Supporting Information

"Long Range" Metal-Ligand Cooperation in H_2 Activation and Ammonia-Promoted Hydride Transfer with a Ruthenium-Acridine Pincer Complex

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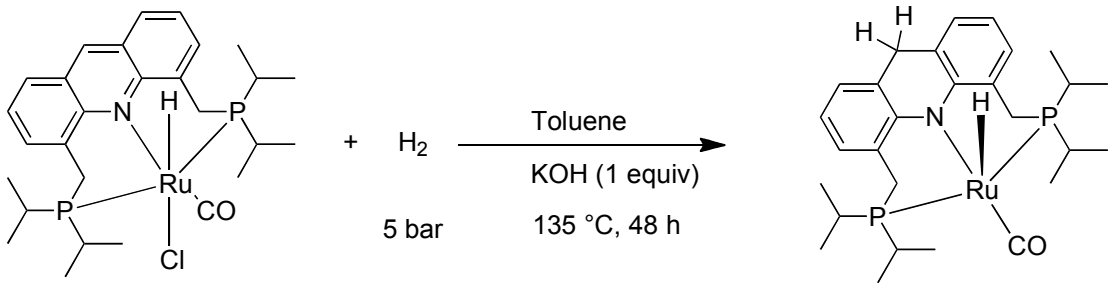
General Experimental

All experiments with metal complexes and phosphine ligands were carried out under an atmosphere of purified nitrogen in a Vacuum Atmospheres glovebox equipped with a MO 40-2 inert gas purifer or using standard Schlenk techniques. All solvents were reagent grade or better. All non-deuterated solvents were refluxed over sodium/benzophenone ketyl and distilled under argon atmosphere. Deuterated solvents were used as received. All solvents were degassed with argon and kept in the glove box over 4Å molecular sieves. The $RuHCl(CO)(PPh_3)_3$[1], 4,5-bis(bromomethyl)acridine[2], 4,5-bis(di-*iso*-propylphosphinomethyl)acridine (A-^{i}Pr-PNP)[3] and [RuH(Cl)(A-^{i}Pr-PNP)(CO)][3] **1** were prepared according to literature procedures.

^{1}H, ^{13}C and ^{31}P NMR spectra were recorded at 500, 100, and 162 MHz, respectively, using a Bruker AMX-500 NMR spectrometers. ^{1}H and ^{13}C{^{1}H} NMR chemical shifts are reported in ppm downfield from tetramethylsilane. ^{31}P NMR chemical shifts are reported in parts per millon downfield from H_3PO_4 and referenced to an external 85% solution of phosphoric acid in D_2O. Abbreviations used in the NMR follow-up experiments: b, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet, v, virtual.

Synthesis of RuH(AH-^{i}Pr-PNP)(CO) 2:

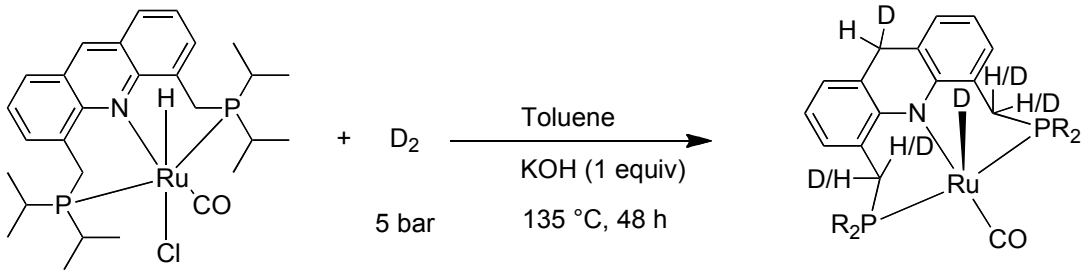


1 **2**

Complex **1** (20 mg, 0.033 mmol), KOH (1.9 mg, 1 equiv) and toluene (2 ml) were charged in a Fischer-Porter tube under N_2 atmosphere. The Fischer-Porter tube was pressurized with H_2 (5 bar) and the reaction mixture was heated at 135 °C for 2 days. The reaction mixture was cooled and the solvents were removed under vacuum. ^{31}P{^{1}H} NMR of the reaction mixture indicated the formation of complex **2**. Pentane wash of the residue gave the clean complex **2** quantitatively.

$^{31}P\{^{1}H\}$ NMR (Benzene-d_6): 74.73 (s). ^{1}H NMR (benzene-d_6): - 21.09 (t, $^{2}J_{PH}$ = 22.3 Hz, 1H, Ru-H), 0.37 (vq, $^{3}J_{PH}$ = 13.4 Hz, $^{3}J_{HH}$ = 6.6 Hz, 6H, P(CH(CH_3)$_2$)$_2$), 0.68 (vq, $^{3}J_{PH}$ = 13.9 Hz, $^{3}J_{HH}$ = 6.9 Hz, 6H, P(CH(CH_3)$_2$)$_2$), 0.85 (vq, $^{3}J_{PH}$ = 13.6 Hz, $^{3}J_{HH}$ = 6.8 Hz, 6H, P(CH(CH_3)$_2$)$_2$), 0.92 (vq, $^{3}J_{PH}$ = 14.9 Hz, $^{3}J_{HH}$ = 7.5 Hz, 6H, P(CH(CH_3)$_2$)$_2$), 1.12 (m, 2H, P(C*H*(CH$_3$)$_2$)$_2$), 1.65 (m, 2H, P(C*H*(CH$_3$)$_2$)$_2$), 2.36 (m, 2H, -CH*H*P), 2.61 (overlapping two d, $^{2}J_{HH}$ = 12.6 Hz, 2H, -C*H*HP), 3.24 (d, $^{2}J_{HH}$ = 14.3 Hz, 1H, Ar-C*H*H-Ar), 3.41(d, $^{2}J_{HH}$ = 14.9 Hz, 1H, Ar-CH*H*-Ar), 6.60 (m, 4H, Ar*H*), 6.87 (m, 2H, Ar*H*). $^{13}C\{^{1}H\}$ NMR (C_6D_6): 17.56 (s, P(CH(*C*H$_3$)$_2$)$_2$), 18.65 (s, P(CH(*C*H$_3$)$_2$)$_2$), 19.14 (s, P(CH(*C*H$_3$)$_2$)$_2$), 20.32 (s, P(CH(*C*H$_3$)$_2$)$_2$), 24.20 (t, $^{1}J_{PC}$ = 7.8 Hz, P(*C*H(CH$_3$)$_2$)$_2$), 25.58 (t, $^{1}J_{PC}$ = 15.2 Hz, P(*C*H(CH$_3$)$_2$)$_2$), 27.71 (t, $^{1}J_{PC}$ = 8.5 Hz, 2 × *C*H$_2$P), 36.48 (s, C_9, Ar*C*H$_2$Ar), 119.36 (s, C_2, C_7, A-PNP), 121.59 (s, C_4, C_5, A-PNP), 126.51 (s, C_1, C_8, A-PNP), 128.29 (s, C_3, C_6, A-PNP), 141.12 (s, C_{8a}, C_{9a}, A-PNP), 152.98 (m, C_{4a}, C_{10a}, A-PNP), 209.7 (m, Ru-CO); IR (KBr, pellet): 2959, 2871, 1922, 1898, 1458, 1435 cm.$^{-1}$; MS (ESI, MeOH): 570 (60%, M^+), 568 (100%, $(M-2H)^+$); Anal. Calcd. for $C_{28}H_{41}NOP_2Ru$: C, 58.93; H, 7.24. Found: C 58.39; H, 7.05.

Synthesis of RuH/D(AH/D-*i*Pr-PNP)(CO) 3:



1 **3**

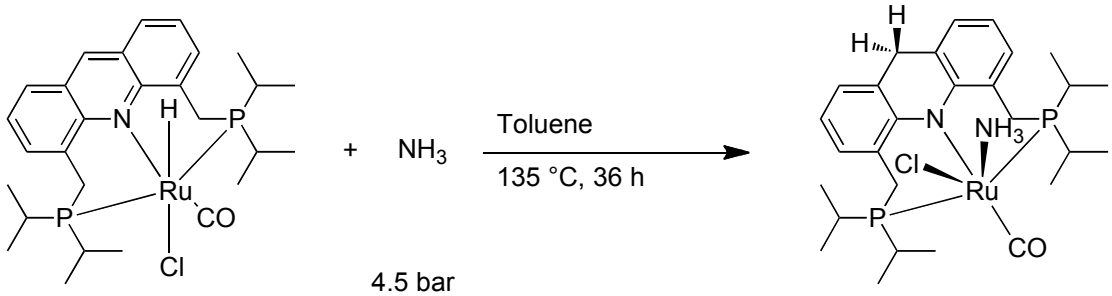
R = -C(H/D)(C(H/D)$_3$)$_2$

Complex **1** (20 mg, 0.033 mmol), KOH (1.9 mg, 1 equiv) and toluene (2 ml) were charged in a Fischer-Porter tube under the N_2 atmosphere. The Fischer-Porter tube was pressurized with D_2 (5 bar) and the reaction mixture was heated at 135 °C for 2 days. The reaction mixture was cooled and the solvents were removed under vacuum. Pentane wash of the residue gave a clean complex **3** as an orange colored solid**.** $^{31}P\{^{1}H\}$ NMR (Benzene-d_6): 74.61 (s). ^{1}H NMR (benzene-d_6): - 20.85 (t, $^{2}J_{PH}$ = 22.3 Hz, Ru-H, minor peak, approx 0.1H), 0.64 (m, P(CH(CH_3)$_2$)$_2$, minor peak), 0.96 (vq, $^{3}J_{PH}$ = 13.7 Hz, $^{3}J_{HH}$ = 6.9 Hz, 6H, P(CH(CH_3)$_2$)$_2$), 1.14 (vq, $^{3}J_{PH}$ = 13.6 Hz, $^{3}J_{HH}$ = 6.9 Hz, 6H, P(CH(CH_3)$_2$)$_2$), 1.46 (m, 2H, P(C*H*(CH$_3$)$_2$)$_2$), 1.93 (m, 2H, P(C*H*(CH$_3$)$_2$)$_2$), 2.10 (s, minor peak), 2.52 (m, minor peak), 2.88 (s, minor peak), 3.51 (s, minor peak), 3.55 (s, minor peak), 3.68 (s, 1H), 3.73 (s, minor peak), 6.88-6.90 (m, 4H, Ar*H*), 7.14-7.16 (m, 2H, Ar*H*). ^{2}H NMR (benzene): -20.75 (s, 1D), 0.59 (s, 5D), 1.14 (s, 1D), 1.40 (s, 6D), 2.48 (s, 2D), 2.83 (s, 2D), 3.55 (m, 1D), $^{13}C\{^{1}H\}$ NMR (C_6D_6): 17.4 (m, P(CH(*C*D$_3$)$_2$)$_2$), 18.6 (m, P(CH(*C*D$_3$)$_2$)$_2$), 19.0 (s, P(CH(*C*H$_3$)$_2$)$_2$), 19.4 (s, P(CH(*C*H$_3$)$_2$)$_2$), 20.1 (m, P(CH(*C*D$_3$)$_2$)$_2$), 24.3 (m, P(*C*H(CH$_3$)$_2$)$_2$), 25.7 (m, P(*C*H(CD$_3$)$_2$)$_2$), 27.6 (m, *C*D$_2$P), 36.5 (t, C_9, Ar*C*HDAr, J_{CD} = 21 Hz), 36.9 (C_9, Ar*C*H$_2$Ar), 119.7, 121.9, 122.0,126.8, 126.9, 126.9, 128.3, 128.6, 128.9, 153.3 (t, J_{PC} = 5 Hz), 210.5 (m, Ru-CO). ^{1}H and D NMR indicate that, under these experimental conditions all the aliphatic protons (CH_3, CH_2 and CH) of complex **3** are deuterated. MS (ESI, CH_3CN): 605 (20%), 591 (100%).

X-ray Crystal Structure Determination of 2. A crystal was mounted on a nylon loop and flash frozen in a nitrogen stream at 100(2) K. Data were collected on a Bruker Appex2 Kappa CCD diffractometer mounted on a FR590 generator equipped with a sealed tube with Mo *Kα* radiation (λ = 0.71073 Å) and a graphite monochromator. Structure was solved using direct methods with SHELXS-97 based on F^2.

Complex 2: $C_{86}H_{110}N_2O_7P_4Ru_2$ (2*$C_{28}H_{40}N_1O_1P_2Ru$+5*C_6H_6+5*O), yellow, 0.50×0.50×0.10 mm^3, monoclinic, $P2_1/c$ (No. 14), a = 14.941(3) Å, b = 12.640 (3) Å, c = 20.960 (4) Å, β = 97.94(3)° from 20 degrees of data, V = 3920.5 (14) Å^3, Z = 2, Fw = 1609.78 g/mol, D_c = 1.364 Mg/m^3, μ = 0.523 mm^{-1}. Full matrix least-square refinement based on F^2 with SHELXS-97, 466 parameters with 1 restraints gave an agreement factor R_1 = 0.0266 (based on F^2) for data with $I > 2\sigma(I)$ and R_1 = 0.035 for all data (14926 reflections) with a goodness-of-fit on F^2 1.079. The largest electron density peak = 0.855 e/ Å^{-3} and deepest hole = -0.557 eÅ^{-3}.

Synthesis of Ru(NH$_3$)(AH-^{i}Pr-PNP)(Cl)(CO) 4:



1 **4**

Complex **1** (121 mg, 0.2 mmol) in toluene (4 mL) was added to a 90 mL Fischer-Porter tube under an atmosphere of purified nitrogen in a Vacuum Atmospheres glovebox. The tube was taken out of the box and ammonia (65 psi) was charged into the Fischer-Porter tube and heated in an oil bath at 135 ^{o}C for 36 h. After cooling to room temperature, the ammonia gas was released under vacuum and toluene was completely evaporated. The crude products was dissolved in methylene chloride (15 mL) and filtered. The filtrate was concentrated to 3 ml and pentane (8 ml) was added, causing precipitation of a yellow solid. The solid was filtered, washed with 10% methylene chloride in pentane (3 x 3 ml), and dried under vacuum for overnight to afford complex **4** (65 mg, 52.4%). $^{31}P\{^1H\}$ (162 MHz, CD_2Cl_2): 79.5 (d, J = 11.8 Hz), 82.9 (d, J = 11.8 Hz), ^1H (500 MHz, CD_2Cl_2): 1.32-1.48 (m, 25H, P(CH(CH_3)$_2$)$_4$ and P(CH(CH$_3$)$_2$), 1.73 (br s, 3H, NH_3), 2.28-2.36 (m, 1H, P(CH(CH$_3$)$_2$)), 2.38-2.47 (m, 2H, P(CH(CH$_3$)$_2$)), 2.51 (dd, J_{HH} = 12.5 Hz, J_{PH} = 7.0 Hz, 1H, -CHHP), 2.59 (dd, J_{HH} = 12.5 Hz, J_{PH} = 7.5 Hz, 1H, -CHHP), 3.12-3.23 (m, 2H, -CHHP), 3.67 (d, J = 16.5 Hz, 1H, Ar-CHH-Ar), 3.78 (d, J = 16.5 Hz, 1H, Ar-CHH-Ar), 6.68 (dd, 2H, J_{HH} = 13.7 Hz, J_{HH} = 7.5 Hz, 2H, Ar-CH), 6.91 (d, J_{HH} = 7.5 Hz, 2H, Ar-CH), 6.94 (d, J_{HH} = 7.5 Hz, 1H, Ar-CH), 6.99 (d, J_{HH} = 7.5 Hz, 1H, Ar-CH). $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2): 19.7 (s, P(CH(CH_3)$_3$)$_2$), 19.8 (d, J_{PC} = 6.3 Hz, P(CH(CH_3)$_3$)$_2$), 19.8 (d, J_{PC} = 6.1 Hz, P(C(CH_3)$_3$)$_2$), 19.9 (d, J_{PC} = 5.7 Hz, P(CH(CH_3)$_3$)$_2$)), 20.0 (d, J_{PC} = 5.6 Hz, P(CH(CH_3)$_3$)$_2$)), 20.3 (s, P(CH(CH_3)$_3$)$_2$), 20.7 (d, J_{PC} = 2.1 Hz, P(CH(CH_3)$_3$)$_2$)), 21.1 (d, J_{PC} = 1.0 Hz, P(CH(CH_3)$_3$)$_2$)), 26.1 (d, J_{PC} = 25.3 Hz, P(CH(CH$_3$)$_3$)$_2$)), 27.2 (d, J_{PC} = 26.4 Hz, P(CH(CH$_3$)$_3$)$_2$)), 28.3 (d, J_{PC} = 16.9 Hz, PCH_2)), 28.6 (d, J_{PC} = 17.7 Hz, PCH_2)), 30. 9 (br m, P(CH(CH$_3$)$_3$)$_2$)), 34.3 (s, Ar-CH_2-Ar), 118.1 (d, J_{PC} = 14.0 Hz, Ar-CH), 122.6 (d, J_{PC} = 4.8 Hz, quat-C), 123.6 (d, J_{PC} = 4.5 Hz, quat-C), 124.9

(d, J_{PC} = 1.1 Hz, Ar-*C*H), 126.1 (d, J_{PC} = 1.2 Hz, Ar-*C*H), 127.4 (d, J_{PC} = 4.6 Hz, Ar-*C*H), 127.9 (d, J_{PC} = 4.6 Hz, Ar-*C*H), 129.8 (s, quat-*C*), 131.4 (s, quat-*C*), 152.6 (d, J_{PC} = 1.1 Hz, quat-*C*), 154.2 (d, J_{PC} = 1.6 Hz, quat-*C*), 203.8 (t, J_{PC} = 14.7 Hz, Ru-CO). **Assignment of signals was confirmed by DEPT 135, H-H and C-H correlation**. IR (KBr, pellet): 3355, 3302, 2962, 2922, 2873, 1922 (ν_{CO}), 1583, 1436 cm.$^{-1}$ MS (ESI, CH3CN): 611 [54%, (M-(Cl,NH_3)+(CH_3CN)$^+$], 570 (100%, (M-(Cl,NH_3)$^+$); MS (ESI, MeOH): 644 (20%, (M+Na-H)$^+$), 604 (8%, (M-NH_3-H)$^+$), 568 (100%, (M-(Cl,NH_3,2H)$^+$). Anal. Calcd. for $C_{29}H_{45}Cl_3N_2OP_2Ru$ (M+CH_2Cl_2): C, 49.26; H, 6.41, N, 3.96; Found: C, 49.40; H, 6.45, N, 3.95.

X-ray Crystal Structure Determination of 4. A crystal was mounted on a nylon loop and flash frozen in a nitrogen stream at 120(2) K. Data were collected on a Nonius Kappa CCD diffractometer mounted on a FR590 generator equipped with a sealed tube with Mo *Kα* radiation (λ = 0.71073 Å) and a graphite monochromator. Structure was solved using direct methods with SHELXS-97 based on F^2.
Complex 4: $C_{28}H_{43}ClN_2OP_2Ru$+ C_7H_8, Orange plate, 0.30×0.30×0.10 mm^3, monoclinic, $P2_1/c$, a = 11.7947(4) Å, b = 12.4346 (5) Å, c = 21.5285 (12) Å, a = 90° β = 102.34(3)°, γ = 90° from 8819 reflections, V = 3133.1 (2) Å^3, Z = 4, Fw = 668.17, D_c = 1.417 Mg/m^3, μ = 0.715 mm^{-1}. Full matrix least-square refinement based on F^2 with SHELXS-97, 362 parameters with 2 restraints gave an agreement factor R_1 = 0.0428 (based on F^2) for data with $I > 2\sigma(I)$ and R_1 = 0.0693 for all data (11875 reflections) with a goodness-of-fit on F^2 1.036. The largest electron density peak = 2.495 eÅ^{-3} and hole = -1.041 eÅ^{-3}. Disordered toluene solvent has been modeled.

Computational Details:

All calculations were carried out using Gaussian 03 Revision E.01[4] or Gaussian 09 Revision A.02.[5] The former was locally modified with the MNGFM patch;[6] this patch from the University of Minnesota adds the M06 (*vide infra*) family of DFT exchange-correlation functionals to the commercial version. The Minnesota06 (M06) hybrid meta-GGA DFT functional was used.[7] This functional has been shown to yield more reliable reaction barrier heights for transition metal reactions than other "conventional" exchange-correlation functionals.[7-8] Two basis set-RECP (relativistic effective core potential) combinations were used. The first, denoted SDD(d), is the combination of the Huzinaga-Dunning double-ζ basis set[9] on lighter elements with the Stuttgart-Dresden basis set-RECP combination[10] on transition metals; polarization functions (i.e., the D95(d) basis set) was used on second-row (i.e., phosphorus) atoms. The second, denoted SDB-cc-pVDZ, combines the Dunning cc-pVDZ basis set[11] on the main group elements, and the Stuttgart-Dresden basis set-RECP[10] on the transition metals with an added *f*-type polarization exponent taken as the average of the two *f*-exponents given in the appendix of ref [12]. Geometry optimizations were carried out using the former basis set while the energetics of the reaction were calculated at these geometries with the latter basis set.

The accuracy of the DFT method was improved by adding an *a posteriori* empirical dispersion correction as recommended by Grimme.[13] This is a

correction that is added to the final energy and is a function of the geometry of the final, optimized geometry. Briefly, the dispersion energy is equal to:[13]

$$E_{disp} = -s_6 \sum_{i=1}^{N_{at}-1} \sum_{j=i+1}^{N_{at}} \frac{C_6^{ij}}{R_{ij}^6} f_{dmp}\left(R_{ij}\right)$$

$$f_{dmp}\left(R_{ij}\right) = \left(1 + \exp\left(-d\left(\frac{R_{ij}}{R_r} - 1\right)\right)\right)^{-1}$$

$$C_6^{ij} = \sqrt{C_6^i C_6^j}$$

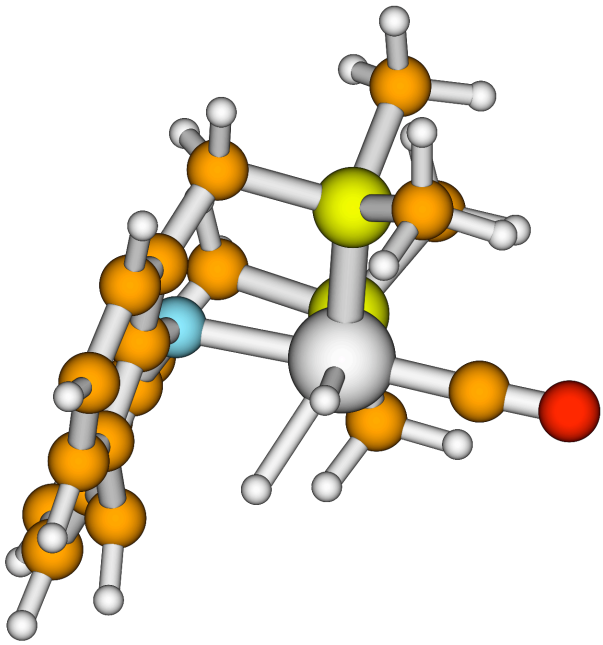
where R_r is the sum of van der Waal radii (r_{vdW}) of the two atoms in question and C_6^i is an empirical constant; these values for H-Xe have been determined by Grimme.[14] The s_6 is an empirical scaling factor unique for each DFT functional. For M06, it has been determined to be 0.25.[15] The use of this correction is identified by appending "+d" to the common name of the DFT functional used. The r_{vdW} and C_6^i values are missing for the third-row transition metals (i.e., the entire 6th row of the periodic table). These values for the first and second row transition metals were determined by Grimme by averaging the values for the Groups 2 and 13 elements of the same row.[14] Thus, the r_{vdW} and C_6^i parameters for the third row transition metals were determined by averaging the parameters for Ba and Tl; the lanthanides were assigned parameters in the same manner. The parameters for these two elements, as well as the rest of the 6th row of the periodic table, were determined by a geometric extrapolation of the parameters for the preceding two rows.

Bulk solvent effects were approximated by single point energy calculations using a polarizable continuum model (PCM),[16] specifically the integral equation formalism model (IEF-PCM)[16a,b,17] with tetrahydrofuran (THF) as the solvent as in the experiments. Since there are some definition changes in the solvation (SCRF) module between Gaussian 03 and 09, all solvation calculations were performed consistently using the latter programme.

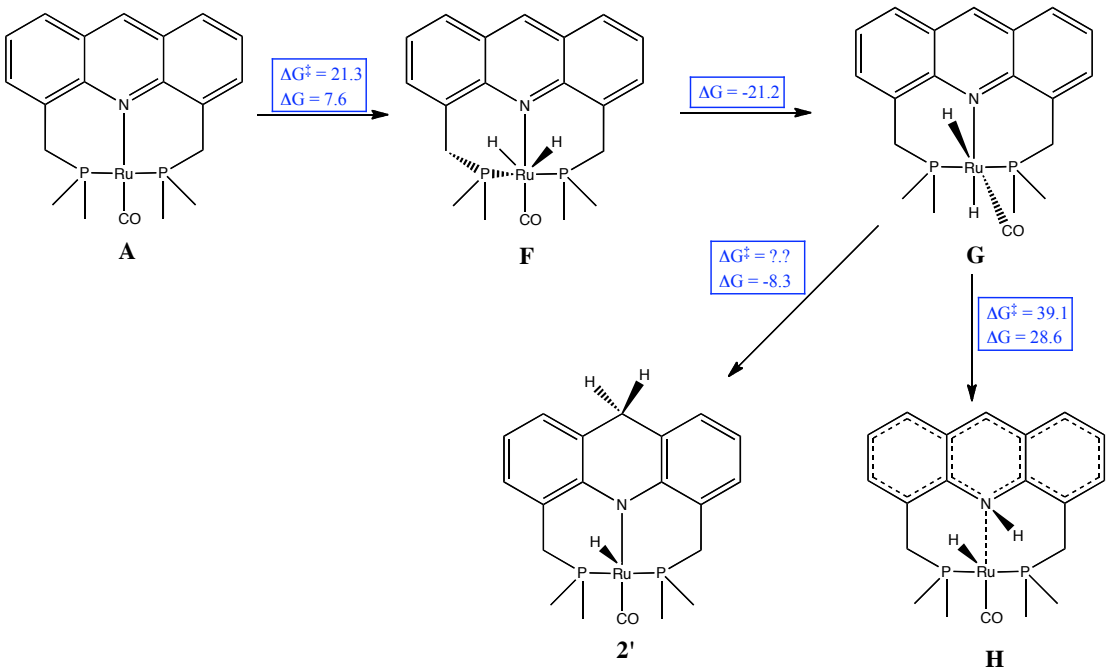
Geometries were optimized using the default pruned (75,302) grid, while the "ultrafine" (i.e., a pruned (99,590)) grid was used for energy and solvation calculations.

The connectivity of the transition states were confirmed by performing intrinsic reaction coordinate (IRC) calculations.[18]

Figure S1. Calculated (DFT) structure of **TS(C-D)** (see Scheme 2 in the paper). Color scheme: H – white, C – brown, N – blue, O – red, P – yellow, Ru – grey.



Scheme S1. An alternative pathway to H_2 addition across acridine-Ru system. The intermediates connecting **H** to **2'** (i.e., proton migration around the acridine central ring, **I** and **J**) and the three connecting transition states were located but involve barriers even higher that **TS(G-H)**.



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Cartesian coordinates of all DFT-optimized geometries:

```
Geometry of complex: 2'
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50
Stoichiometry = H25C20NOP2Ru
   C    -3.480501    2.056755   -0.866160
   C    -2.365872    1.201427   -0.877868
   C    -1.192934    1.560169   -0.159093
   C    -1.218206    2.767877    0.584676
   C    -2.331985    3.610484    0.568740
   C    -3.474078    3.267023   -0.164957
   C    -0.000001    3.071388    1.409291
   C     1.218203    2.767879    0.584673
   C     1.192933    1.560171   -0.159095
   C     2.365871    1.201430   -0.877870
   C     3.480498    2.056762   -0.866167
   C     3.474072    3.267031   -0.164966
   C     2.331980    3.610490    0.568733
   H    -4.366580    1.759411   -1.425347
   H    -2.303616    4.532349    1.146536
   H    -4.342328    3.918400   -0.180154
   H    -0.000001    4.107921    1.765647
   H     4.366577    1.759419   -1.425354
   H     4.342320    3.918410   -0.180166
   H     2.303609    4.532356    1.146529
   N     0.000000    0.760263   -0.167890
   Ru    0.000002   -1.306593    0.228461
   H     0.000002   -2.308675   -1.011821
   C    -2.498721   -0.137893   -1.546761
   H    -1.692437   -0.339039   -2.265877
   H    -3.469951   -0.238943   -2.049576
   C     2.498724   -0.137891   -1.546760
   H     1.692442   -0.339039   -2.265878
   H     3.469955   -0.238942   -2.049573
   P    -2.300769   -1.386164   -0.192154
   P     2.300770   -1.386161   -0.192152
   C     3.638237   -0.951082    1.004711
   H     3.737837   -1.762706    1.733919
   H     4.593375   -0.808465    0.482356
   H     3.379811   -0.028369    1.534111
   C     2.929172   -2.965487   -0.905548
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H	3.991615	-2.883910	-1.165878
H	2.793773	-3.774010	-0.178012
H	2.347862	-3.210356	-1.801011
C	-3.638240	-0.951081	1.004704
H	-4.593372	-0.808446	0.482343
H	-3.737856	-1.762709	1.733905
H	-3.379806	-0.028375	1.534112
C	-2.929173	-2.965487	-0.905556
H	-2.793781	-3.774012	-0.178021
H	-3.991614	-2.883906	-1.165891
H	-2.347858	-3.210356	-1.801016
C	0.000005	-2.870629	1.197793
O	0.000004	-3.863313	1.859720
H	0.000001	2.415612	2.298813

Geometry of complex: TS(A-B)

48

Stoichiometry = H23C20NOP2Ru

C	-3.401255	2.067372	-0.308355
C	-2.351652	1.245774	-0.691264
C	-1.005455	1.629684	-0.347619
C	-0.774638	2.931831	0.235548
C	-1.897225	3.722662	0.640104
C	-3.180086	3.290750	0.391011
C	0.542172	3.402873	0.326142
C	1.612566	2.642172	-0.193516
C	1.340732	1.323440	-0.685229
C	2.413883	0.513841	-1.173558
C	3.701508	1.033176	-1.181939
C	3.975573	2.346682	-0.711100
C	2.951426	3.132659	-0.221737
H	-4.417587	1.778714	-0.570633
H	-1.711640	4.679564	1.122806
H	-4.031911	3.893811	0.690616
H	0.736639	4.383621	0.756986
H	4.517826	0.415867	-1.552794
H	4.994577	2.720731	-0.732078
H	3.146727	4.134748	0.153722
N	0.063064	0.787868	-0.633323
Ru	-0.176663	-0.863490	0.706319
C	-2.629511	-0.004302	-1.483701
H	-1.923151	-0.092621	-2.321601
H	-3.655681	0.000393	-1.877805
C	2.148940	-0.899993	-1.602678
H	1.319397	-0.955022	-2.323369
H	3.044153	-1.354689	-2.050632
P	-2.316108	-1.488335	-0.394283
P	1.593821	-1.919739	-0.133695
C	3.160815	-2.142472	0.808676
H	2.974883	-2.766424	1.689268
H	3.930263	-2.607479	0.178515
H	3.505873	-1.161772	1.154733
C	1.371615	-3.586823	-0.905734
H	2.279057	-3.903725	-1.437695
H	1.132397	-4.313047	-0.121597
H	0.530159	-3.545136	-1.607464
C	-3.853280	-1.485738	0.639700

H	-4.753393	-1.497666	0.009774
H	-3.852548	-2.360902	1.297624
H	-3.859751	-0.585870	1.265253
C	-2.664818	-2.881950	-1.568009
H	-2.571209	-3.838310	-1.042032
H	-3.672348	-2.798059	-1.996104
H	-1.927874	-2.857820	-2.380238
C	0.674270	-0.942917	2.323457
O	1.202213	-0.975205	3.403557

Geometry of complex: TS(A-F)

50

Stoichiometry = H25C20NOP2Ru

C	0.932336	3.899344	0.375733
C	0.458899	2.683946	-0.109857
C	1.333419	1.524141	-0.067362
C	2.733230	1.823417	0.155593
C	3.176401	3.102095	0.608179
C	2.272865	4.119151	0.784944
C	3.679333	0.846275	-0.165910
C	3.287340	-0.457326	-0.463294
C	1.889984	-0.805689	-0.283466
C	1.632108	-2.227037	-0.119128
C	2.623914	-3.128845	-0.501376
C	3.919475	-2.747236	-0.933937
C	4.267500	-1.422889	-0.846278
H	0.244426	4.741885	0.386120
H	4.237690	3.238831	0.801734
H	2.576532	5.091298	1.158726
H	4.737337	1.102463	-0.164385
H	2.399273	-4.189800	-0.408978
H	4.634003	-3.502241	-1.245201
H	5.279906	-1.078889	-1.043321
N	0.923985	0.204624	-0.260733
Ru	-1.144466	-0.505154	-0.694067
C	-0.901433	2.751784	-0.758353
H	-0.817817	2.507228	-1.827751
H	-1.292034	3.777229	-0.671828
C	0.487143	-2.911587	0.620993
H	-0.004220	-3.626872	-0.054363
H	0.928572	-3.492299	1.452426
P	-2.097714	1.521417	-0.098993
P	-0.880668	-1.820938	1.195116
C	-0.222012	-1.200514	2.816434
H	-1.019444	-0.673732	3.353201
H	0.145793	-2.028130	3.438562
H	0.597056	-0.494699	2.631655
C	-2.098330	-3.083654	1.777582
H	-1.629660	-3.802275	2.463592
H	-2.926943	-2.582357	2.289778
H	-2.505187	-3.613363	0.908951
C	-2.310914	2.130469	1.641169
H	-2.602022	3.190102	1.668158
H	-3.077248	1.528977	2.144335
H	-1.361070	2.000863	2.174793
C	-3.671692	2.103368	-0.874214
H	-4.505569	1.478930	-0.534646

H	-3.877072	3.153138	-0.624186
H	-3.586461	1.988639	-1.960651
C	-2.808512	-1.145821	-1.138418
O	-3.900776	-1.554213	-1.403361
H	-0.320589	-1.461540	-1.940671
H	-0.571037	-0.652812	-2.361125

Geometry of complex: B

48

Stoichiometry = H23C20NOP2Ru

C	-3.278727	2.173630	-0.308322
C	-2.316899	1.276253	-0.737322
C	-0.921970	1.563222	-0.489748
C	-0.543719	2.863983	0.026537
C	-1.584505	3.738487	0.486868
C	-2.908842	3.395490	0.336362
C	0.803397	3.233458	-0.008736
C	1.783659	2.335876	-0.509073
C	1.371851	1.026532	-0.913435
C	2.344621	0.041694	-1.259966
C	3.687787	0.403100	-1.295528
C	4.098255	1.724814	-0.980052
C	3.166126	2.667272	-0.578478
H	-4.330307	1.952146	-0.480766
H	-1.301851	4.689394	0.933128
H	-3.688743	4.068638	0.680759
H	1.106480	4.217542	0.344333
H	4.434268	-0.347502	-1.550208
H	5.152273	1.982569	-1.023638
H	3.478337	3.666827	-0.283697
N	0.037593	0.639246	-0.885721
Ru	-0.309688	-0.617402	0.821936
C	-2.691371	0.012648	-1.467935
H	-2.087286	-0.091705	-2.380019
H	-3.756773	0.002452	-1.734639
C	1.910377	-1.385674	-1.443603
H	1.055366	-1.458994	-2.131765
H	2.734540	-2.010314	-1.818866
P	-2.251838	-1.429593	-0.374867
P	1.293394	-2.097099	0.192341
C	2.871081	-2.261082	1.136024
H	2.670825	-2.702086	2.118318
H	3.586718	-2.888194	0.587382
H	3.303243	-1.265403	1.287027
C	0.981132	-3.858689	-0.291848
H	1.876198	-4.302620	-0.748363
H	0.702950	-4.433443	0.598192
H	0.151935	-3.901296	-1.007720
C	-3.734915	-1.516030	0.724668
H	-4.650196	-1.675235	0.139610
H	-3.614818	-2.325402	1.451932
H	-3.813901	-0.568835	1.271591
C	-2.509073	-2.874902	-1.502963
H	-2.402565	-3.810435	-0.942689
H	-3.508095	-2.837152	-1.955368
H	-1.757615	-2.850492	-2.301531
C	0.846973	0.100355	2.086829

O	1.518425	0.564787	2.957260

Geometry of complex: TS(B-C)

50
Stoichiometry = H25C20NOP2Ru

C	-3.710592	1.562860	-0.545680
C	-2.545080	0.870005	-0.821086
C	-1.280409	1.499528	-0.553898
C	-1.248723	2.852211	-0.062740
C	-2.481744	3.518040	0.221533
C	-3.683628	2.884860	-0.008076
C	0.003747	3.464275	0.114089
C	1.183735	2.786393	-0.238700
C	1.073784	1.436963	-0.725725
C	2.254060	0.737370	-1.153379
C	3.482122	1.363448	-1.034439
C	3.600491	2.686365	-0.511329
C	2.477048	3.385299	-0.130531
H	-4.669419	1.088655	-0.748516
H	-2.449278	4.531550	0.615270
H	-4.620459	3.390639	0.205334
H	0.059758	4.479556	0.504196
H	4.378426	0.834981	-1.354656
H	4.584365	3.136577	-0.423072
H	2.552877	4.397029	0.261403
N	-0.133003	0.786054	-0.783946
Ru	-0.008628	-0.863192	0.971760
C	-2.572258	-0.526417	-1.370879
H	-1.865058	-0.626200	-2.207072
H	-3.580454	-0.800949	-1.712584
C	2.128212	-0.654778	-1.700263
H	1.311243	-0.704248	-2.434783
H	3.063160	-0.982331	-2.176913
P	-1.987771	-1.751136	-0.080838
P	1.651923	-1.870311	-0.353936
C	3.300475	-2.200682	0.413203
H	3.182411	-2.910018	1.239104
H	4.009919	-2.600574	-0.323552
H	3.690706	-1.262923	0.826353
C	1.425262	-3.398156	-1.378224
H	2.340049	-3.630255	-1.939417
H	1.169722	-4.243909	-0.730602
H	0.604282	-3.239240	-2.088236
C	-3.469239	-1.828582	1.024358
H	-4.371516	-2.107038	0.464070
H	-3.288022	-2.560490	1.819222
H	-3.617322	-0.846290	1.487532
C	-2.179959	-3.341605	-1.012527
H	-1.907961	-4.179503	-0.361422
H	-3.214687	-3.468162	-1.356336
H	-1.513227	-3.346917	-1.882247
C	1.367929	-0.185953	2.030568
O	2.233445	0.250334	2.725146
H	-1.176969	-0.088902	2.022822
H	-0.943108	-0.932611	2.407085

Geometry of complex: C

50
Stoichiometry = H25C20NOP2Ru

C	-4.042225	-0.760138	-0.387191
C	-2.746601	-0.521026	-0.803007
C	-2.159876	0.764151	-0.525580
C	-2.889872	1.735300	0.251145
C	-4.228236	1.436602	0.656926
C	-4.792285	0.224188	0.329857
C	-2.232937	2.932729	0.580057
C	-0.908807	3.155633	0.168769
C	-0.280767	2.140187	-0.638823
C	1.080871	2.305414	-1.074874
C	1.759923	3.450163	-0.707093
C	1.136698	4.466406	0.084450
C	-0.164559	4.328270	0.511264
H	-4.500803	-1.724807	-0.596805
H	-4.781759	2.175657	1.231706
H	-5.809262	-0.005919	0.632757
H	-2.749889	3.687647	1.171227
H	2.791727	3.584338	-1.027184
H	1.707621	5.351020	0.349922
H	-0.638660	5.094373	1.120512
N	-0.911997	0.998214	-0.982630
Ru	1.025031	-1.283267	0.975162
C	-1.901749	-1.568131	-1.464011
H	-1.260586	-1.122294	-2.234942
H	-2.523774	-2.359175	-1.907853
C	1.698577	1.206582	-1.878478
H	0.963210	0.789333	-2.577356
H	2.575328	1.563524	-2.437979
P	-0.741495	-2.409254	-0.239693
P	2.279229	-0.252740	-0.832921
C	3.913338	0.431238	-0.284318
H	4.466980	-0.336122	0.268261
H	4.515841	0.779106	-1.134211
H	3.727154	1.268710	0.399705
C	2.827834	-1.338456	-2.242686
H	3.511865	-0.807871	-2.918573
H	3.328805	-2.231778	-1.852215
H	1.942723	-1.654979	-2.810026
C	-1.975048	-3.249379	0.847727
H	-2.746532	-3.767799	0.261538
H	-1.442804	-3.965538	1.483135
H	-2.439548	-2.502854	1.500846
C	-0.203123	-3.846827	-1.289809
H	0.442736	-4.504987	-0.697464
H	-1.068444	-4.421902	-1.644998
H	0.368696	-3.487030	-2.153288
C	2.088029	-0.543405	2.303288
O	2.710783	-0.060151	3.193141
H	0.080012	-0.064519	1.230431
H	0.194608	-1.945807	2.232536

Geometry of complex: TS(C-D)

```
50
Stoichiometry = H25C20NOP2Ru
   C    -3.943290    0.818968   -0.922537
   C    -2.615315    0.423784   -1.121585
   C    -1.580178    1.239725   -0.607465
   C    -1.901799    2.295878    0.286871
   C    -3.244050    2.661057    0.497136
   C    -4.261171    1.956505   -0.151372
   C    -0.771192    2.749983    1.070142
   C     0.479623    2.883876    0.377365
   C     0.726945    1.832895   -0.550871
   C     2.038278    1.620831   -1.059500
   C     3.034430    2.536284   -0.735176
   C     2.776498    3.627555    0.133924
   C     1.523102    3.775258    0.717050
   H    -4.742577    0.211180   -1.343761
   H    -3.479637    3.477522    1.175724
   H    -5.299034    2.246507   -0.019390
   H    -0.953283    3.347996    1.962639
   H     4.038112    2.393137   -1.132449
   H     3.575046    4.324374    0.369512
   H     1.336201    4.567373    1.438213
   N    -0.244862    0.857201   -0.735846
   Ru    0.350113   -0.644409    0.740541
   C    -2.245068   -0.926121   -1.657842
   H    -1.444180   -0.866838   -2.408297
   H    -3.108320   -1.465502   -2.071148
   C     2.317973    0.332616   -1.777095
   H     1.583221    0.150109   -2.573363
   H     3.331345    0.309548   -2.201428
   P    -1.526300   -1.877901   -0.201542
   P     2.123675   -1.112581   -0.589445
   C     3.772875   -1.217208    0.219844
   H     3.759389   -2.000438    0.985545
   H     4.562956   -1.428212   -0.511851
   H     3.968576   -0.258608    0.713597
   C     2.155082   -2.547100   -1.755997
   H     3.076327   -2.549622   -2.353261
   H     2.084693   -3.481166   -1.187596
   H     1.290554   -2.476706   -2.427801
   C    -3.008363   -2.073676    0.887730
   H    -3.874905   -2.450743    0.327689
   H    -2.762497   -2.770179    1.697712
   H    -3.254963   -1.102301    1.331559
   C    -1.367448   -3.590611   -0.889576
   H    -0.980239   -4.256357   -0.109565
   H    -2.336176   -3.968373   -1.240711
   H    -0.657011   -3.588334   -1.724541
   C     0.787802   -1.883607    2.024363
   O     1.058361   -2.702701    2.847684
   H    -0.357971    1.022032    1.640175
   H     1.477528    0.344663    1.400808


Geometry of complex: D
----------------------

50
Stoichiometry = H25C20NOP2Ru
   C     2.346669   -3.247139    0.866366
```

C	1.427592	-2.184834	0.844231
C	1.762646	-0.991310	0.151699
C	3.036260	-0.885178	-0.462507
C	3.946291	-1.942195	-0.390688
C	3.604558	-3.136973	0.261203
C	3.319761	0.385976	-1.225878
C	2.756243	1.574514	-0.487728
C	1.500412	1.383511	0.128598
C	0.879360	2.468013	0.798174
C	1.501052	3.725703	0.788079
C	2.745598	3.914775	0.170466
C	3.375397	2.827025	-0.452274
H	2.075031	-4.161137	1.393491
H	4.920909	-1.834820	-0.863495
H	4.307752	-3.963150	0.303019
H	4.392191	0.503544	-1.423656
H	1.016547	4.557478	1.297928
H	3.219418	4.891635	0.182459
H	4.343750	2.955115	-0.932800
N	0.873033	0.113949	0.085536
Ru	-1.036084	-0.002015	-0.755385
C	0.105716	-2.320357	1.549421
H	-0.050344	-1.497375	2.264867
H	0.036168	-3.277553	2.085494
C	-0.394513	2.251903	1.569885
H	-0.246939	1.466880	2.329035
H	-0.712902	3.174358	2.077193
P	-1.262651	-2.173260	0.304032
P	-1.799179	1.632599	0.532730
C	-2.482279	3.127694	-0.288077
H	-3.249813	2.830455	-1.011086
H	-2.913209	3.819725	0.445907
H	-1.668773	3.620224	-0.832239
C	-3.088461	1.228177	1.787496
H	-3.380001	2.124421	2.350317
H	-3.967919	0.809143	1.285609
H	-2.687477	0.481594	2.483632
C	-1.002666	-3.681574	-0.732752
H	-0.945485	-4.579276	-0.103235
H	-1.830537	-3.785064	-1.442563
H	-0.067670	-3.581721	-1.294267
C	-2.776752	-2.644901	1.256366
H	-3.659736	-2.521811	0.619091
H	-2.716354	-3.685573	1.599084
H	-2.884315	-1.989313	2.127724
C	-2.649780	-0.096290	-1.666927
O	-3.696398	-0.149390	-2.236822
H	-0.647352	1.377145	-1.544077
H	2.813537	0.321903	-2.207008

Geometry of complex: E

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Stoichiometry = H25C20NOP2Ru

C	3.391206	2.236072	0.829580
C	2.324842	1.322018	0.855567
C	1.106794	1.630300	0.186902
C	1.051713	2.850150	-0.536601

C	2.119341	3.750966	-0.538031
C	3.299761	3.458068	0.155337
C	-0.197490	3.105322	-1.328261
C	-1.379304	2.720277	-0.486804
C	-1.276934	1.494466	0.221590
C	-2.438686	1.039178	0.907289
C	-3.593498	1.838000	0.937484
C	-3.651553	3.078652	0.293657
C	-2.534774	3.503575	-0.436074
H	4.309547	1.973835	1.353233
H	2.024066	4.678580	-1.099226
H	4.132418	4.154479	0.158351
H	-0.259406	4.147661	-1.662111
H	-4.464456	1.467700	1.476508
H	-4.550566	3.685100	0.341176
H	-2.558013	4.442522	-0.985952
N	-0.039963	0.771063	0.238257
Ru	0.077219	-1.305054	-0.224484
C	2.558702	-0.022911	1.480544
H	1.785747	-0.292501	2.216652
H	3.546500	-0.078847	1.957336
C	-2.526609	-0.350670	1.470244
H	-1.725185	-0.577382	2.190987
H	-3.499763	-0.529957	1.946855
P	2.397871	-1.242914	0.094896
P	-2.252976	-1.476370	0.020561
C	-3.515428	-0.941057	-1.212486
H	-3.553439	-1.679010	-2.021093
H	-4.504379	-0.855236	-0.744021
H	-3.231784	0.030407	-1.630254
C	-2.911590	-3.106126	0.578713
H	-3.976596	-3.029349	0.830110
H	-2.776038	-3.852972	-0.211060
H	-2.350508	-3.437953	1.459434
C	3.627554	-0.676011	-1.156443
H	4.602330	-0.488261	-0.687990
H	3.730958	-1.450972	-1.923807
H	3.272244	0.245348	-1.629201
C	3.177899	-2.781610	0.748600
H	3.114304	-3.577214	-0.001947
H	4.229410	-2.607034	1.007860
H	2.631497	-3.111419	1.639309
C	0.179520	-3.102987	-0.625141
O	0.246734	-4.251115	-0.944353
H	-0.182796	2.468892	-2.231726
H	0.119925	-1.177328	-1.790966

Geometry of complex: TS(E-2')

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Stoichiometry = H25C20NOP2Ru

C	-1.635336	-3.396573	1.518000
C	-0.853227	-2.447393	0.828600
C	-1.469984	-1.258176	0.301335
C	-2.899924	-1.313464	0.261138
C	-3.645744	-2.261991	0.959320
C	-3.017678	-3.296296	1.658068
C	-3.609048	-0.390912	-0.674762

C	-2.978297	0.962266	-0.664771
C	-1.562525	1.059570	-0.502970
C	-1.029420	2.377585	-0.727028
C	-1.883925	3.469177	-0.973236
C	-3.271072	3.348856	-1.038207
C	-3.801396	2.067465	-0.891254
H	-1.119620	-4.257976	1.940952
H	-4.731826	-2.200555	0.915571
H	-3.582390	-4.032155	2.220911
H	-3.552572	-0.808304	-1.697037
H	-1.428649	4.447063	-1.120869
H	-3.903325	4.211754	-1.218827
H	-4.873932	1.900790	-0.975354
N	-0.771724	-0.092261	-0.163460
Ru	1.405711	0.057143	0.001805
C	0.583601	-2.911319	0.649484
H	0.577643	-4.004957	0.519415
H	1.207280	-2.687027	1.528180
C	0.433330	2.750308	-0.701844
H	1.004564	2.237349	-1.501090
H	0.553661	3.829514	-0.868623
P	1.422820	-2.129339	-0.776982
P	1.195463	2.206165	0.883883
C	0.037298	2.767940	2.197205
H	0.502169	2.621109	3.177827
H	-0.211303	3.828154	2.061924
H	-0.881372	2.176178	2.146495
C	2.664169	3.293839	1.107581
H	2.358144	4.339420	1.233563
H	3.237512	2.975310	1.984621
H	3.312190	3.205566	0.228506
C	3.007295	-3.059723	-0.895216
H	2.823495	-4.131353	-1.040396
H	3.605727	-2.677253	-1.728956
H	3.575783	-2.907721	0.029511
C	0.467777	-2.722359	-2.236954
H	0.989870	-2.449131	-3.159996
H	0.342332	-3.811714	-2.196807
H	-0.516966	-2.243572	-2.232143
C	3.231622	0.225957	-0.142602
O	4.414345	0.338868	-0.244515
H	-4.676395	-0.327095	-0.429033
H	1.744676	-0.553736	1.407753

Geometry of complex: F

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Stoichiometry = H25C20NOP2Ru

C	1.096047	3.865482	0.329742
C	0.553634	2.663345	-0.111294
C	1.402014	1.470855	-0.103255
C	2.820326	1.742823	0.054673
C	3.327705	3.019094	0.446640
C	2.464749	4.060204	0.655966
C	3.725942	0.724844	-0.234892
C	3.292258	-0.582421	-0.436013
C	1.888286	-0.875536	-0.226885
C	1.583781	-2.284189	-0.023732

C	2.551164	-3.223821	-0.357981
C	3.864916	-2.905962	-0.790695
C	4.248376	-1.591089	-0.764762
H	0.436954	4.729703	0.367041
H	4.401553	3.125620	0.579414
H	2.810815	5.031091	0.993877
H	4.790615	0.949060	-0.274382
H	2.290665	-4.273332	-0.233850
H	4.556394	-3.696965	-1.060627
H	5.269994	-1.283433	-0.973977
N	0.956269	0.160462	-0.227471
Ru	-1.179627	-0.449223	-0.732349
C	-0.845518	2.783621	-0.661366
H	-0.843513	2.557916	-1.736411
H	-1.198661	3.816375	-0.524441
C	0.382231	-2.916298	0.666453
H	-0.092113	-3.619162	-0.033502
H	0.754556	-3.500648	1.525778
P	-2.047878	1.580601	0.044107
P	-0.987592	-1.795986	1.166006
C	-0.397316	-1.172541	2.812055
H	-1.212882	-0.634975	3.310059
H	-0.063946	-1.996588	3.456909
H	0.433758	-0.473271	2.655984
C	-2.253481	-3.036218	1.690809
H	-1.829241	-3.771799	2.387050
H	-3.090483	-2.521452	2.175133
H	-2.635868	-3.548100	0.800490
C	-2.201446	2.230529	1.778223
H	-2.490111	3.290906	1.783206
H	-2.951249	1.649483	2.327615
H	-1.233738	2.120010	2.283815
C	-3.621819	2.182067	-0.712236
H	-4.458163	1.569605	-0.357218
H	-3.811496	3.236993	-0.474489
H	-3.547310	2.051072	-1.797989
C	-2.786136	-1.083066	-1.328683
O	-3.829829	-1.503615	-1.724240
H	-0.471547	-1.643324	-1.621068
H	-1.008851	0.307138	-2.197136

Geometry of complex: G

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Stoichiometry = H25C20NOP2Ru

C	-3.618195	1.710558	-0.656870
C	-2.454082	0.991278	-0.875456
C	-1.184034	1.574441	-0.493787
C	-1.214249	2.909708	0.064385
C	-2.447843	3.593734	0.290494
C	-3.635410	3.003254	-0.061262
C	0.000065	3.528892	0.369150
C	1.214345	2.909643	0.064394
C	1.184046	1.574391	-0.493799
C	2.454045	0.991162	-0.875508
C	3.618211	1.710342	-0.656899
C	3.635515	3.003016	-0.061244
C	2.447989	3.593575	0.290524

H	-4.562507	1.261654	-0.959297
H	-2.415361	4.588641	0.728269
H	-4.581814	3.510826	0.094044
H	0.000089	4.520766	0.819067
H	4.562485	1.261363	-0.959334
H	4.581956	3.510513	0.094086
H	2.415583	4.588471	0.728326
N	-0.000007	0.901174	-0.674666
Ru	-0.000031	-1.450249	0.277516
C	-2.570984	-0.374414	-1.476814
H	-1.806104	-0.563629	-2.239525
H	-3.568301	-0.519312	-1.915525
C	2.570795	-0.374528	-1.476880
H	1.805752	-0.563726	-2.239428
H	3.568033	-0.519494	-1.915749
P	-2.244088	-1.646711	-0.148153
P	2.244079	-1.646712	-0.148058
C	3.573735	-1.294960	1.088656
H	3.556902	-2.087546	1.845464
H	4.568092	-1.257857	0.622954
H	3.364574	-0.342531	1.588273
C	2.881138	-3.189133	-0.933199
H	3.951406	-3.110348	-1.164381
H	2.711210	-4.030577	-0.252906
H	2.308477	-3.371211	-1.848404
C	-3.573566	-1.295280	1.088838
H	-4.568201	-1.259490	0.623637
H	-3.555590	-2.087300	1.846215
H	-3.365053	-0.342307	1.587690
C	-2.881095	-3.189090	-0.933409
H	-2.711275	-4.030549	-0.253107
H	-3.951334	-3.110271	-1.164715
H	-2.308328	-3.371168	-1.848546
C	-0.000076	-0.816370	2.055768
O	-0.000151	-0.494992	3.204975
H	-0.000004	-2.946144	0.844727
H	-0.000052	-2.226069	-1.248999

Geometry of complex: TS(G-H)

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Stoichiometry = H25C20NOP2Ru

C	-3.630765	1.934042	-0.388601
C	-2.468111	1.254103	-0.735764
C	-1.193554	1.851560	-0.414107
C	-1.204579	3.127395	0.263724
C	-2.431386	3.776287	0.594670
C	-3.631640	3.189473	0.273780
C	0.016754	3.729340	0.586729
C	1.232727	3.117412	0.262547
C	1.210536	1.841410	-0.414670
C	2.479789	1.232945	-0.736624
C	3.648379	1.903282	-0.390889
C	3.660264	3.159249	0.270399
C	2.465256	3.756272	0.591916
H	-4.585205	1.474902	-0.638767
H	-2.386707	4.734260	1.107232
H	-4.573715	3.668855	0.518823

H	0.020975	4.693547	1.092088
H	4.598767	1.436017	-0.641385
H	4.606524	3.630966	0.514179
H	2.429121	4.714901	1.103911
N	0.005841	1.241775	-0.725376
Ru	-0.007677	-1.704393	0.080925
C	-2.637083	-0.086565	-1.391054
H	-1.958680	-0.231658	-2.240604
H	-3.669603	-0.184018	-1.756739
C	2.636665	-0.109819	-1.390597
H	1.957176	-0.249672	-2.240158
H	3.668311	-0.217129	-1.756003
P	-2.293756	-1.534146	-0.229748
P	2.279882	-1.553108	-0.227845
C	3.494359	-1.259238	1.133817
H	3.494604	-2.136746	1.790730
H	4.508364	-1.089994	0.745712
H	3.175614	-0.392293	1.722216
C	3.125484	-2.901004	-1.179687
H	4.177510	-2.656335	-1.381142
H	3.067821	-3.831768	-0.605701
H	2.592225	-3.049948	-2.125542
C	-3.507846	-1.232377	1.130491
H	-4.520408	-1.057403	0.741176
H	-3.514055	-2.109506	1.787882
H	-3.184751	-0.367010	1.718807
C	-3.149078	-2.873669	-1.184789
H	-3.098433	-3.806139	-0.612923
H	-4.199226	-2.620789	-1.385922
H	-2.616764	-3.024408	-2.130891
C	-0.011302	-2.354818	1.815820
O	-0.013678	-2.740562	2.948219
H	-0.004255	-1.007731	-1.580999
H	0.000019	-0.118378	-1.133568

Geometry of complex: H

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Stoichiometry = H25C20NOP2Ru

C	3.677546	1.887100	0.652718
C	2.492391	1.174161	0.906430
C	1.263449	1.627073	0.377886
C	1.218959	2.812901	-0.425561
C	2.459155	3.458706	-0.721267
C	3.655989	3.025064	-0.175963
C	0.000136	3.360115	-0.864137
C	-1.218700	2.812989	-0.425488
C	-1.263238	1.627158	0.377954
C	-2.492199	1.174251	0.906456
C	-3.677313	1.887273	0.652746
C	-3.655708	3.025276	-0.175884
C	-2.458853	3.458885	-0.721163
H	4.613637	1.521554	1.069076
H	2.425994	4.342065	-1.355016
H	4.578344	3.558722	-0.388007
H	0.000148	4.261589	-1.471021
H	-4.613433	1.521747	1.069059
H	-4.578042	3.558979	-0.387909

H	-2.425638	4.342260	-1.354886
N	0.000094	0.907271	0.712880
Ru	-0.000188	-1.160387	-0.277199
H	-0.000185	-1.904301	1.140855
C	2.630879	-0.181489	1.543756
H	1.905056	-0.412598	2.335696
H	3.641407	-0.328212	1.945738
C	-2.630893	-0.181416	1.543757
H	-1.905043	-0.412720	2.335615
H	-3.641411	-0.327894	1.945849
P	2.296452	-1.354265	0.138550
P	-2.296722	-1.354176	0.138460
C	-3.626752	-0.976004	-1.081986
H	-3.577569	-1.721681	-1.883583
H	-4.617443	-1.010436	-0.611054
H	-3.464729	0.019090	-1.509357
C	-2.825053	-3.003162	0.774742
H	-3.889124	-2.996823	1.040714
H	-2.647753	-3.766818	0.008790
H	-2.226099	-3.256823	1.656102
C	3.626403	-0.976311	-1.082037
H	4.617139	-1.010779	-0.611198
H	3.577081	-1.722062	-1.883562
H	3.464399	0.018755	-1.509481
C	2.824880	-3.003111	0.775124
H	2.648474	-3.766886	0.009095
H	3.888772	-2.996312	1.041822
H	2.225445	-3.256964	1.656099
C	0.000093	-2.783401	-1.151791
O	0.000632	-3.872970	-1.634235
H	0.000147	0.706670	1.718134

Geometry of complex: TS(H-I)

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Stoichiometry = H25C20NOP2Ru

C	3.417238	2.349696	0.579370
C	2.330109	1.470486	0.807766
C	1.073033	1.751547	0.246058
C	0.894187	2.939924	-0.518816
C	2.000921	3.780272	-0.751223
C	3.257824	3.489988	-0.206911
C	-0.424286	3.316890	-0.963991
C	-1.542436	2.748313	-0.384887
C	-1.427519	1.560250	0.454717
C	-2.626575	0.900294	0.912380
C	-3.856668	1.522638	0.752080
C	-3.966204	2.739335	0.012292
C	-2.858085	3.312683	-0.560614
H	4.383881	2.112062	1.019649
H	1.852037	4.676447	-1.349457
H	4.099304	4.152567	-0.387692
H	-0.530706	4.202894	-1.586810
H	-4.746832	1.055392	1.167074
H	-4.944450	3.194500	-0.117964
H	-2.943142	4.210475	-1.168657
N	-0.057142	0.787475	0.362676
Ru	0.156905	-1.276080	-0.181681

H	0.224090	-2.199789	1.108745
C	2.616625	0.176528	1.516886
H	1.878964	-0.069775	2.292391
H	3.620029	0.180940	1.962488
C	-2.601506	-0.486111	1.485106
H	-1.836964	-0.640405	2.258925
H	-3.584553	-0.754792	1.893359
P	2.462936	-1.136240	0.218334
P	-2.143688	-1.602709	0.069588
C	-3.380016	-1.193116	-1.234309
H	-3.336122	-1.959994	-2.015907
H	-4.393036	-1.147641	-0.813203
H	-3.137965	-0.220720	-1.676175
C	-2.679459	-3.276238	0.623927
H	-3.756150	-3.291997	0.832720
H	-2.450545	-4.013177	-0.154205
H	-2.124800	-3.548781	1.528171
C	3.695902	-0.653794	-1.063857
H	4.675605	-0.456275	-0.609818
H	3.785538	-1.470342	-1.789176
H	3.354053	0.246634	-1.584140
C	3.238801	-2.632239	0.965933
H	3.181282	-3.469371	0.260734
H	4.289357	-2.441772	1.217596
H	2.688188	-2.908202	1.871671
C	0.356802	-2.853829	-1.100009
O	0.489691	-3.855552	-1.733527
H	-0.569248	1.343886	1.412884

Geometry of complex: I

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Stoichiometry = H25C20NOP2Ru

C	-4.073591	0.447247	-0.985827
C	-2.714844	0.100567	-0.932879
C	-1.750838	1.022236	-0.417819
C	-2.273338	2.251373	0.118285
C	-3.648257	2.550971	0.077931
C	-4.557765	1.669122	-0.498480
C	-1.367933	3.136029	0.812453
C	-0.031275	3.042670	0.585482
C	0.383854	2.070409	-0.520273
C	1.890435	2.006994	-0.680578
C	2.713891	2.878389	-0.038047
C	2.247333	3.839417	0.947287
C	0.924341	3.893458	1.255779
H	-4.769470	-0.271030	-1.417004
H	-3.984183	3.491920	0.509871
H	-5.614957	1.907512	-0.554314
H	-1.772709	3.863627	1.515184
H	3.780086	2.851919	-0.265200
H	2.968231	4.486964	1.436866
H	0.545567	4.581683	2.009435
N	-0.350330	0.757401	-0.360793
Ru	0.496284	-1.091236	0.180777
H	0.664182	-2.216774	-0.936176
C	-2.352710	-1.306442	-1.320698
H	-1.564702	-1.359880	-2.084728

H	-3.236234	-1.856577	-1.671529
C	2.472969	0.995838	-1.621411
H	1.793814	0.757636	-2.450969
H	3.448350	1.308513	-2.017934
P	-1.634052	-2.061536	0.205783
P	2.625173	-0.525628	-0.582424
C	4.023736	-0.168341	0.565846
H	4.238186	-1.081058	1.135247
H	4.923821	0.135647	0.015397
H	3.735003	0.618515	1.268131
C	3.401276	-1.773572	-1.699730
H	4.375353	-1.424623	-2.064657
H	3.532484	-2.712321	-1.148712
H	2.734443	-1.962792	-2.547541
C	-2.954551	-1.838410	1.478154
H	-3.928112	-2.161785	1.086550
H	-2.699487	-2.434915	2.361006
H	-3.017540	-0.784712	1.768584
C	-1.692684	-3.880149	-0.089944
H	-1.223719	-4.406075	0.749484
H	-2.728033	-4.224698	-0.202061
H	-1.126307	-4.112396	-0.998189
C	1.213617	-2.374307	1.284646
O	1.693166	-3.169948	2.035165
H	0.007619	2.504353	-1.478129

Geometry of complex: TS(I-J)

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Stoichiometry = H25C20NOP2Ru

C	3.774332	1.580323	0.782846
C	2.510858	0.953131	0.907695
C	1.384706	1.488545	0.254542
C	1.532689	2.689487	-0.517136
C	2.817559	3.263069	-0.659468
C	3.928607	2.719192	-0.011284
C	0.366220	3.326335	-1.040879
C	-0.861828	3.011899	-0.406652
C	-1.011894	1.682790	0.265902
C	-2.319889	1.381621	0.831075
C	-3.398224	2.230148	0.621554
C	-3.283191	3.450948	-0.108943
C	-2.068180	3.825526	-0.609503
H	4.631269	1.137046	1.286510
H	2.913983	4.162369	-1.264230
H	4.906105	3.181299	-0.119800
H	0.456793	4.260737	-1.589796
H	-4.363344	1.951953	1.039590
H	-4.158437	4.075505	-0.255050
H	-1.937749	4.750971	-1.164105
N	0.077489	0.809347	0.274691
Ru	-0.136022	-1.246372	-0.211720
H	-0.201594	-2.259275	1.023073
C	2.486073	-0.398995	1.566379
H	1.664031	-0.528169	2.282472
H	3.441141	-0.618651	2.061031
C	-2.581686	0.069589	1.507765
H	-1.815366	-0.179544	2.253790

H	-3.572492	0.060948	1.979971
P	2.150277	-1.569559	0.170644
P	-2.431215	-1.217417	0.182954
C	-3.745376	-0.771351	-1.034422
H	-3.848427	-1.595762	-1.749117
H	-4.707428	-0.602959	-0.532610
H	-3.457965	0.130605	-1.583030
C	-3.135162	-2.738959	0.948992
H	-4.196130	-2.602562	1.191779
H	-3.025735	-3.578794	0.253190
H	-2.574143	-2.974855	1.859439
C	3.474253	-1.223197	-1.063495
H	4.465080	-1.244895	-0.591356
H	3.424304	-1.983845	-1.850864
H	3.313242	-0.235885	-1.508027
C	2.626945	-3.235961	0.798748
H	2.418545	-3.992919	0.033830
H	3.693307	-3.262554	1.054361
H	2.029615	-3.470394	1.686259
C	-0.251003	-2.767891	-1.235727
O	-0.317556	-3.743224	-1.920046
H	-0.776369	3.127517	0.863997

Geometry of complex: J

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Stoichiometry = H25C20NOP2Ru

C	-1.717591	3.233100	0.781948
C	-1.221052	2.339522	-0.157469
C	0.079026	1.769640	0.037046
C	0.967755	2.380995	1.019345
C	0.349494	3.140853	2.074750
C	-0.956300	3.563970	1.945750
C	2.325363	2.267405	0.783537
C	2.661530	1.853180	-0.643404
C	1.915827	0.535405	-0.760600
C	2.662706	-0.690015	-0.978456
C	4.026689	-0.639142	-1.151896
C	4.774213	0.598687	-1.101333
C	4.141173	1.770126	-0.852741
H	-2.694777	3.686723	0.624055
H	0.964007	3.472018	2.909210
H	-1.397095	4.203728	2.705606
H	3.104662	2.533711	1.492094
H	4.570859	-1.570366	-1.299057
H	5.851818	0.567810	-1.236462
H	4.694246	2.704492	-0.778789
N	0.566020	0.605657	-0.614853
Ru	-0.875064	-0.877057	0.052339
H	-0.998439	-1.969858	-1.086102
C	-2.036177	1.953702	-1.362646
H	-1.415322	1.905482	-2.267049
H	-2.869772	2.648107	-1.528090
C	1.999998	-2.042624	-0.944895
H	1.300253	-2.187053	-1.779272
H	2.758696	-2.836899	-0.983381
P	-2.644672	0.246636	-1.009105
P	0.985210	-2.182028	0.600381

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   C     2.199499   -1.822048    1.940201
   H     1.773596   -2.120204    2.904152
   H     3.135426   -2.369180    1.764736
   H     2.413068   -0.747233    1.964536
   C     0.712285   -3.995961    0.768051
   H     1.667391   -4.532678    0.823435
   H     0.127284   -4.202579    1.671130
   H     0.141380   -4.349521   -0.097717
   C    -4.150611    0.556388    0.005106
   H    -4.897375    1.129977   -0.557787
   H    -4.583758   -0.396177    0.328957
   H    -3.849725    1.121766    0.895333
   C    -3.320900   -0.398271   -2.596562
   H    -3.767736   -1.383550   -2.424603
   H    -4.079417    0.279037   -3.007122
   H    -2.500733   -0.511080   -3.313383
   C    -2.049437   -1.930891    0.996816
   O    -2.799681   -2.617023    1.617546
   H     2.200570    2.577385   -1.348199


Geometry of complex: TS(J-2')
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Stoichiometry = H25C20NOP2Ru
   C     3.698832    1.728828    0.777441
   C     2.455614    1.052725    0.910162
   C     1.313928    1.534241    0.247981
   C     1.429505    2.743990   -0.516452
   C     2.684408    3.372140   -0.662732
   C     3.819721    2.867268   -0.017014
   C     0.237652    3.313076   -1.060607
   C    -1.024855    2.982907   -0.358796
   C    -1.097551    1.646305    0.293832
   C    -2.330226    1.291801    0.894694
   C    -3.486298    2.083088    0.704553
   C    -3.478269    3.234170   -0.107854
   C    -2.293766    3.653737   -0.678626
   H     4.571720    1.313312    1.277738
   H     2.744398    4.276255   -1.265198
   H     4.780974    3.360450   -0.127995
   H     0.284675    4.237117   -1.635412
   H    -4.416043    1.757377    1.167296
   H    -4.397805    3.783241   -0.285165
   H    -2.241644    4.550314   -1.293225
   N     0.037852    0.807908    0.244333
   Ru   -0.077366   -1.248068   -0.230990
   H    -0.112699   -2.278391    0.990596
   C     2.484109   -0.297007    1.572055
   H     1.657924   -0.458728    2.276782
   H     3.440448   -0.473486    2.081576
   C    -2.523604   -0.043443    1.558146
   H    -1.726015   -0.284378    2.274481
   H    -3.498070   -0.100923    2.060732
   P     2.214013   -1.489553    0.177184
   P    -2.370819   -1.286105    0.195466
   C    -3.696940   -0.832293   -1.005237
   H    -3.773050   -1.629059   -1.753864
   H    -4.663793   -0.714041   -0.498772
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H	-3.437474	0.103190	-1.510746
C	-3.025973	-2.856601	0.904846
H	-4.087009	-2.756164	1.164365
H	-2.904760	-3.665420	0.175067
H	-2.449515	-3.114500	1.799698
C	3.563185	-1.113862	-1.024192
H	4.538582	-1.078673	-0.521579
H	3.573970	-1.898974	-1.788739
H	3.373356	-0.150289	-1.507483
C	2.738175	-3.130788	0.834432
H	2.554740	-3.903943	0.079365
H	3.803415	-3.123821	1.096136
H	2.142074	-3.369750	1.721575
C	-0.148841	-2.771888	-1.258391
O	-0.190970	-3.742682	-1.951516
H	-0.652253	3.704912	0.448921