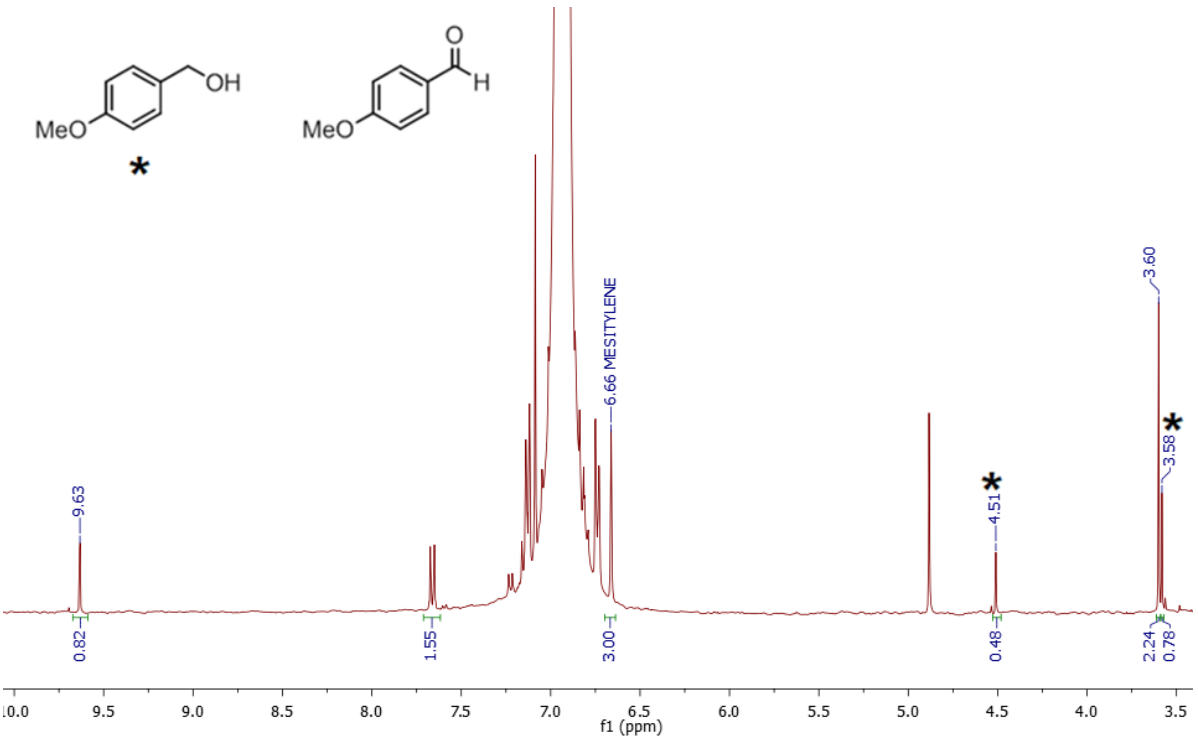


Figure S35. ^{1}H NMR spectrum of the reaction mixture in Scheme 5, 24 h (CD_3OD, 20 °C, 400 MHz). MeO peaks integration was used to determine yield and conversion.

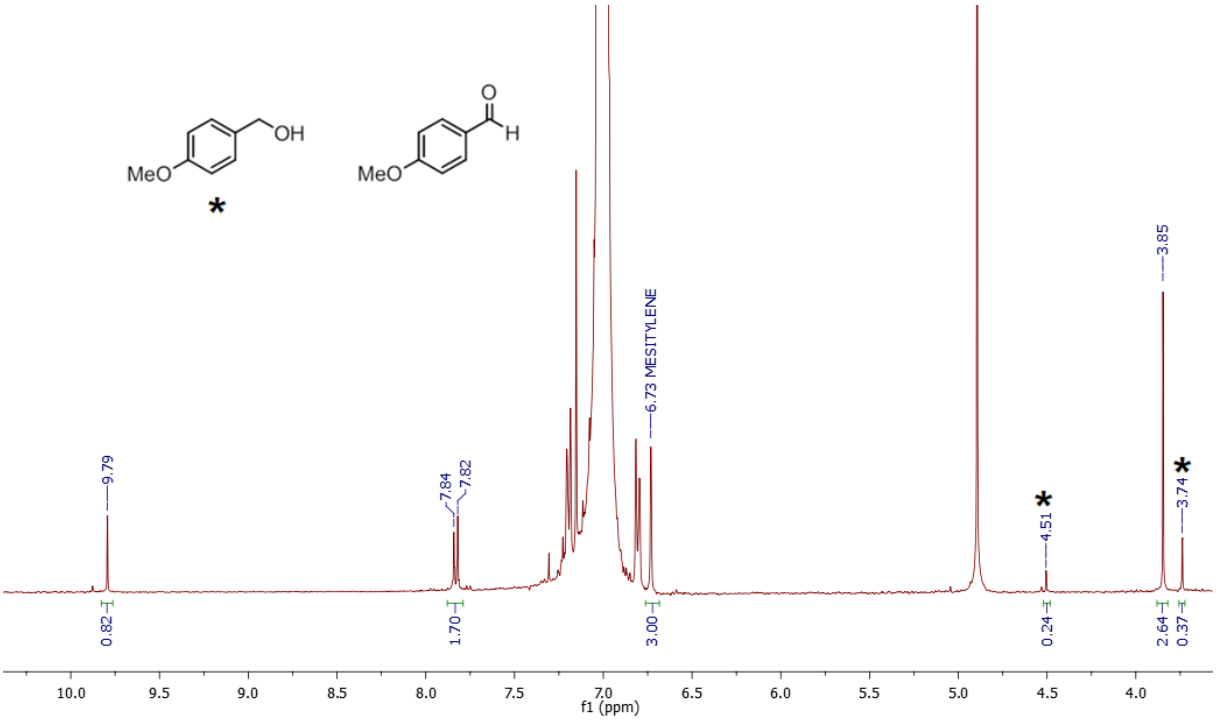


Figure S36. ^{1}H NMR spectrum of the reaction mixture in Scheme 5, 72 h (CD_3OD, 20 °C, 400 MHz). MeO peaks integration was used to determine yield and conversion.

Reaction with D_2O

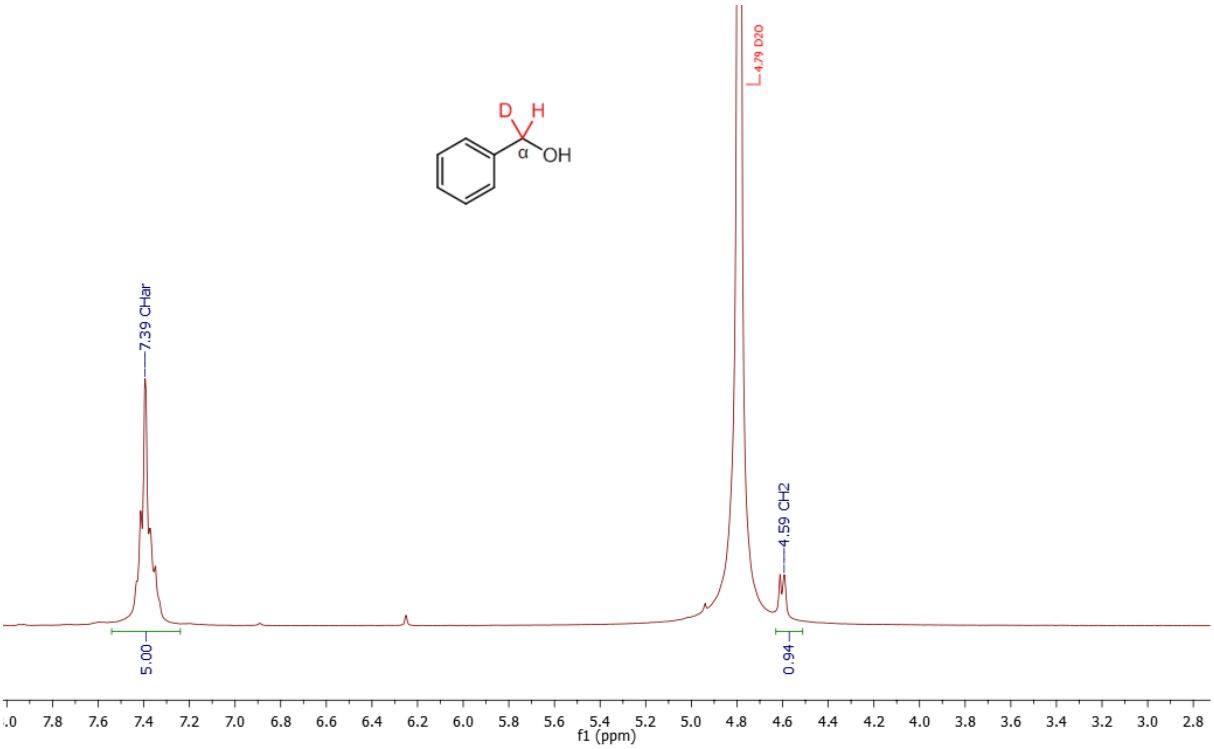


Figure S37. ^{1}H NMR spectrum of H/D scrambling reaction mixture with *para*-anisyl alcohol in Scheme 6 (D_2O, 20 °C, 400 MHz).

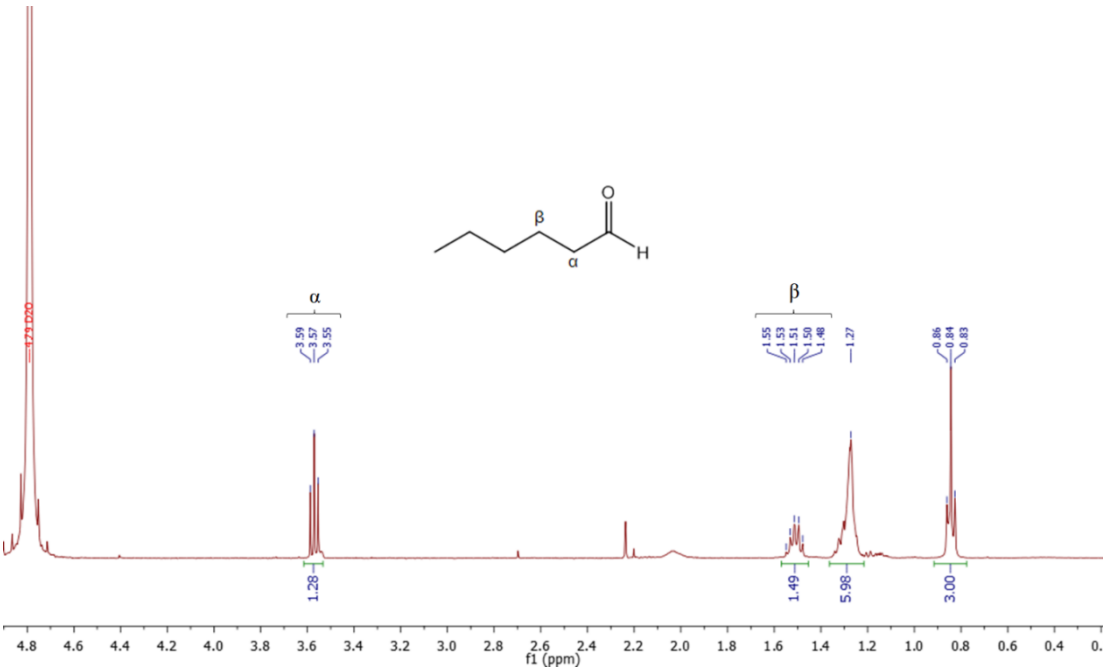


Figure S38. ^{1}H NMR spectrum of H/D scrambling reaction mixture with 1-hexanol in Scheme 6 (D_2O, 20 °C, 400 MHz).

III. Computational details

DFT calculation was carried out using Gaussian 09 rev. E.01[1] at B3LYP[2-4] level of theory. LANL2DZ[5] and valence-basis sets was used at Ru. For other atoms, 6–31+G (d, p)[6-8] was employed. The structures reported are either minima (NIMAG=0) or transition states (NIMAG=1) on the potential energy surface. Important bond parameters for the intermediates and the transition states are provided below. Cartesian coordinates and corresponding Gibbs energies for all intermediates and transition states are given below.

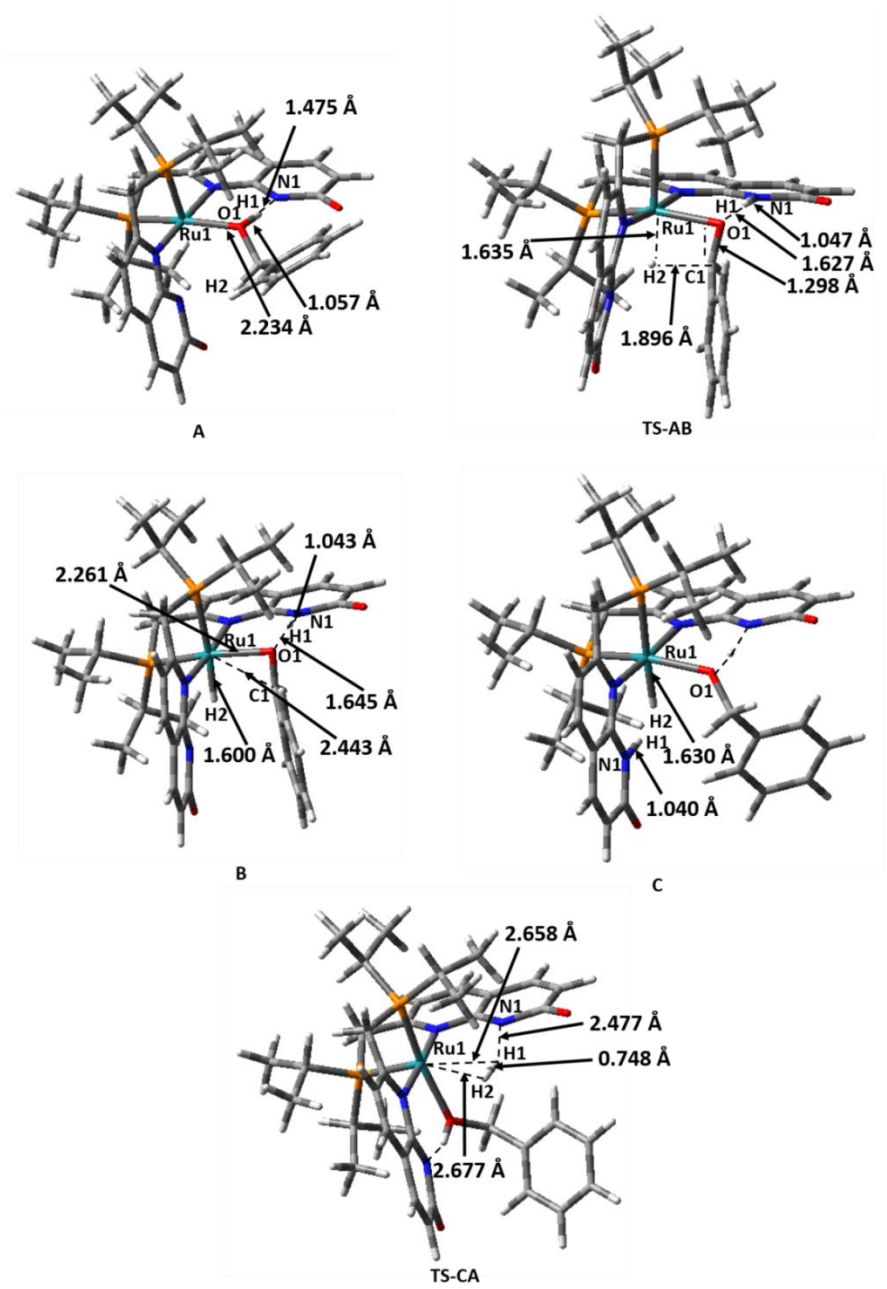


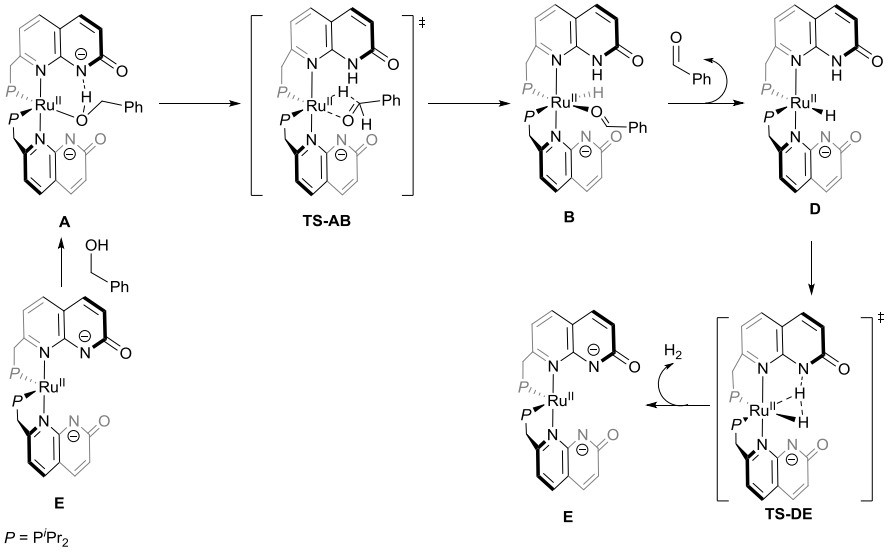
Figure S39. Geometry-optimized intermediates and transition states for alcohol dehydrogenation and important bond lengths for the mechanism presented in Scheme 7 (in angstrom).

The following alternative mechanisms were considered, in addition to the mechanism shown in Scheme 7.

Path B. Hydrogen elimination via five-coordinate intermediate **D**.

In this pathway, we considered β-hydride elimination to follow the same pathway as in the mechanism shown in Scheme 7. The, upon the formation of intermediate **B**, aldehyde dissociation leads to the formation of a five-coordinate hydride complex **D**, which then eliminates H_2 via protonation by the NH group of a protonated ligand, leading to the formation of a coordinately-unsaturated intermediate **E**, which then coordinates another molecule of benzyl alcohol to re-form **A**. Formally coordinatively unsaturated intermediate **E** shows weak interactions (2.475 Å) with two terminal N-atom of napthyridinones (adjacent to O).

Although the barrier for such mechanism is feasible and the rate-limiting step does not change, formation of **E** is unlikely as such complex is likely to dimerize to form a stable binuclear complex **2**. Experimental observations also indicate that complex **2** reacts with excess protic solvents (see manuscript) leading to solvent coordination. From compound **E**, the total barrier for β-hydride elimination is 31.41 kcal mol^{-1}. However mechanism **2** cannot be completely excluded at this stage.



Scheme S1. Schematic representation of path B.

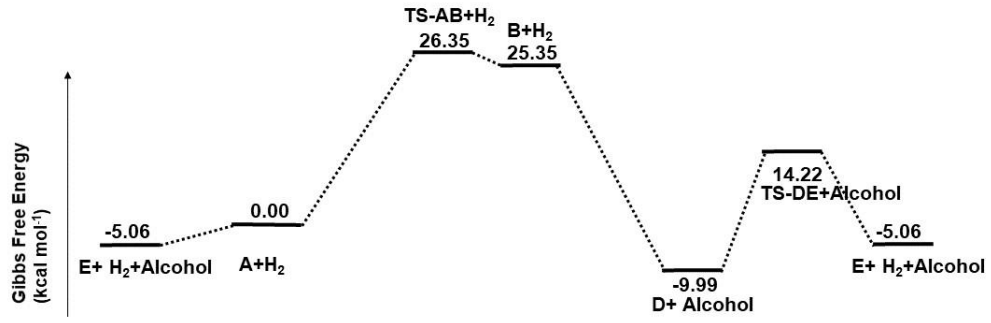


Figure S40. Calculated energy profile for path B.

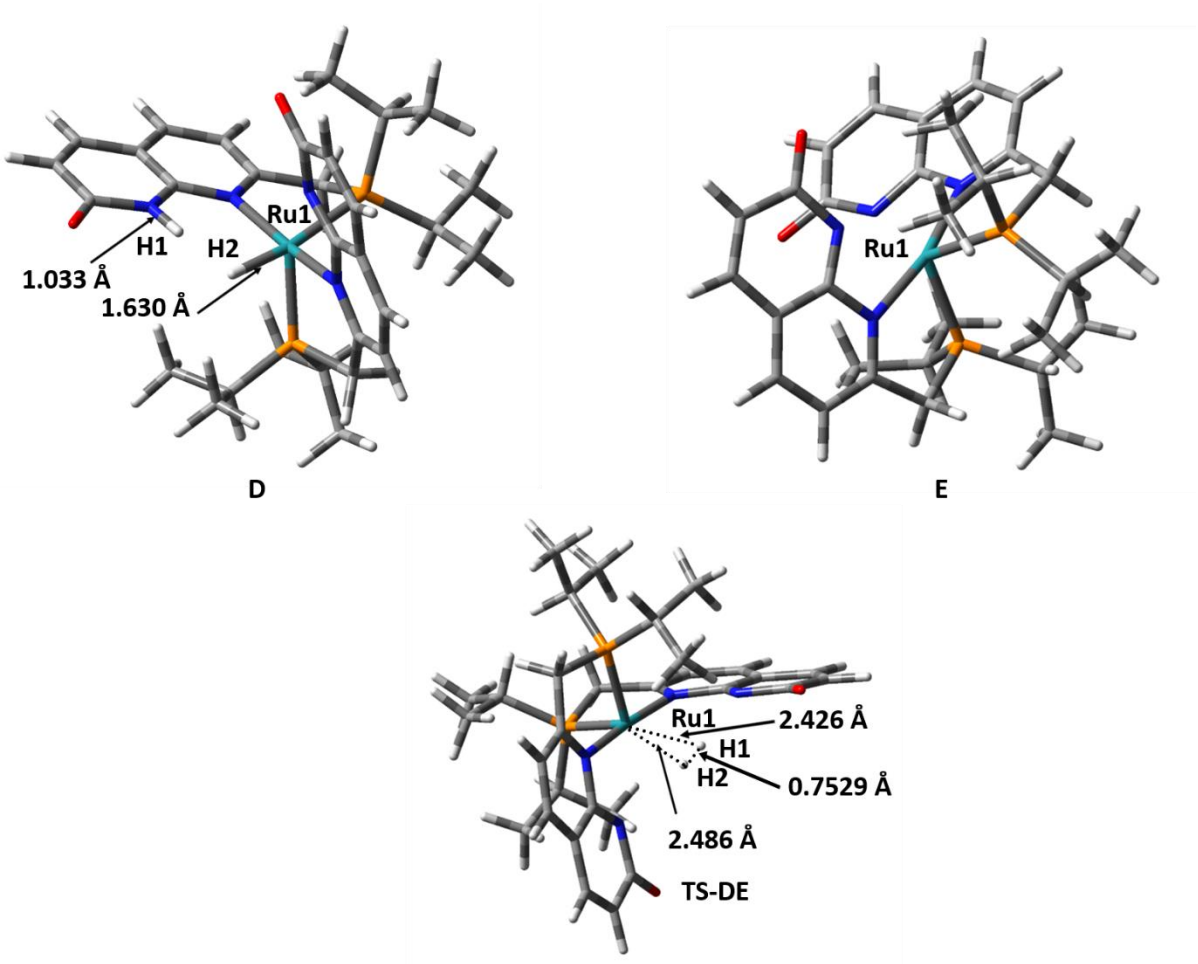
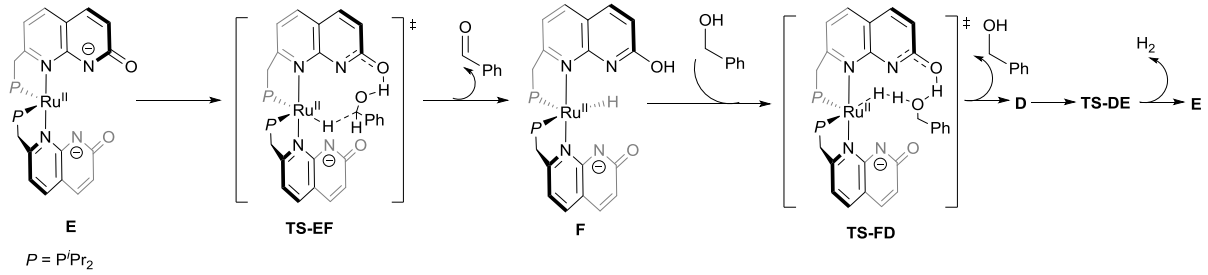


Figure S41. Geometry-optimized intermediates and transition states for alcohol dehydrogenation and important bond lengths (in angstrom).

Path C. Metal-ligand cooperative mechanism via participation of an O-atom.

In this mechanism, the concerted hydride abstraction by the metal and the proton abstraction by the O-atom is considered, followed by alcohol-assisted proton exchange.



Scheme S2. Schematic representation of path C.

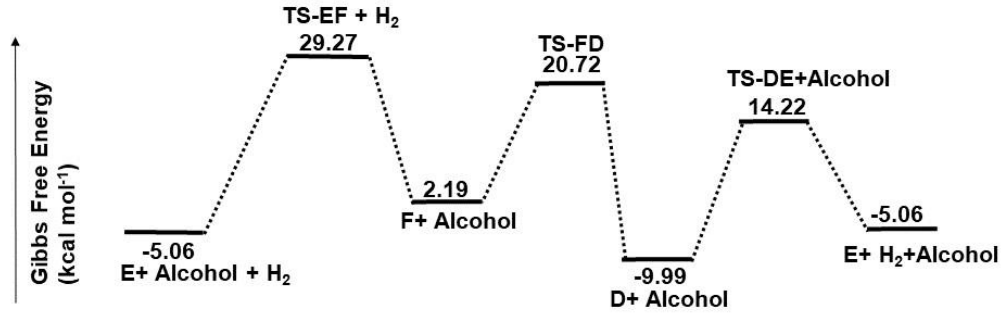


Figure S42. Calculated energy profile for path C.

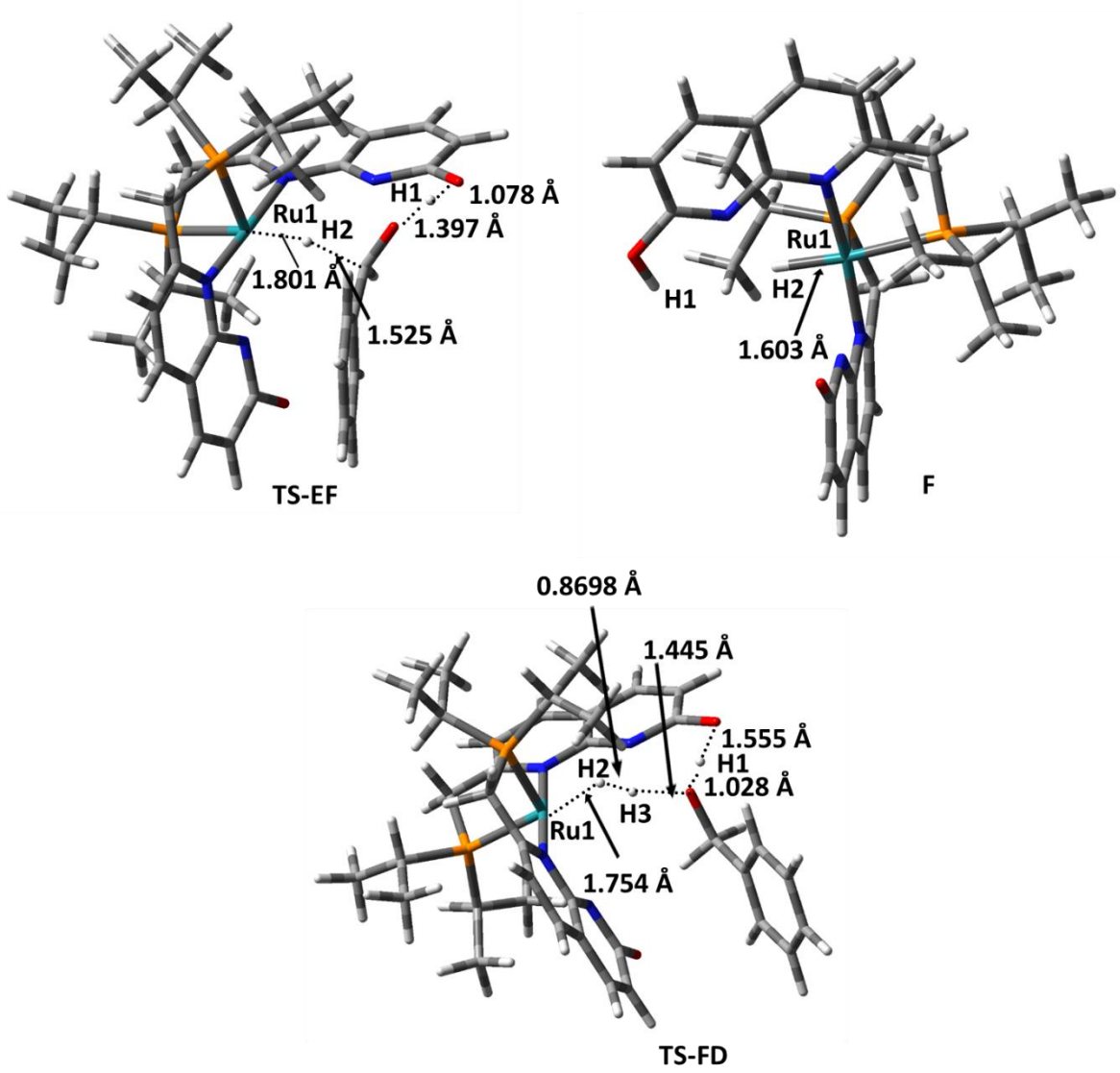
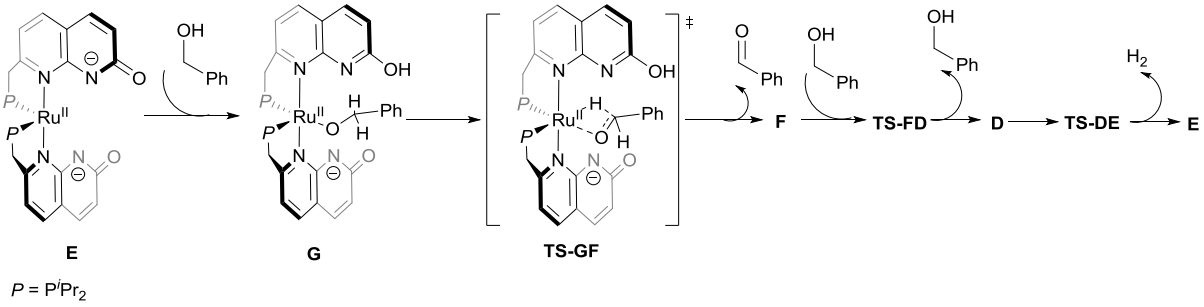


Figure S43. Geometry-optimized intermediates and transition states for alcohol dehydrogenation and important bond lengths (in angstrom).

Path D. Proton abstraction by O-atom.

Stepwise proton abstraction by O-atom of napthyridonate and subsequent β-hydride elimination are considered.



Scheme S3. Schematic representation of path D.

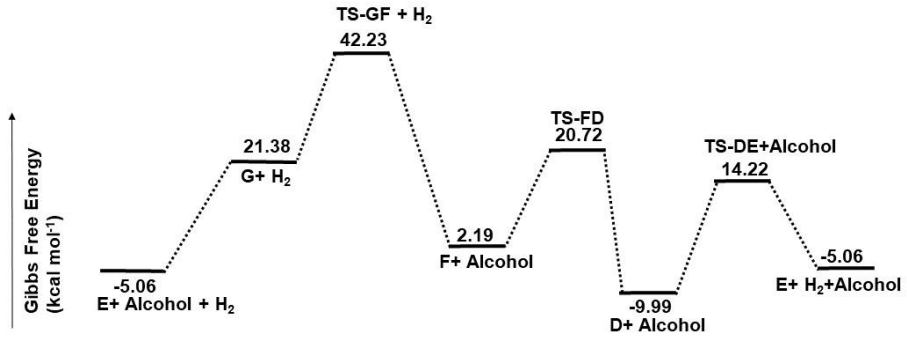


Figure S44. Calculated energy profile for path D.

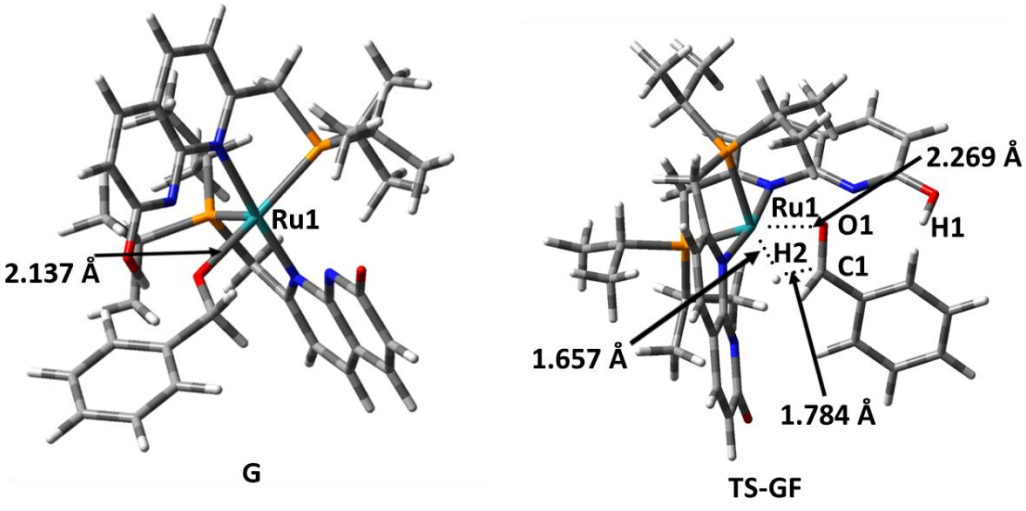


Figure S45. Geometry-optimized intermediates and transition states for alcohol dehydrogenation and important bond lengths (in angstrom).

Both Paths C and D appear generally less favorable compared to other pathways and involve intermediate **E**. As discussed above, formation of **E** is unlikely as such complex is likely to dimerize to

form a stable dimeric complex **2** or will likely react immediately with a protic solvent (alcohol or trace water).

Gas-phase values are given in the manuscript for Gibbs energies. For comparison, solvent corrected values of Gibbs energies were calculated using the CPCM (toluene, ε = 2.3741) model.[9-10] The comparison of solvent-corrected and gas phase values for relative Gibbs energies is given in Table S1.

Table S1. Comparison of solvent-corrected (CPCM) and gas phase Gibbs energy values for each step of the proposed reaction pathways.[a]

Step in a catalytic cycle	ΔG, kcal mol^{-1}	ΔG(Solvent Corrected, CPCM), kcal mol^{-1}
A	0	0
TS-AB	26.34598636	26.39411634
B	25.34887376	25.20831163
C	1.07931634	2.422563176
TS-CA	18.98718245	18.99157502
D	-9.994971316	-11.65366718
TS-DE	14.22062029	10.36375865
E	-5.060236608	-7.867902364
TS-EF	29.26516055	30.18527773
F	2.185615588	1.423881807
TS-FD	20.72412875	21.14041855
G	21.38113119	23.11061013
TS-GF	42.23138935	44.21494688

[a]Mass balanced was ensured through every step of the proposed pathways.

Cartesian coordinates and sum of electronic and thermal Free Energies (hartrees) of the optimized geometries

2

H_2, G = -1.179853 hartrees

H	0.000000	0.000000	0.371396
H	0.000000	0.000000	-0.371396

3

H_2O, G = -76.430410 hartrees

O	0.000000	0.000000	0.116500
H	-0.000000	0.769500	-0.466000
H	-0.000000	-0.769500	-0.466000

16

$PhCH_2OH$, G = -346.701945 hartrees

O	2.696236	-0.516079	0.234883
H	3.622891	-0.331298	0.039737
C	1.908307	0.606812	-0.159742
H	2.125453	1.477225	0.476777
H	2.146000	0.888701	-1.197903
C	0.437934	0.265880	-0.059677
C	-0.507281	1.297744	0.022399
C	-0.005753	-1.061501	-0.085146
C	-1.873204	1.011164	0.065959
H	-0.173864	2.332957	0.055931
C	-1.373098	-1.349251	-0.034552
H	0.724913	-1.861284	-0.133726

C	-2.311015	-0.316432	0.037809
H	-2.593251	1.822118	0.130595
H	-1.704633	-2.383863	-0.050285
H	-3.372744	-0.542417	0.077511

14

PhCHO, G = -345.518755 hartrees

O	-2.855405	0.394097	0.000007
C	-1.993256	-0.467187	-0.000012
H	-2.274995	-1.542400	-0.000025
C	-0.535482	-0.207639	0.000016
C	0.356116	-1.290407	-0.000015
C	-0.039955	1.107093	0.000002
C	1.733769	-1.065714	0.000009
H	-0.033380	-2.305983	0.000046
C	1.334357	1.329802	-0.000010
H	-0.746537	1.931154	-0.000032
C	2.221329	0.244371	0.000006
H	2.423437	-1.904399	-0.000022
H	1.720465	2.344835	0.000021
H	3.292979	0.422105	-0.000016

85

3, G = -2465.835111 hartrees

Ru	-0.000017	-0.085076	-0.000038
P	0.104344	1.427192	1.760712
P	-0.103778	1.425525	-1.762044
O	-2.760942	-4.066587	-1.700442

O	2.758820	-4.067010	1.702099
O	-0.159592	-1.732183	-1.458439
H	-1.125733	-2.035178	-1.156501
H	0.463041	-2.431716	-1.212263
O	0.158889	-1.730927	1.460131
H	1.124467	-2.034704	1.158161
H	-0.464161	-2.430327	1.214688
N	-2.126321	-0.112996	0.599872
N	-2.479261	-2.116103	-0.548746
N	2.126286	-0.113930	-0.599663
N	2.478166	-2.116715	0.549840
C	-1.674881	1.970220	1.834990
H	-1.965834	2.364642	2.813146
H	-1.774017	2.797506	1.121261
C	-2.600990	0.848581	1.428629
C	-3.915080	0.859863	1.911208
H	-4.234373	1.657994	2.572207
C	-4.785472	-0.156550	1.536949
H	-5.811830	-0.170058	1.896182
C	-4.333400	-1.175141	0.702330
C	-5.154844	-2.277007	0.277415
H	-6.187824	-2.311025	0.617904
C	-4.647551	-3.245745	-0.521465
H	-5.237757	-4.090916	-0.859245
C	-3.249450	-3.192782	-0.971247
C	-2.973392	-1.147503	0.236715
C	1.675487	1.968415	-1.836474
H	1.966600	2.361794	-2.815009
H	1.774711	2.796425	-1.123605

C	2.601394	0.847057	-1.428811
C	3.915762	0.857960	-1.910680
H	4.235480	1.655672	-2.571978
C	4.785837	-0.158336	-1.535382
H	5.812404	-0.172119	-1.894014
C	4.333196	-1.176498	-0.700530
C	5.154244	-2.278316	-0.274730
H	6.187438	-2.312586	-0.614547
C	4.646312	-3.246729	0.524144
H	5.236195	-4.091855	0.862600
C	3.247904	-3.193485	0.972936
C	2.972956	-1.148477	-0.235652
C	1.006393	3.090852	1.695632
H	0.739808	3.471745	0.702288
C	2.539200	2.953456	1.743205
H	2.884132	2.712779	2.752926
H	3.003444	3.906559	1.462849
H	2.915450	2.182078	1.066227
C	0.529244	4.131325	2.725567
H	-0.544782	4.328985	2.663523
H	1.046979	5.081974	2.549058
H	0.759475	3.826960	3.751655
C	0.469331	0.806290	3.510631
H	0.537818	1.726340	4.106787
C	1.809937	0.055172	3.620757
H	1.760409	-0.908583	3.112536
H	2.025243	-0.135111	4.679026
H	2.653551	0.615095	3.211051
C	-0.665085	-0.051719	4.100419

H	-1.623050	0.474769	4.137952
H	-0.402763	-0.324051	5.129727
H	-0.790208	-0.972886	3.528633
C	-0.468277	0.803082	-3.511492
H	-0.536052	1.722581	-4.108590
C	-1.809088	0.052331	-3.621634
H	-1.760130	-0.910983	-3.112539
H	-2.023925	-0.138726	-4.679854
H	-2.652700	0.612874	-3.212783
C	0.666073	-0.056070	-4.099850
H	1.624284	0.469956	-4.137537
H	0.404078	-0.329396	-5.128977
H	0.790505	-0.976703	-3.527068
C	-1.005855	3.089203	-1.698475
H	-0.739093	3.471066	-0.705551
C	-2.538656	2.951622	-1.745501
H	-2.883902	2.709788	-2.754832
H	-3.002933	3.904970	-1.466029
H	-2.914527	2.180897	-1.067549
C	-0.528952	4.128701	-2.729494
H	0.545157	4.326117	-2.668106
H	-1.046350	5.079629	-2.553518
H	-0.759751	3.823541	-3.755212

95

A, G = -2659.655632 hartrees

Ru	0.477600	0.066100	-0.000600
P	0.205000	-0.062000	2.291700

P	2.767400	0.477100	-0.162100
O	0.183000	1.655800	-4.186500
O	-3.036600	-3.477100	-1.515900
N	-0.152600	1.974000	0.331600
N	0.024500	1.818600	-1.900800
N	1.218700	-2.031100	-0.471100
N	-0.915800	-2.787600	-1.022300
C	-0.014400	1.771000	2.716200
H	-0.691600	1.922300	3.560500
H	0.972000	2.133400	3.034400
C	-0.434200	2.563100	1.499600
C	-0.993100	3.850300	1.516400
H	-1.228600	4.329000	2.460600
C	-1.238400	4.500200	0.300800
H	-1.678900	5.494700	0.301000
C	-0.921800	3.887800	-0.919800
C	-1.114500	4.410600	-2.246700
H	-1.550300	5.399200	-2.376500
C	-0.753000	3.656200	-3.318600
H	-0.886200	4.011700	-4.335500
C	-0.153700	2.305400	-3.186300
C	-0.351600	2.584500	-0.869400
C	3.445800	-1.213500	0.200000
H	4.460300	-1.345300	-0.188800
H	3.510400	-1.306600	1.291400
C	2.542000	-2.293900	-0.346000
C	3.119200	-3.523100	-0.688900
H	4.188100	-3.662900	-0.570900
C	2.311100	-4.536600	-1.186900

H	2.733800	-5.497700	-1.470500
C	0.943200	-4.316100	-1.323000
C	0.028200	-5.304700	-1.823200
H	0.426500	-6.269800	-2.129700
C	-1.295900	-5.032700	-1.905800
H	-2.017700	-5.752100	-2.277500
C	-1.820300	-3.730900	-1.478000
C	0.397500	-3.040500	-0.943000
C	1.573900	-0.575900	3.492900
H	2.465800	-0.102600	3.067600
C	1.803800	-2.098600	3.504800
H	1.003100	-2.614500	4.043300
H	2.741800	-2.325900	4.024900
H	1.860900	-2.527600	2.500900
C	1.413700	-0.051500	4.932400
H	1.341900	1.038300	4.985100
H	2.286800	-0.349300	5.525400
H	0.532000	-0.473300	5.425700
C	-1.313600	-0.913200	3.037600
H	-1.054900	-0.998000	4.101700
C	-1.533100	-2.332200	2.481000
H	-1.914400	-2.293300	1.461000
H	-2.276900	-2.846200	3.101300
H	-0.626100	-2.941000	2.478200
C	-2.608700	-0.092000	2.931700
H	-2.551900	0.864100	3.460200
H	-3.426800	-0.662500	3.386400
H	-2.875600	0.094400	1.891300
C	3.502700	0.807200	-1.873900

H	4.557100	0.524400	-1.742600
C	3.456900	2.278000	-2.318800
H	2.433900	2.657100	-2.340300
H	3.853300	2.351900	-3.337700
H	4.063500	2.930000	-1.685000
C	2.893400	-0.102800	-2.956800
H	2.937600	-1.162700	-2.692300
H	3.467200	0.027400	-3.882100
H	1.858400	0.171600	-3.177300
C	3.773900	1.553000	1.022400
H	3.575100	1.074900	1.989800
C	3.271100	3.004600	1.123200
H	3.510300	3.583600	0.228200
H	3.754800	3.502100	1.972600
H	2.190600	3.058600	1.268200
C	5.295400	1.506000	0.792400
H	5.687500	0.484400	0.782700
H	5.804700	2.044600	1.600600
H	5.579100	1.987500	-0.148200
O	-1.668800	-0.511900	-0.231200
C	-2.611100	0.049800	-1.177500
H	-2.245400	1.020700	-1.506700
H	-2.642000	-0.612300	-2.050200
C	-3.993900	0.192700	-0.579200
C	-4.809000	-0.935000	-0.388000
C	-4.487900	1.455900	-0.224600
C	-6.086800	-0.794600	0.158800
H	-4.431500	-1.912400	-0.678800
C	-5.768300	1.597500	0.320900

H	-3.868100	2.335900	-0.382200
C	-6.570300	0.469700	0.516200
H	-6.711500	-1.673400	0.296400
H	-6.139400	2.584200	0.586000
H	-7.567900	0.575300	0.934700
H	-1.445700	-1.493400	-0.554600

95

TS-AB, G = -2659.613647 hartrees

Ru	-0.237000	-0.148600	-0.002200
P	-0.164600	-1.824700	-1.595400
O	-2.855500	4.320600	1.180000
H	-1.741600	2.177400	0.579500
N	-2.217600	0.331300	-1.073000
N	-2.598100	2.375500	0.010600
C	-1.980700	-1.931400	-2.017700
H	-2.164900	-2.399700	-2.989500
H	-2.433500	-2.583800	-1.258900
C	-2.670000	-0.596600	-1.956900
C	-3.787200	-0.384400	-2.778900
H	-4.083700	-1.158600	-3.477400
C	-4.496700	0.801300	-2.685400
H	-5.359800	0.990300	-3.317900
C	-4.101300	1.755100	-1.745000
C	-4.794000	3.000400	-1.534900
H	-5.654600	3.215900	-2.164100
C	-4.398400	3.877400	-0.581900
H	-4.907500	4.817600	-0.404000
C	-3.249700	3.587000	0.276100

C	-2.958700	1.471500	-0.943800
C	0.542600	-1.564100	-3.333400
H	-0.053900	-2.261900	-3.938700
C	2.027600	-1.908500	-3.524200
H	2.666600	-1.240300	-2.945600
H	2.283800	-1.770400	-4.581800
H	2.257700	-2.945800	-3.269100
C	0.271600	-0.137100	-3.838200
H	-0.779200	0.158400	-3.754900
H	0.552900	-0.072000	-4.895900
H	0.883300	0.581300	-3.286400
C	0.176600	-3.639400	-1.179100
H	-0.541300	-3.814900	-0.365300
C	1.582600	-3.899600	-0.607600
H	2.357900	-3.804700	-1.371100
H	1.630700	-4.923200	-0.216100
H	1.834200	-3.212400	0.201100
C	-0.146600	-4.632000	-2.311300
H	-1.168400	-4.527600	-2.689800
H	-0.040400	-5.658400	-1.939400
H	0.540500	-4.520500	-3.155500
P	-1.267200	-1.231400	1.954700
O	4.172500	0.631800	-2.580800
N	1.602300	-0.756800	0.996500
N	2.916400	-0.040300	-0.794800
C	0.256800	-2.063900	2.608300
H	0.229700	-2.199200	3.694000
H	0.262900	-3.073000	2.171300
C	1.547400	-1.394400	2.191900

C	2.667900	-1.589600	3.007800
H	2.551100	-2.086800	3.964500
C	3.916700	-1.170900	2.559300
H	4.801600	-1.298100	3.179600
C	4.038300	-0.629500	1.285000
C	5.296200	-0.253400	0.703400
H	6.195900	-0.345900	1.309300
C	5.347100	0.192600	-0.575200
H	6.277500	0.482800	-1.053200
C	4.121800	0.281800	-1.384300
C	2.861200	-0.457600	0.462500
C	-2.468000	-2.699600	1.911700
H	-1.988900	-3.348200	1.164900
C	-3.864300	-2.333400	1.375900
H	-4.459500	-1.817800	2.135500
H	-4.411100	-3.244600	1.104500
H	-3.820500	-1.689300	0.493400
C	-2.591800	-3.506300	3.216400
H	-1.623400	-3.838600	3.602100
H	-3.199600	-4.402700	3.041300
H	-3.089400	-2.929000	4.002800
C	-1.822000	-0.218100	3.455200
H	-2.107600	-0.967200	4.205800
C	-3.042700	0.674400	3.172800
H	-2.781300	1.509100	2.519000
H	-3.405200	1.103800	4.114300
H	-3.875000	0.132600	2.716700
C	-0.674200	0.627600	4.037100
H	0.166400	0.018700	4.381500

H	-1.047000	1.189600	4.901900
H	-0.300500	1.342600	3.301000
O	-0.219300	1.817600	1.026100
C	0.427900	2.139400	-0.052000
H	-0.155000	2.505500	-0.907700
C	1.791900	2.709100	0.027600
C	2.395600	3.226200	-1.127600
C	2.423300	2.868900	1.270800
C	3.617300	3.891500	-1.045400
H	1.920600	3.084900	-2.094300
C	3.643100	3.538500	1.352400
H	1.938000	2.484600	2.161300
C	4.242000	4.051000	0.195600
H	4.088400	4.267700	-1.948000
H	4.126200	3.665600	2.317200
H	5.193800	4.570800	0.261300
H	0.736900	0.584100	-1.091600

95

B, G = -2659.615236 hartrees

Ru	-0.247400	-0.148600	-0.047000
P	-0.268500	-2.094300	-1.291200
O	-2.815100	4.472500	0.421800
H	-1.773200	2.225300	0.225700
H	0.570000	0.202800	-1.375700
N	-2.291100	0.126800	-1.066400
N	-2.619500	2.340100	-0.372200
C	-2.106000	-2.273600	-1.568500

H	-2.348700	-2.927200	-2.411800
H	-2.503000	-2.754600	-0.664500
C	-2.789800	-0.946100	-1.734400
C	-3.938500	-0.879000	-2.537500
H	-4.269800	-1.768900	-3.060500
C	-4.630000	0.315200	-2.652700
H	-5.513900	0.394300	-3.279700
C	-4.188400	1.425100	-1.928600
C	-4.857400	2.700800	-1.937900
H	-5.736300	2.809500	-2.569100
C	-4.418900	3.735500	-1.181900
H	-4.910300	4.701500	-1.170100
C	-3.247700	3.591000	-0.317700
C	-3.020900	1.279000	-1.127600
C	0.339600	-2.184000	-3.081400
H	-0.243300	-3.023200	-3.487900
C	1.832700	-2.496600	-3.262900
H	2.454900	-1.695600	-2.861000
H	2.046400	-2.573700	-4.335800
H	2.123900	-3.445600	-2.805900
C	-0.026700	-0.917900	-3.873000
H	-1.089900	-0.665200	-3.814300
H	0.219700	-1.075600	-4.929500
H	0.555800	-0.064000	-3.517800
C	0.113100	-3.796700	-0.553700
H	-0.559000	-3.810500	0.316200
C	1.549600	-3.949200	-0.022800
H	2.277800	-4.028900	-0.833200
H	1.621100	-4.867200	0.573300

H	1.848700	-3.109100	0.604200
C	-0.264500	-4.986600	-1.454900
H	-1.302900	-4.948500	-1.798900
H	-0.140500	-5.921800	-0.895400
H	0.383100	-5.047400	-2.334900
P	-1.161200	-0.812900	2.203400
O	4.009000	0.271500	-2.943200
N	1.657200	-0.576700	0.942000
N	2.864200	-0.147600	-1.011000
C	0.407600	-1.577600	2.833800
H	0.475400	-1.575300	3.925900
H	0.358300	-2.632900	2.529700
C	1.671400	-1.006300	2.228700
C	2.839400	-1.086700	2.996700
H	2.778200	-1.417500	4.027600
C	4.062700	-0.778600	2.409600
H	4.984200	-0.826100	2.986300
C	4.109000	-0.450700	1.060400
C	5.332500	-0.199000	0.352300
H	6.268300	-0.228000	0.908000
C	5.307300	0.057300	-0.978100
H	6.209500	0.249900	-1.550400
C	4.031900	0.072000	-1.711400
C	2.883400	-0.379300	0.294200
C	-2.374400	-2.245300	2.477500
H	-1.973600	-3.005600	1.792800
C	-3.802500	-1.911900	2.010600
H	-4.312100	-1.257900	2.725000
H	-4.398300	-2.829600	1.933500

H	-3.815200	-1.415900	1.035600
C	-2.394700	-2.856500	3.888600
H	-1.398800	-3.147500	4.235600
H	-3.020300	-3.758000	3.894800
H	-2.820600	-2.165500	4.623600
C	-1.605100	0.420900	3.571900
H	-1.910700	-0.195500	4.427700
C	-2.780700	1.337000	3.185800
H	-2.482900	2.053400	2.417100
H	-3.097200	1.914600	4.062700
H	-3.653700	0.788900	2.822000
C	-0.402300	1.276100	4.010700
H	0.425700	0.676700	4.398900
H	-0.719200	1.954400	4.812300
H	-0.031600	1.881700	3.181100
O	-0.255400	1.949600	0.795900
C	0.430500	2.188200	-0.261000
H	-0.103600	2.382300	-1.199600
C	1.804500	2.705800	-0.213400
C	2.436600	3.075000	-1.411700
C	2.438100	2.962800	1.014200
C	3.685900	3.690900	-1.386400
H	1.960600	2.851200	-2.361900
C	3.685600	3.582500	1.037100
H	1.937400	2.687500	1.935800
C	4.310600	3.947500	-0.161600
H	4.177700	3.951900	-2.318100
H	4.171500	3.784900	1.987400
H	5.285000	4.427800	-0.140300

97

C, G = -2660.833765 hartrees

Ru	-0.288400	0.237400	-0.110500
P	-1.316100	1.115900	-1.968000
O	4.322900	-0.375000	2.270800
H	-0.149200	-1.044800	-1.107600
N	1.527600	1.094200	-1.093500
N	2.977000	0.276400	0.547000
C	-0.022000	2.294300	-2.582200
H	-0.088400	2.483200	-3.658300
H	-0.215400	3.251500	-2.078400
C	1.368800	1.846600	-2.208000
C	2.437200	2.309600	-2.988000
H	2.232600	2.888300	-3.882100
C	3.737300	2.038900	-2.586800
H	4.586600	2.382800	-3.172600
C	3.951100	1.349800	-1.395700
C	5.258800	1.101100	-0.855900
H	6.124500	1.418600	-1.433900
C	5.400300	0.507200	0.353600
H	6.370400	0.319400	0.801600
C	4.221200	0.105200	1.126400
C	2.820500	0.885200	-0.636000
C	-2.828900	2.264400	-1.926200
H	-2.502200	3.008300	-1.188200
C	-4.108100	1.604700	-1.380100
H	-4.589500	0.978900	-2.137200
H	-4.833800	2.377000	-1.096600

H	-3.917900	0.981000	-0.503800
C	-3.133300	3.012700	-3.235900
H	-2.260400	3.534700	-3.639000
H	-3.911400	3.765700	-3.058700
H	-3.511900	2.336200	-4.009200
C	-1.598100	0.053400	-3.508700
H	-1.962000	0.768300	-4.259000
C	-2.657500	-1.047500	-3.337700
H	-2.302700	-1.837400	-2.672800
H	-2.857300	-1.513000	-4.310100
H	-3.609000	-0.675000	-2.950600
C	-0.290000	-0.561500	-4.036300
H	0.453600	0.191800	-4.310700
H	-0.505600	-1.152800	-4.934200
H	0.160200	-1.226300	-3.293600
P	-0.508300	2.021900	1.589800
O	-1.808500	-4.435100	-1.414800
N	-2.091800	-0.492700	0.952700
N	-1.987600	-2.541600	-0.152500
C	-2.311200	1.739300	1.992600
H	-2.600900	2.118800	2.978000
H	-2.880200	2.319300	1.253900
C	-2.721000	0.294900	1.865100
C	-3.782500	-0.173400	2.657700
H	-4.233200	0.497200	3.380500
C	-4.247400	-1.469100	2.505900
H	-5.067500	-1.845100	3.111400
C	-3.652600	-2.294100	1.546300
C	-4.065100	-3.646900	1.270200

H	-4.881200	-4.061400	1.857400
C	-3.466700	-4.386700	0.304500
H	-3.768200	-5.402600	0.076400
C	-2.373100	-3.838800	-0.498500
C	-2.574900	-1.758700	0.794400
C	0.257900	1.980900	3.322800
H	-0.193000	2.830500	3.853300
C	1.784600	2.164500	3.303300
H	2.281700	1.333500	2.798700
H	2.158200	2.198200	4.333800
H	2.092700	3.092500	2.814700
C	-0.109000	0.696800	4.089400
H	-1.188100	0.583100	4.234900
H	0.350900	0.731200	5.084200
H	0.268100	-0.185800	3.568400
C	-0.558800	3.867500	1.151600
H	-1.259700	3.871400	0.305500
C	0.790300	4.392600	0.626800
H	1.503600	4.547100	1.441200
H	0.646900	5.362700	0.135200
H	1.250300	3.709800	-0.091700
C	-1.125100	4.806700	2.229700
H	-2.102700	4.483700	2.602400
H	-1.249500	5.815000	1.815400
H	-0.447900	4.892000	3.085700
H	-1.202300	-2.084000	-0.658200
C	1.019700	-2.342500	1.643100
H	0.012400	-2.755700	1.548300
H	1.334800	-2.467700	2.688000

C	1.978200	-3.108500	0.749400
C	1.532500	-3.782700	-0.397300
C	3.336700	-3.192200	1.093900
C	2.424800	-4.510000	-1.190900
H	0.484100	-3.768800	-0.675800
C	4.230600	-3.913900	0.299300
H	3.699100	-2.665300	1.972000
C	3.777700	-4.574700	-0.847100
H	2.056000	-5.030600	-2.070500
H	5.279700	-3.961500	0.579200
H	4.471600	-5.142100	-1.462000
O	0.922200	-0.928600	1.400000
H	1.843000	-0.498600	1.158800

97

TS-CA, G = -2660.805227 hartrees

Ru	-0.393100	-0.160400	-0.017200
P	-1.954200	-0.873000	1.577500
P	-1.082100	-1.397800	-1.807700
O	4.530800	-0.957500	-1.632700
O	-0.021000	4.138400	2.261700
N	0.841600	-1.765200	1.000200
N	2.766000	-1.258700	-0.218700
N	-1.635800	1.297300	-0.938900
N	-0.794600	2.738800	0.629400
C	-1.272200	-2.540700	2.012000
H	-1.598600	-2.886700	2.996600
H	-1.677000	-3.252000	1.280900

C	0.235700	-2.564500	1.914900
C	0.931000	-3.469200	2.724600
H	0.387800	-4.064600	3.450100
C	2.306700	-3.598500	2.573700
H	2.871900	-4.288800	3.195600
C	2.959700	-2.858600	1.593500
C	4.365300	-2.978100	1.316100
H	4.963000	-3.631300	1.948700
C	4.916500	-2.309400	0.275100
H	5.968000	-2.390000	0.020700
C	4.085100	-1.465300	-0.591300
C	2.200900	-1.940400	0.783300
C	-2.583500	-0.437000	-2.357900
H	-2.783800	-0.552800	-3.427100
H	-3.447000	-0.859000	-1.827300
C	-2.448600	1.017300	-1.977600
C	-3.191700	2.007300	-2.631500
H	-3.824400	1.739400	-3.470600
C	-3.112000	3.323500	-2.176700
H	-3.677800	4.110700	-2.670100
C	-2.316300	3.633700	-1.074600
C	-2.177900	4.942400	-0.497600
H	-2.708300	5.776700	-0.952600
C	-1.399100	5.115100	0.600300
H	-1.270500	6.085000	1.070100
C	-0.691300	3.981900	1.224100
C	-1.568500	2.582300	-0.440000
C	-3.764300	-1.256000	1.179900
H	-3.693100	-1.786100	0.222700

C	-4.607000	0.011400	0.944700
H	-4.832000	0.518800	1.887300
H	-5.565300	-0.263900	0.488600
H	-4.111600	0.728400	0.285300
C	-4.469200	-2.196900	2.173700
H	-3.949500	-3.151300	2.298100
H	-5.478700	-2.420200	1.808000
H	-4.581000	-1.739300	3.162000
C	-2.054400	-0.023300	3.274300
H	-2.919000	-0.521400	3.733500
C	-2.332100	1.488200	3.219700
H	-1.452600	2.040700	2.886100
H	-2.586900	1.835100	4.228200
H	-3.160100	1.753800	2.558900
C	-0.836300	-0.290200	4.177400
H	-0.659300	-1.352200	4.364700
H	-1.013600	0.187700	5.147800
H	0.076300	0.144600	3.765100
C	-0.043800	-1.470900	-3.388500
H	-0.655500	-2.123200	-4.027500
C	1.344600	-2.112700	-3.227100
H	2.027100	-1.465000	-2.676500
H	1.771700	-2.278700	-4.223200
H	1.316900	-3.077900	-2.718100
C	0.081900	-0.111300	-4.097000
H	-0.883000	0.345800	-4.333200
H	0.613900	-0.258600	-5.044100
H	0.658900	0.588300	-3.492000
C	-1.775300	-3.150200	-1.638700

H	-2.451600	-3.049900	-0.782100
C	-0.718900	-4.211300	-1.278200
H	-0.133200	-4.500900	-2.154900
H	-1.219400	-5.116000	-0.913100
H	-0.023900	-3.872200	-0.507300
C	-2.621200	-3.623700	-2.836200
H	-3.431200	-2.933400	-3.088300
H	-3.078600	-4.590300	-2.593700
H	-2.009900	-3.774300	-3.731600
H	1.249500	0.693300	1.915900
H	0.830500	1.306600	1.830900
C	1.803900	1.941200	-1.424200
H	0.965700	2.616000	-1.251100
H	2.062800	1.974000	-2.490900
C	3.005200	2.384300	-0.613800
C	2.848700	3.110300	0.577600
C	4.302200	2.117000	-1.078800
C	3.966500	3.555700	1.288400
H	1.859300	3.335700	0.961100
C	5.419800	2.557200	-0.365300
H	4.440000	1.535300	-1.984800
C	5.254700	3.280200	0.820000
H	3.823100	4.121000	2.205100
H	6.416100	2.333500	-0.736700
H	6.123400	3.629400	1.372300
O	1.330200	0.603300	-1.142200
H	2.058600	-0.082900	-0.844700

81

D, G = -2314.149468 hartrees

Ru	0.106000	-0.043600	0.200300
P	0.444500	-2.234400	0.782600
O	0.235000	4.272200	0.381500
H	-0.467500	-0.011200	1.726600
N	1.909000	0.127600	1.088300
N	1.088900	2.168400	0.738600
C	2.298100	-2.211900	1.242700
H	2.534100	-2.916300	2.045900
H	2.841200	-2.553700	0.351300
C	2.729000	-0.802100	1.578600
C	3.861800	-0.402700	2.310400
H	4.541900	-1.146100	2.712200
C	4.088800	0.964000	2.522400
H	4.955900	1.280600	3.097600
C	3.203300	1.932200	2.018800
C	3.245900	3.362800	2.172400
H	4.064400	3.823500	2.722000
C	2.251800	4.119300	1.631600
H	2.246500	5.200300	1.730200
C	1.110000	3.544100	0.875200
C	2.086700	1.459000	1.284900
C	0.411600	-3.710300	-0.407100
H	0.993900	-3.321600	-1.253100
C	-1.004400	-4.030700	-0.919800
H	-1.581900	-4.580500	-0.169900
H	-0.946000	-4.667700	-1.810700
H	-1.569200	-3.131000	-1.180600
C	1.102000	-4.992300	0.091400

H	2.133300	-4.821500	0.413100
H	1.129600	-5.734700	-0.715900
H	0.557700	-5.446800	0.926000
C	-0.371300	-2.900800	2.354400
H	-0.081000	-3.958300	2.411600
C	-1.906300	-2.811300	2.289000
H	-2.228200	-1.767300	2.254700
H	-2.339100	-3.263700	3.189100
H	-2.330500	-3.325900	1.423300
C	0.135500	-2.195900	3.624800
H	1.208800	-2.329700	3.786800
H	-0.381500	-2.609000	4.498800
H	-0.073700	-1.122600	3.587900
P	0.681600	0.095400	-2.174800
O	-3.594700	1.437100	3.371100
H	-1.889700	0.672200	1.673100
N	-1.929800	0.073800	-0.716500
N	-2.846400	0.805500	1.305700
C	-0.912900	-0.625200	-2.844800
H	-1.085200	-0.405800	-3.904200
H	-0.797400	-1.712900	-2.755300
C	-2.107800	-0.188200	-2.036600
C	-3.354500	-0.061800	-2.668500
H	-3.437300	-0.287300	-3.725900
C	-4.456600	0.362500	-1.942300
H	-5.428700	0.473500	-2.415100
C	-4.304700	0.666200	-0.586300
C	-5.370200	1.139600	0.261000
H	-6.354500	1.270400	-0.182500

C	-5.162400	1.418500	1.570500
H	-5.950700	1.775400	2.223100
C	-3.844100	1.241100	2.184700
C	-3.014600	0.508200	-0.013300
C	0.769400	1.756100	-3.070900
H	0.694700	1.521600	-4.141700
C	2.105200	2.476200	-2.815700
H	2.256900	2.650600	-1.747000
H	2.093200	3.453900	-3.311300
H	2.964400	1.922300	-3.204500
C	-0.407500	2.673100	-2.690700
H	-1.378800	2.224800	-2.921800
H	-0.334600	3.601700	-3.269700
H	-0.385300	2.949500	-1.632100
C	1.943300	-1.004000	-3.063800
H	1.569300	-2.009800	-2.826600
C	3.352700	-0.890300	-2.453900
H	3.834900	0.054800	-2.719500
H	3.990700	-1.698400	-2.832500
H	3.332800	-0.951800	-1.362800
C	1.991500	-0.872300	-4.595000
H	1.005100	-0.977200	-5.058700
H	2.636400	-1.653400	-5.016700
H	2.408400	0.092100	-4.902400

81

TS-DE, G = -2314.110878 hartrees

Ru	0.072600	-0.035400	-0.129900

P	0.790500	-0.914300	1.863400
P	-0.553700	2.134000	0.405200
O	-3.348500	0.340800	-3.594100
O	2.265100	-3.297300	-2.284600
N	-1.694100	-1.152000	0.405200
N	-2.526800	-0.431200	-1.605900
N	1.761700	0.957900	-0.775200
N	2.024000	-1.151200	-1.501000
C	-0.785000	-1.567900	2.623500
H	-0.592400	-2.470400	3.212200
H	-1.155500	-0.808600	3.323800
C	-1.831700	-1.824300	1.564900
C	-2.910300	-2.681900	1.810600
H	-2.973900	-3.213000	2.754000
C	-3.884600	-2.840200	0.823500
H	-4.721400	-3.517100	0.981700
C	-3.796900	-2.118700	-0.365600
C	-4.747500	-2.176200	-1.442700
H	-5.592900	-2.856600	-1.360800
C	-4.581100	-1.387200	-2.534600
H	-5.276400	-1.402200	-3.367900
C	-3.453300	-0.440300	-2.631400
C	-2.684200	-1.228400	-0.555000
C	1.079900	3.066700	0.154900
H	0.897200	4.051800	-0.286300
H	1.515300	3.243700	1.146600
C	2.042400	2.265000	-0.691300
C	3.161000	2.788000	-1.356200
H	3.390700	3.845600	-1.286600

C	3.958700	1.928400	-2.122000
H	4.820900	2.324600	-2.653500
C	3.649800	0.567100	-2.230700
C	4.331800	-0.430100	-3.012300
H	5.212100	-0.151400	-3.587700
C	3.855700	-1.702900	-3.028500
H	4.334100	-2.482700	-3.612500
C	2.659200	-2.123200	-2.259600
C	2.510700	0.094300	-1.517800
C	1.523000	0.095300	3.275400
H	0.709800	0.796800	3.499600
C	2.755900	0.920000	2.868100
H	3.643600	0.291900	2.760000
H	2.975000	1.665300	3.641800
H	2.607700	1.440800	1.920600
C	1.795800	-0.716200	4.555100
H	0.923300	-1.287300	4.886900
H	2.068700	-0.032600	5.367900
H	2.629300	-1.412600	4.423000
C	1.810200	-2.502600	1.788100
H	1.750700	-2.857600	2.827100
C	3.292200	-2.302900	1.436300
H	3.407000	-1.801500	0.474300
H	3.773900	-3.283900	1.357300
H	3.831600	-1.734500	2.199000
C	1.154900	-3.567000	0.888800
H	0.106700	-3.747300	1.145900
H	1.691100	-4.513500	1.024700
H	1.220700	-3.308200	-0.170700

C	-1.680800	3.097500	-0.769700
H	-1.487600	4.134500	-0.460100
C	-3.179200	2.805500	-0.595700
H	-3.392700	1.750000	-0.775900
H	-3.739600	3.384200	-1.338400
H	-3.554300	3.087100	0.391700
C	-1.276600	2.958700	-2.248600
H	-0.197400	3.046300	-2.411900
H	-1.760300	3.762700	-2.815400
H	-1.627200	2.012400	-2.666900
C	-1.038500	2.718500	2.134000
H	-0.156300	2.434300	2.721700
C	-2.252100	1.970800	2.714700
H	-3.191600	2.346800	2.302900
H	-2.291800	2.114800	3.801000
H	-2.214400	0.899300	2.509300
C	-1.207800	4.242400	2.269700
H	-0.339300	4.797800	1.902100
H	-1.338900	4.501800	3.327000
H	-2.092500	4.600900	1.735200
H	-0.602100	0.072500	-2.457900
H	0.128400	0.178000	-2.606400

79

E, G = -2312.961751 hartrees

Ru	-0.016400	-0.000100	0.000000
P	-1.444100	-0.496000	-1.767300
P	-1.446400	0.500600	1.764400

O	3.384300	1.622700	2.074300
O	3.382400	-1.633500	-2.068100
N	0.200700	1.683500	-1.145100
N	1.751200	1.671200	0.457200
N	0.192800	-1.684400	1.145600
N	1.746300	-1.676800	-0.453900
C	-1.586800	1.197800	-2.633600
H	-1.688000	1.076600	-3.716500
H	-2.512700	1.669200	-2.279500
C	-0.398400	2.061800	-2.275200
C	0.110500	3.157200	-2.991200
H	-0.367800	3.482900	-3.908500
C	1.259900	3.804500	-2.514100
H	1.671500	4.643200	-3.070900
C	1.903100	3.374600	-1.343100
C	3.111100	3.875600	-0.741700
H	3.633100	4.715500	-1.195300
C	3.589500	3.278000	0.382800
H	4.502700	3.618200	0.860500
C	2.921300	2.126900	1.041300
C	1.319500	2.277400	-0.659100
C	-1.595200	-1.192300	2.631500
H	-1.696900	-1.070000	3.714300
H	-2.522200	-1.661200	2.277000
C	-0.409100	-2.060300	2.275000
C	0.095300	-3.157000	2.992000
H	-0.385300	-3.481000	3.908800
C	1.243400	-3.808200	2.516900
H	1.651500	-4.648000	3.074600

C	1.889800	-3.380500	1.346800
C	3.097300	-3.885300	0.747600
H	3.616000	-4.726700	1.202100
C	3.579400	-3.289200	-0.376200
H	4.492400	-3.632300	-0.852300
C	2.916000	-2.136200	-1.035900
C	1.310700	-2.281700	0.661600
C	-3.268900	-0.966500	-1.628300
H	-3.676900	-0.108700	-1.078900
C	-3.500300	-2.226900	-0.777600
H	-3.259100	-3.136800	-1.334300
H	-4.555200	-2.294900	-0.485800
H	-2.891500	-2.226600	0.130100
C	-4.021700	-1.057800	-2.967200
H	-3.890200	-0.164300	-3.585200
H	-5.096000	-1.171300	-2.778100
H	-3.702100	-1.925900	-3.552400
C	-0.758200	-1.559700	-3.166400
H	-1.542500	-1.516200	-3.934400
C	-0.552900	-3.027100	-2.755600
H	0.190800	-3.105100	-1.959300
H	-0.180300	-3.593600	-3.616900
H	-1.475800	-3.508300	-2.420200
C	0.532900	-0.977800	-3.771000
H	0.402800	0.045000	-4.137500
H	0.823300	-1.593200	-4.630900
H	1.369100	-0.993500	-3.066700
C	-0.760100	1.563400	3.164000
H	-1.546000	1.522700	3.930600

C	-0.549900	3.029700	2.752100
H	0.195200	3.104500	1.956800
H	-0.176800	3.596000	3.613400
H	-1.470800	3.513300	2.414800
C	0.528100	0.978300	3.771600
H	0.394300	-0.043900	4.138700
H	0.818800	1.593600	4.631400
H	1.365700	0.990700	3.068800
C	-3.270000	0.975600	1.622600
H	-3.679200	0.118500	1.073000
C	-3.497800	2.236200	0.771200
H	-3.254000	3.145700	1.327500
H	-4.552500	2.307000	0.479400
H	-2.889000	2.233800	-0.136400
C	-4.024100	1.069300	2.960600
H	-3.895000	0.176000	3.579400
H	-5.098000	1.184600	2.770100
H	-3.703600	1.937200	3.545400

95

TS-EF, G = -2659.608995 hartrees

Ru	-0.242300	-0.202200	0.064900
P	-0.719700	-0.122800	2.311400
P	-1.085900	-2.373300	-0.576200
O	2.096300	-0.466100	-3.728200
O	-1.246500	4.799200	-0.701000
N	1.550600	-0.833300	0.762400

N	1.810800	-0.670500	-1.458100
N	-2.310800	0.345200	-0.851700
N	-1.795600	2.599200	-0.847200
C	0.784500	-1.034700	3.026500
H	1.109900	-0.612300	3.981300
H	0.454700	-2.061000	3.235200
C	1.911800	-1.101000	2.021300
C	3.227700	-1.509100	2.297800
H	3.527900	-1.715900	3.319400
C	4.128400	-1.665900	1.239600
H	5.145600	-1.994000	1.440500
C	3.732100	-1.417400	-0.083100
C	4.507600	-1.579100	-1.282300
H	5.534500	-1.932900	-1.215000
C	3.942400	-1.286400	-2.484100
H	4.492500	-1.396200	-3.413500
C	2.558100	-0.776100	-2.616600
C	2.399600	-0.970500	-0.292500
C	-2.912100	-2.031900	-0.652100
H	-3.442600	-2.749100	-1.286900
H	-3.305700	-2.158400	0.364900
C	-3.203500	-0.626000	-1.114400
C	-4.429700	-0.395200	-1.777600
H	-5.090800	-1.233400	-1.969300
C	-4.765400	0.882600	-2.172800
H	-5.699100	1.083000	-2.693000
C	-3.884500	1.934200	-1.878100
C	-4.145400	3.301800	-2.195300
H	-5.060500	3.552800	-2.725900

C	-3.262100	4.272100	-1.820500
H	-3.421600	5.324300	-2.027300
C	-2.076700	3.872300	-1.111100
C	-2.657400	1.637300	-1.199800
C	-2.132000	-1.110900	3.103400
H	-2.029100	-2.085500	2.613100
C	-3.527500	-0.555200	2.764600
H	-3.762100	0.321500	3.375700
H	-4.291700	-1.311400	2.982400
H	-3.624100	-0.263600	1.715600
C	-2.011200	-1.345900	4.620900
H	-1.055500	-1.791700	4.911000
H	-2.803100	-2.031200	4.947600
H	-2.137200	-0.418000	5.187700
C	-0.783700	1.501700	3.275000
H	-1.136900	1.213300	4.273800
C	-1.784800	2.489100	2.648800
H	-1.466300	2.759600	1.640500
H	-1.818400	3.403100	3.253600
H	-2.800900	2.091200	2.593600
C	0.583000	2.184800	3.428100
H	1.356800	1.526900	3.833800
H	0.478700	3.031700	4.117100
H	0.914800	2.588500	2.471400
C	-0.805700	-3.023000	-2.333800
H	-1.626200	-3.742000	-2.469500
C	0.518500	-3.779400	-2.530900
H	1.380200	-3.166300	-2.262700
H	0.623900	-4.044600	-3.589000

H	0.559000	-4.708200	-1.955800
C	-0.965300	-1.911400	-3.386800
H	-1.928800	-1.399000	-3.311500
H	-0.914600	-2.363100	-4.384700
H	-0.162500	-1.172000	-3.324100
C	-1.060700	-3.921800	0.514100
H	-1.578400	-3.571300	1.416300
C	0.356700	-4.343500	0.941800
H	0.911600	-4.803600	0.120500
H	0.293100	-5.085600	1.747100
H	0.947300	-3.499800	1.303300
C	-1.855100	-5.122200	-0.030200
H	-2.890700	-4.866800	-0.276200
H	-1.886000	-5.915100	0.727200
H	-1.389600	-5.547400	-0.924500
O	0.637300	3.692500	0.458000
C	1.115400	2.740200	-0.260700
H	0.678200	2.570000	-1.252900
C	2.603300	2.532700	-0.217800
C	3.269800	2.193800	-1.403100
C	3.358900	2.850700	0.921500
C	4.666300	2.166400	-1.449600
H	2.694700	1.966700	-2.296300
C	4.752000	2.802200	0.882200
H	2.851100	3.168600	1.824700
C	5.411200	2.462900	-0.305800
H	5.167600	1.914200	-2.379500
H	5.326400	3.049900	1.771200
H	6.497300	2.442000	-0.340300

H	-0.436500	4.333500	-0.164300
H	0.488300	1.436900	0.223200

81

F, G = -2314.130057 hartrees

Ru	0.123100	0.031800	-0.201600
P	0.500500	2.066100	-1.147200
O	0.229800	-4.297400	0.314100
N	1.945100	-0.314000	-1.002400
N	1.107200	-2.277600	-0.346600
C	2.362900	1.962200	-1.549400
H	2.631300	2.516300	-2.454000
H	2.882100	2.450900	-0.714200
C	2.788400	0.514000	-1.621500
C	3.940500	-0.003700	-2.241700
H	4.635100	0.662000	-2.743200
C	4.169200	-1.384400	-2.209300
H	5.052900	-1.795300	-2.692500
C	3.262300	-2.251000	-1.575000
C	3.311000	-3.685600	-1.480600
H	4.150900	-4.226800	-1.912400
C	2.298500	-4.346400	-0.854500
H	2.299100	-5.428400	-0.764700
C	1.129900	-3.655500	-0.253400
C	2.122500	-1.663000	-0.968100
C	0.450700	3.747200	-0.268000
H	1.001200	3.529000	0.656900

C	-0.978800	4.165600	0.117900
H	-1.526500	4.545100	-0.750600
H	-0.949900	4.973400	0.859400
H	-1.555000	3.336600	0.538600
C	1.171700	4.903900	-0.982700
H	2.215100	4.672600	-1.215500
H	1.169400	5.794800	-0.342000
H	0.669700	5.178900	-1.916500
C	-0.292100	2.431200	-2.828500
H	-0.049500	3.476300	-3.062500
C	-1.822100	2.271900	-2.771000
H	-2.082500	1.233000	-2.548200
H	-2.257500	2.535900	-3.742800
H	-2.290800	2.907800	-2.015200
C	0.276000	1.542400	-3.948400
H	1.344100	1.703800	-4.120900
H	-0.244300	1.762400	-4.888600
H	0.123000	0.483800	-3.715800
H	-0.447300	-0.235400	-1.676100
P	0.605800	0.290700	2.193400
O	-3.447000	-2.408100	-2.922700
H	-2.479300	-2.384400	-3.020000
N	-1.940900	0.089800	0.644800
N	-2.759000	-1.140200	-1.159000
C	-0.996100	1.153300	2.652600
H	-1.233200	1.098000	3.721800
H	-0.840300	2.213600	2.417100
C	-2.166400	0.633600	1.854700
C	-3.459900	0.731800	2.425300

H	-3.568500	1.201300	3.397100
C	-4.550000	0.229100	1.755300
H	-5.551100	0.296600	2.173600
C	-4.343800	-0.414400	0.518100
C	-5.389200	-1.030600	-0.227200
H	-6.406800	-0.979000	0.151000
C	-5.107400	-1.692600	-1.391800
H	-5.864000	-2.190500	-1.987000
C	-3.742800	-1.724900	-1.798000
C	-3.015800	-0.484300	-0.007600
C	0.596800	-1.187800	3.372000
H	0.463900	-0.779100	4.383600
C	1.925200	-1.962600	3.321200
H	2.132600	-2.314400	2.306600
H	1.860600	-2.844800	3.969100
H	2.775600	-1.366100	3.663500
C	-0.577400	-2.136800	3.069100
H	-1.549000	-1.639800	3.156100
H	-0.569100	-2.959600	3.794400
H	-0.494300	-2.580700	2.072000
C	1.847400	1.505600	2.956700
H	1.505600	2.464000	2.541500
C	3.279200	1.275400	2.439400
H	3.724600	0.370700	2.863200
H	3.921500	2.118500	2.723200
H	3.307300	1.174700	1.351100
C	1.822200	1.625700	4.489300
H	0.819600	1.836800	4.876000
H	2.477400	2.444400	4.812900

H	2.182700	0.711400	4.972100

97

TS-FD, G = -2660.802459 hartrees

Ru	-0.626900	-0.162800	0.077900
P	-1.563400	-0.343900	2.166600
P	-2.166500	-1.336200	-1.278900
O	2.445900	-0.615800	-3.146200
O	1.561000	4.391900	0.395600
N	0.465600	-1.740700	0.780400
N	1.434700	-1.191000	-1.167200
N	-1.810000	1.545200	-0.812400
N	-0.138600	3.027200	-0.222800
C	-0.921700	-2.040300	2.712100
H	-0.751800	-2.088600	3.791800
H	-1.716300	-2.764600	2.488000
C	0.315000	-2.414700	1.926600
C	1.233800	-3.416400	2.275000
H	1.118600	-3.961200	3.205800
C	2.288800	-3.703700	1.400200
H	3.005900	-4.479900	1.657100
C	2.433800	-3.004600	0.194200
C	3.443900	-3.184800	-0.813000
H	4.212000	-3.942700	-0.675400
C	3.425500	-2.396600	-1.920100
H	4.171600	-2.497900	-2.701600
C	2.412300	-1.337400	-2.135900
C	1.480000	-1.987500	-0.091300

C	-3.543700	-0.091200	-1.388200
H	-4.192800	-0.254300	-2.254900
H	-4.162800	-0.235700	-0.493600
C	-3.002500	1.318800	-1.398600
C	-3.767400	2.330800	-2.004500
H	-4.715700	2.077700	-2.466200
C	-3.291400	3.634600	-2.007500
H	-3.863700	4.434000	-2.473200
C	-2.061200	3.915300	-1.409900
C	-1.469400	5.220300	-1.353300
H	-2.004900	6.055500	-1.799900
C	-0.261700	5.401100	-0.753200
H	0.217900	6.372500	-0.692300
C	0.431000	4.257500	-0.168300
C	-1.315800	2.841600	-0.808600
C	-3.413800	-0.509800	2.511700
H	-3.722500	-1.241500	1.753700
C	-4.192800	0.793600	2.256800
H	-4.054400	1.502000	3.078800
H	-5.265800	0.576600	2.196000
H	-3.892800	1.292300	1.332000
C	-3.772600	-1.086200	3.893600
H	-3.302900	-2.054400	4.088000
H	-4.857800	-1.231300	3.957500
H	-3.491700	-0.403800	4.702400
C	-0.938700	0.824600	3.515900
H	-1.569000	0.596500	4.386200
C	-1.128300	2.303800	3.133900
H	-0.540700	2.560800	2.248800

H	-0.790800	2.936700	3.962800
H	-2.170200	2.558800	2.926800
C	0.525200	0.565600	3.916300
H	0.701700	-0.457200	4.260900
H	0.787700	1.237400	4.741600
H	1.213900	0.775100	3.094200
C	-1.732900	-1.597500	-3.098900
H	-2.708100	-1.756900	-3.580400
C	-0.856300	-2.834300	-3.357700
H	0.076500	-2.785300	-2.791800
H	-0.592300	-2.868000	-4.420700
H	-1.366100	-3.771000	-3.118100
C	-1.085900	-0.344000	-3.717600
H	-1.696900	0.553800	-3.591300
H	-0.963400	-0.508900	-4.794600
H	-0.091600	-0.158600	-3.302000
C	-3.114000	-2.881800	-0.747600
H	-3.617300	-2.533100	0.164800
C	-2.209800	-4.060700	-0.344300
H	-1.761500	-4.545600	-1.214800
H	-2.805800	-4.818600	0.178300
H	-1.395900	-3.752900	0.314600
C	-4.205600	-3.336400	-1.732900
H	-4.909000	-2.535800	-1.982000
H	-4.784600	-4.154700	-1.288100
H	-3.775800	-3.712800	-2.666300
O	2.418100	1.984200	0.712500
C	4.595300	1.190400	-0.086100
C	5.405800	0.684900	-1.114700

C	5.069600	1.153000	1.230400
C	6.669800	0.163100	-0.832300
H	5.037400	0.692500	-2.138100
C	6.333100	0.623500	1.514500
H	4.441400	1.539900	2.025800
C	7.139400	0.129800	0.485500
H	7.286100	-0.222800	-1.640300
H	6.688300	0.601000	2.541800
H	8.122500	-0.277300	0.706400
C	3.253600	1.798600	-0.440100
H	2.733500	1.171100	-1.171600
H	3.405800	2.780900	-0.905500
H	2.068600	2.949900	0.680600
H	0.489100	0.806700	1.022000
H	1.201600	1.203600	0.719800

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G, G = -2659.621559 hartrees

Ru	-0.503500	-0.037400	0.056300
P	-0.849400	0.184700	2.336600
P	-2.626900	0.543700	-0.797500
O	0.277200	-1.844300	-3.901900
O	4.371900	1.513500	-1.400300
H	4.123200	0.628700	-1.067400
N	-0.852600	-1.975100	0.489100
N	-0.331900	-1.911900	-1.687800
N	-0.146700	2.155400	-0.629000
N	2.134800	1.852900	-1.016800

C	-1.457500	-1.562200	2.767900
H	-1.092600	-1.900400	3.740700
H	-2.550500	-1.498400	2.848200
C	-1.121700	-2.540800	1.667700
C	-1.146200	-3.941900	1.778900
H	-1.365900	-4.407100	2.733800
C	-0.876900	-4.719400	0.647300
H	-0.879000	-5.804300	0.725700
C	-0.593600	-4.117600	-0.588400
C	-0.263700	-4.757600	-1.833100
H	-0.240200	-5.844200	-1.889800
C	0.023500	-3.991600	-2.920500
H	0.283400	-4.436700	-3.876000
C	0.009100	-2.509000	-2.887900
C	-0.593900	-2.697300	-0.635600
C	-2.603400	2.384400	-0.507300
H	-3.315000	2.927600	-1.139800
H	-2.921300	2.547400	0.529000
C	-1.221900	2.959200	-0.715900
C	-1.139500	4.338300	-1.021600
H	-2.051600	4.924600	-1.054400
C	0.083700	4.908600	-1.281900
H	0.176600	5.966300	-1.515500
C	1.224600	4.086400	-1.280300
C	2.521100	4.567100	-1.619500
H	2.648600	5.619800	-1.858000
C	3.577400	3.703000	-1.654800
H	4.585200	4.008900	-1.910400
C	3.315400	2.334400	-1.342700

C	1.080900	2.694500	-0.965700
C	-2.205500	1.245600	3.129100
H	-3.065300	1.094500	2.466700
C	-1.847100	2.743200	3.119700
H	-1.092400	2.971700	3.878800
H	-2.735000	3.342000	3.356100
H	-1.456700	3.079500	2.155600
C	-2.634800	0.818000	4.545700
H	-2.989300	-0.215300	4.589300
H	-3.456700	1.459000	4.887500
H	-1.820200	0.926000	5.269700
C	0.608300	0.531300	3.492200
H	0.147900	0.885200	4.424200
C	1.484900	1.662200	2.920900
H	1.903200	1.350400	1.961800
H	2.299700	1.881200	3.622400
H	0.924100	2.589600	2.771600
C	1.444600	-0.716200	3.824100
H	0.885700	-1.444800	4.419700
H	2.315300	-0.417800	4.420800
H	1.795700	-1.192400	2.907200
C	-2.947200	0.466800	-2.661900
H	-3.791900	1.152400	-2.820000
C	-3.358400	-0.929000	-3.160100
H	-2.597700	-1.673100	-2.916700
H	-3.456900	-0.905400	-4.251400
H	-4.318000	-1.257400	-2.752500
C	-1.744500	0.984600	-3.472200
H	-1.457200	2.003300	-3.195500

H	-2.016000	1.000300	-4.534500
H	-0.878500	0.324900	-3.367500
C	-4.289700	0.085200	-0.014100
H	-4.199800	0.518300	0.990400
C	-4.473300	-1.432700	0.168700
H	-4.621700	-1.945300	-0.785000
H	-5.359800	-1.625700	0.785500
H	-3.612000	-1.893400	0.657000
C	-5.525300	0.720300	-0.676000
H	-5.439600	1.807800	-0.770700
H	-6.415700	0.514300	-0.069200
H	-5.710100	0.308100	-1.672600
O	1.493700	-0.459400	0.690200
C	3.740600	-1.262500	0.155000
C	4.614000	-1.987200	-0.678700
C	4.283400	-0.600200	1.263700
C	5.982200	-2.049100	-0.410300
H	4.210000	-2.505300	-1.546700
C	5.655300	-0.663600	1.538800
H	3.617600	-0.033100	1.901500
C	6.510300	-1.387500	0.705700
H	6.637300	-2.611400	-1.070800
H	6.055000	-0.141000	2.404600
H	7.575300	-1.433100	0.916400
C	2.247300	-1.240700	-0.173300
H	1.930300	-2.302600	-0.172700
H	2.147400	-0.911600	-1.223900

95

TS-GF , G = -2659.588332 hartrees

Ru	-0.089900	-0.277900	-0.063700
P	-0.787400	-1.155900	1.943000
O	4.154800	2.829600	-1.232300
H	3.214500	3.074800	-1.347800
N	1.951000	-0.563600	0.995500
N	3.089300	1.128500	-0.133600
C	0.710200	-2.172400	2.392500
H	0.778000	-2.396400	3.463400
H	0.602300	-3.135800	1.878300
C	1.988600	-1.518000	1.942900
C	3.185700	-1.970100	2.550100
H	3.127100	-2.748300	3.303500
C	4.392700	-1.441800	2.164100
H	5.329300	-1.793500	2.589600
C	4.394900	-0.401900	1.216600
C	5.587100	0.245400	0.786500
H	6.544200	-0.107400	1.161800
C	5.513500	1.306800	-0.069500
H	6.384300	1.846900	-0.422300
C	4.211300	1.729200	-0.468900
C	3.145800	0.056900	0.683000
C	-0.967100	-0.104200	3.504200
H	-0.873300	-0.837400	4.318100
C	-2.314900	0.618700	3.648700
H	-2.473500	1.349500	2.852600
H	-2.325500	1.156500	4.604900
H	-3.162200	-0.072400	3.659100
C	0.189800	0.900400	3.636800

H	1.171900	0.418700	3.668400
H	0.068900	1.465800	4.568100
H	0.186100	1.611200	2.806000
C	-2.113300	-2.504300	2.101700
H	-1.714600	-3.285600	1.438400
C	-3.501000	-2.117100	1.563600
H	-3.958300	-1.312200	2.143600
H	-4.166900	-2.987100	1.622200
H	-3.458500	-1.792000	0.524800
C	-2.232400	-3.107100	3.514200
H	-1.271900	-3.436400	3.923200
H	-2.890400	-3.984100	3.481700
H	-2.675700	-2.396500	4.218500
P	0.165800	-2.241200	-1.483100
O	-3.404400	3.268400	1.692400
N	-2.111900	-0.278100	-0.965200
N	-2.803900	1.497800	0.382400
C	-1.590200	-2.441400	-2.046300
H	-1.671300	-2.851800	-3.056800
H	-2.030600	-3.194200	-1.376400
C	-2.430000	-1.192400	-1.912600
C	-3.587200	-1.114200	-2.698700
H	-3.769000	-1.870400	-3.454400
C	-4.493600	-0.083700	-2.478000
H	-5.392600	0.006900	-3.084300
C	-4.260800	0.820500	-1.447300
C	-5.162800	1.886200	-1.108900
H	-6.066600	2.007500	-1.703600
C	-4.884500	2.711600	-0.069800

H	-5.539500	3.529200	0.214400
C	-3.662000	2.521200	0.726100
C	-3.062400	0.703000	-0.649200
C	0.564800	-4.038400	-1.011000
H	-0.025200	-4.182300	-0.095500
C	2.049100	-4.239900	-0.659800
H	2.676100	-4.194800	-1.556600
H	2.197500	-5.230000	-0.211700
H	2.421500	-3.492500	0.045500
C	0.116900	-5.105200	-2.026800
H	-0.955000	-5.067300	-2.238400
H	0.336100	-6.105400	-1.632300
H	0.652200	-5.010200	-2.977700
C	1.168200	-2.005000	-3.072800
H	1.318700	-3.011300	-3.485900
C	2.544700	-1.388100	-2.762200
H	2.426900	-0.373200	-2.375100
H	3.142000	-1.342300	-3.681500
H	3.112500	-1.970200	-2.030100
C	0.437000	-1.158000	-4.130900
H	-0.500500	-1.613700	-4.462500
H	1.079100	-1.059400	-5.015200
H	0.224100	-0.156400	-3.750500
O	0.553000	1.075100	-1.768300
C	0.470800	3.261900	-0.698200
C	0.030800	3.967900	0.430700
C	1.285300	3.909900	-1.641500
C	0.455600	5.281000	0.641700
H	-0.662300	3.498500	1.124100

C	1.695900	5.232300	-1.434600
H	1.540800	3.387200	-2.561000
C	1.295500	5.913900	-0.282300
H	0.114700	5.816300	1.523300
H	2.317500	5.728800	-2.175200
H	1.615700	6.938700	-0.116300
C	-0.095100	1.917700	-1.058100
H	-1.182500	1.957200	-1.137700
H	-0.295800	1.236400	0.577900

IV. Additional X-ray figures showing hydrogen bonding in 3 and 4

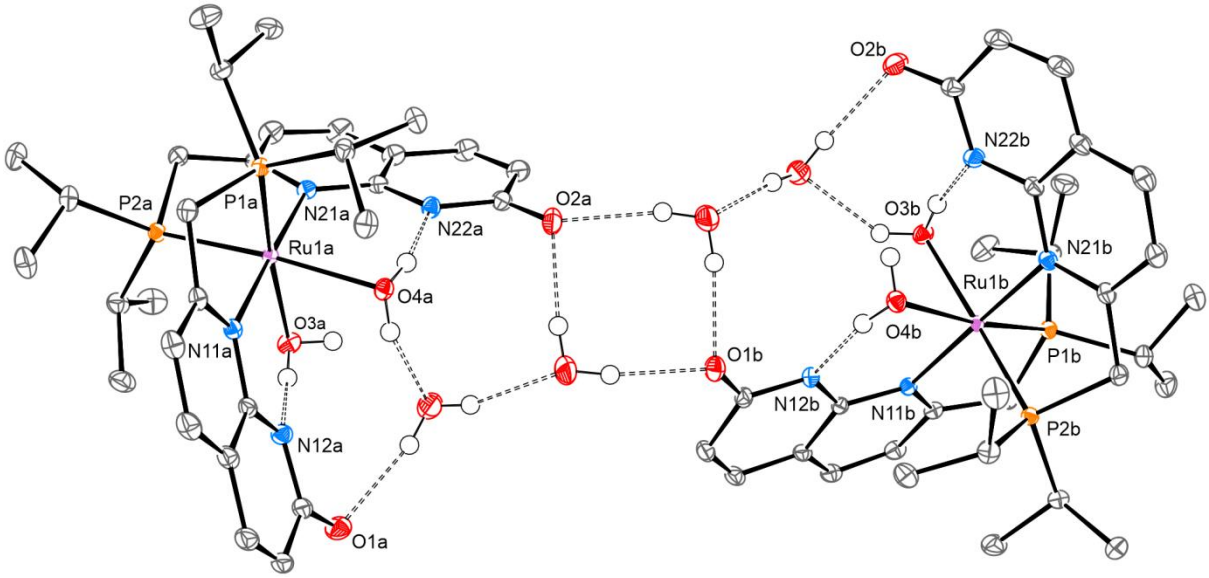

Figure S46. Hydrogen bonding and asymmetric cell of compound **3**.

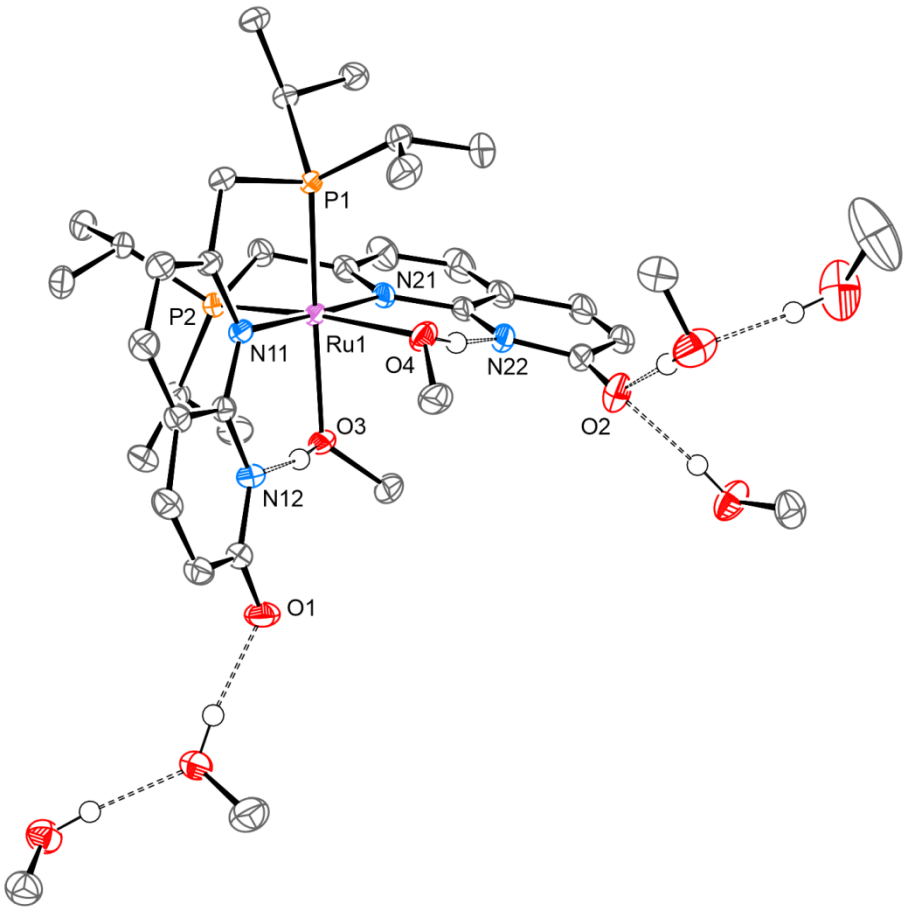

Figure S47. Hydrogen bonding and asymmetric cell of compound **4**. Minor disorder components are omitted for clarity.

V. References

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