Supporting Information for

Ruthenium-Mediated *Phospha*-Buchner Ring Expansion: Phosphorus Insertion into a Pendant Arene

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Experimental Details and Characterization Data for All New Compounds

General Methods. All reactions were performed using standard Schlenk techniques, or in a Vigor glovebox under an inert atmosphere of N_2. Glassware, stir bars, filter aid (Celite) and 4Å molecular sieves were dried in an oven at 105 °C for at least 12 h prior to use. Solvents (*n*-pentane, tetrahydrofuran, diethyl ether) were dried over sodium benzophenone ketyl, deoxygenated by sparging with N_2 for 15 min, and stored over 4Å molecular sieves. Deuterated solvents were purchased from J&K or Cambridge Isotope Laboratories, Inc., and dried over potassium mirror (C_6D_6, toluene-d_8), distilled and stored under N_2 over activated 4Å molecular sieves.

Commercial reagents were purchased from J&K Scientific, Leyan, Bidepharm and other domestic manufacturers. Solid chemicals were used without further purification, while liquid reagents were filtered through a Al_2O_3 column and degassed by a freeze-pump-thaw operation. ^1H, $^{13}C\{^1H\}$, $^{31}P\{^1H\}$, ^1H-^{13}C HSQC and ^1H-^{13}C HMBC spectra were recorded on Bruker Avance III HD 400 MHz or Bruker AV-HD-600X 600 MHz spectrometers at 25 °C, unless otherwise stated. All chemical shifts (δ) are reported in units of ppm, with references to the residues protio-solvent resonance for proton and carbon chemical shifts. ^1H NMR spectroscopy: 7.16 ppm (C_6D_6). ^{13}C NMR spectroscopy: 128.06 ppm (C_6D_6). Elemental analysis was performed on a Vario EL CUBE elemental analyzer (Elementar, Germany) following the standard method JY/T 0580-2020 (General rules for elemental analyzers).

X-ray Crystallography. Data collection was performed on a Rigaku XtaLAB Supernova diffractometer with an HyPix area detector with confocal multilayer optic-monochromated Cu-Kα radiation (λ = 1.54184 Å) at 100 K. The structures were solved by intrinsic phasing using SHELXT and refined by full-matrix least-squares on F^2 with SHELXL-2018. CCDC entries Cp^*Ru(Idmop)Cl (**2**) 2537157, Cp^*Ru(P-Idmop)(CO) (**3**) 2537158, contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre. Crystal parameters and refinement results are given in **Table S1**.

Synthesis of Cp^*Ru(Idmop)Cl (2). Idmop·HCl was prepared according to the literature procedure[1] and subsequently converted to Idmop·HBF_4 by counterion exchange in aqueous tetrafluoroborate solution. Idmop·HBF_4 (103 mg, 0.24 mmol) was dissolved in THF (3 mL) and cooled to −30 °C. A solution of ^{t}BuOK (26 mg, 0.24 mmol) in THF (2 mL) was added dropwise. After 3 min, the solution became clear and colorless. A solution of $[Cp^*RuCl]_4$ (26 mg, 0.06 mmol) in THF (3 mL) was then added, and the reaction mixture was allowed to stir at room temperature for 3 h, giving a brownish-purple solution. Volatiles were removed under reduced pressure, and the residue was extracted with petroleum ether/Et_2O (1:1). The extract

was filtered through a pad of Celite. Single crystals suitable for X-ray diffraction were obtained by storing a saturated filtrate at −35 °C for one week. Yield 45 mg (31 %). ^{1}H NMR (500 MHz, C_6D_6, 298 K) δ 6.99 (t, $^{3}J_{HH}$ = 8.4 Hz, 2H, Ar *p-H*), 6.42 (dd, $^{3}J_{HH}$ = 8.4, $^{4}J_{HH}$ = 1.3 Hz, 2H, Ar *m-H*), 6.26 (dd, $^{3}J_{HH}$ = 8.4, $^{4}J_{HH}$ = 1.2 Hz, 2H, Ar *m-H*), 4.31 – 4.23 (m, 2H, NCH_2), 3.80 (s, 6H, OCH_3), 3.52 – 3.45 (m, 2H, NCH_2), 3.39 (s, 6H, OCH_3), 1.37 (s, 15H, Cp* CH_3). ^{13}C NMR (126 MHz, C_6D_6, 298 K) δ 232.76 (s, NHC *carbene-C*), 158.99 (s, Ar *o-C*), 156.37 (s, Ar *o-C*), 127.30 (s, Ar *p-C*), 121.21 (s, Ar *ipso-C*), 105.42 (s, Ar *m-C*), 103.52 (s, Ar *m-C*), 74.68 (s, Cp* *C*CH_3), 56.07 (s, O*C*H_3), 54.90 (s, O*C*H_3), 50.90 (s, N*C*H_2), 10.23 (s, Cp* *C*H_3). Anal. Calcd. for $C_{29}H_{37}ClN_2O_4Ru$: C, 56.71; H, 6.07; N, 4.56. Found: C, 56.72; H, 6.07; N, 4.56.

Synthesis of Cp*Ru(P-Idmop)(CO) (3). Sodium phosphaethynolate (NaOCP•(dioxane)$_2$, 12 mg, 0.042 mmol) was added into a solution of Cp*Ru(Idmop)Cl (26 mg, 0.042 mmol) in 1 mL C_6D_6 and the resulting solution was allowed to stir under room temperature for 24 h, forming an orange solution. All volatile materials were removed under vacuum. The residues were extracted by Et_2O and filtered through celite. Single crystals of the product suitable for crystallographic analysis were grown by storing the saturated filtrate at -35 °C for a week. Yield 22 mg (85 %). ^{1}H NMR (600 MHz, C_6D_6, 298 K) δ 7.01 (t, $^{3}J_{HH}$ = 8.4 Hz, 1H, Ar *p-H*), 6.57 (dd, $^{3}J_{HH}$ = 11.4, $^{4}J_{HH}$ = 6.5 Hz, 1H, Ar PCCHCHC*H*), 6.37 (dd, $^{3}J_{HH}$ = 8.5, $^{4}J_{HH}$ = 1.2 Hz, 1H, Ar *m-H*), 6.33 (dd, $^{3}J_{HH}$ = 11.5, $^{4}J_{HH}$ = 1.2 Hz, 1H, PCC*H*CHCH), 6.21 (dd, $^{3}J_{HH}$ = 8.5, $^{4}J_{HH}$ = 1.2 Hz, 1H, Ar *m-H*), 5.70 – 5.62 (m, 1H, PCCHC*H*CH), 4.05 (td, $^{3}J_{HH}$ = 11.4, $^{4}J_{HH}$ = 8.2 Hz, 1H, NCH_2CH_2), 3.72 – 3.66 (m, 1H, NCH_2CH_2), 3.63 (s, 3H, OCH_3), 3.62 – 3.56 (m, 1H, NCH_2CH_2), 3.53 (s, 3H, OCH_3), 3.26 (s, 3H, OCH_3), 3.21 (s, 3H, OCH_3), 3.21 – 3.14 (m, 1H, NCH_2CH_2), 1.73 (s, 15H, Cp* CH_3). ^{13}C NMR (151 MHz, C_6D_6, 298 K) δ 217.63 (s, *C*O), 210.91 (s, NH*C*), 157.82 (d, $^{4}J_{CP}$ = 29.1, *ipso-C*),140.32 (br, Ar PCCHCHCH*C*), 130.52 (s, Ar PCCHCH*C*H), 128.75 (s, Ar *p-C*), 128.47 (s, Ar *o-C*), 122.39 (br, PC*C*HCHCH), 120.48 (s, Ar *o-C*), 104.69 (s, Ar *m-C*), 103.52 (s, Ar *m-C*), 102.91 (d, $^{3}J_{CP}$ = 17.2, PCCH*C*HCH), 95.76 (s, Cp* *C*CH_3), 59.52 (s, O*C*H_3), 56.14 (s, O*C*H_3), 55.47 (s, O*C*H_3), 54.62 (s, O*C*H_3), 51.87 (s, NCH_2*C*H_2), 48.77 (s, N*C*H_2CH_2), 10.18 (d, $^{3}J_{Cp}$ = 17.2, Cp* C*C*H_3). ^{31}P NMR (162 MHz, C_6D_6, 298 K) δ 26.45 (s, Ru*P*).

Summary of Crystal Data

Table S1. Summary of crystallographic data for compounds reported in this work.

Complexes	**2**	**3**
Empirical formula	$C_{87}H_{111}Cl_3N_6O_{12}Ru_3$	$C_{34}H_{47}N_2O_6PRu$
Formula weight	1842.37	711.77
Temperature/K	99.9(4)	173.00(10)
Crystal system	monoclinic	monoclinic
Space group	I2/a	P21/c
a/Å	20.3926(2)	12.01230(10)
b/Å	14.92420(10)	12.97590(10)
c/Å	55.1682(6)	22.1429(2)
α/°	90	90
β/°	90.1730(10)	91.1850(10)
γ/°	90	90
Volume/Å^3	16790.0(3)	3450.69(5)
Z	8	4
ρ_{calc}/g•cm^{-3}	1.458	1.370
μ/mm^{-1}	5.708	4.479
F(000)	7632.0	1488.0
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2θ range for data collection/°	6.136 to 154.776	7.36 to 153.634
Index ranges	-25 ≤ h ≤ 25	-14 ≤ h ≤ 15
	-18 ≤ k ≤ 13	-15 ≤ k ≤ 16
	-69 ≤ l ≤ 68	-27 ≤ l ≤ 27
Reflections collected	109188	22014
Independent reflections	17450 [Rint = 0.0411, Rsigma = 0.0233]	7011 [Rint = 0.0250, Rsigma = 0.0232]
Data/restraints/parameters	17450/0/1027	7011/0/409
Goodness-of-fit on F^2	1.035	1.036
Final R indexes [I>=2σ (I)]	R1 = 0.0377	R1 = 0.0238
	wR2 = 0.0946	wR2 = 0.0621
Final R indexes [all data]	R1 = 0.0404	R1 = 0.0252
	wR2 = 0.0962	wR2 = 0.0629
Largest diff. peak/hole / e Å^{-3}	0.97/-1.50	0.41/-0.52

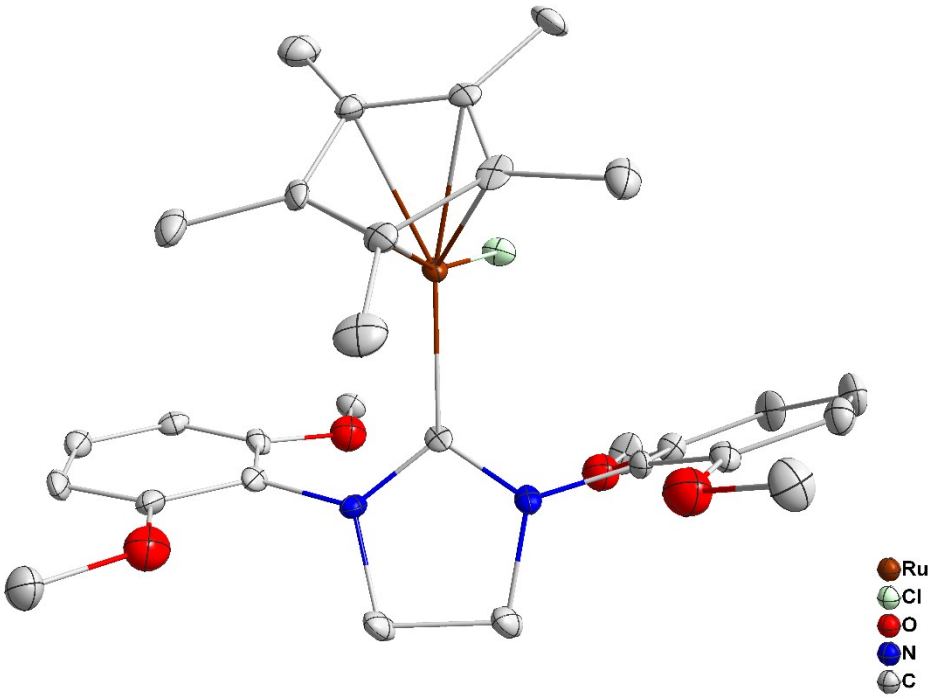


Figure S1. Crystallographic structure of **2**, with thermal ellipsoids at 30% probability level. Hydrogen atoms were omitted for clarity.

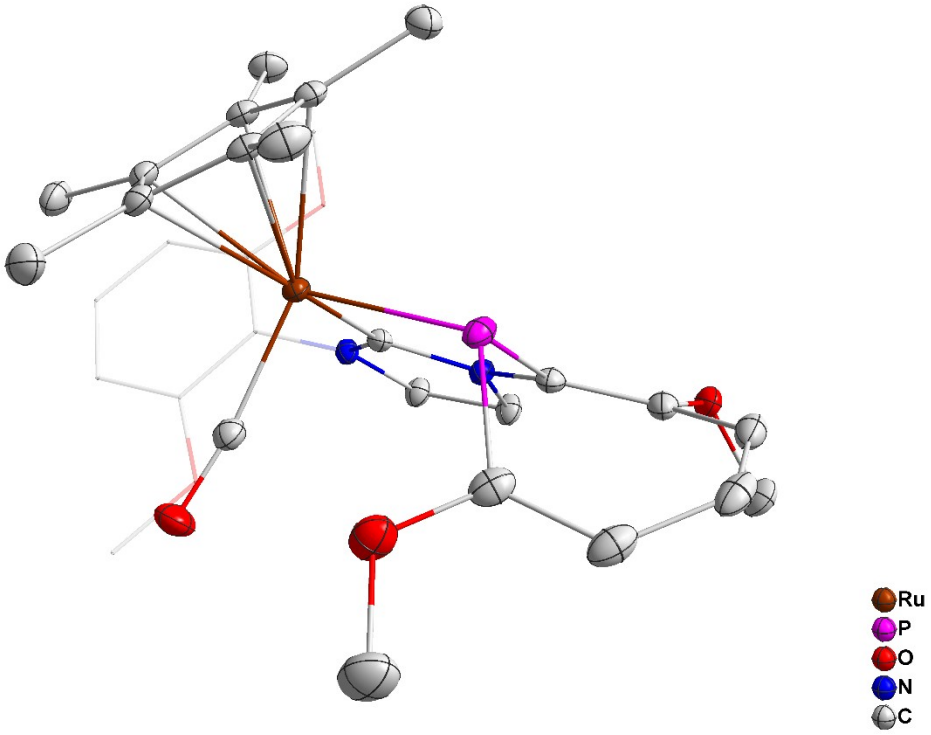


Figure S2. Crystallographic structure of **3**, with thermal ellipsoids at 30% probability level. Hydrogen atoms were omitted for clarity.

Spectroscopic Data

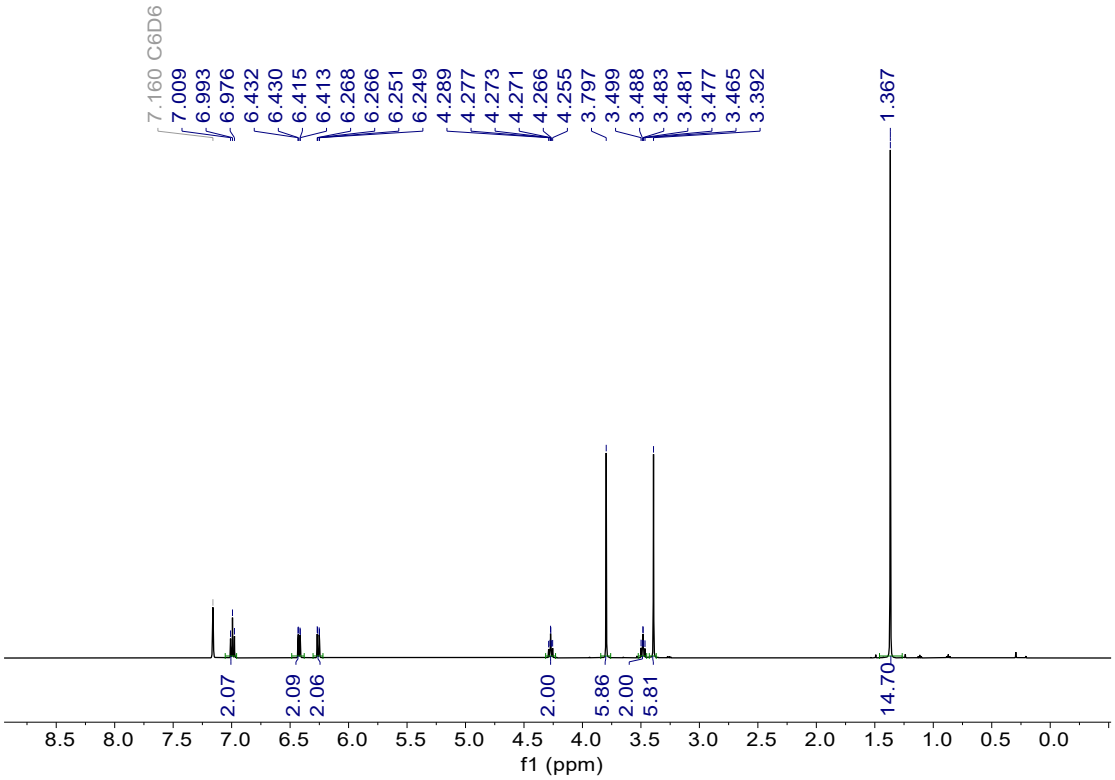


Figure S3. ^{1}H NMR spectrum of **2** in C_6D_6 (298 K).

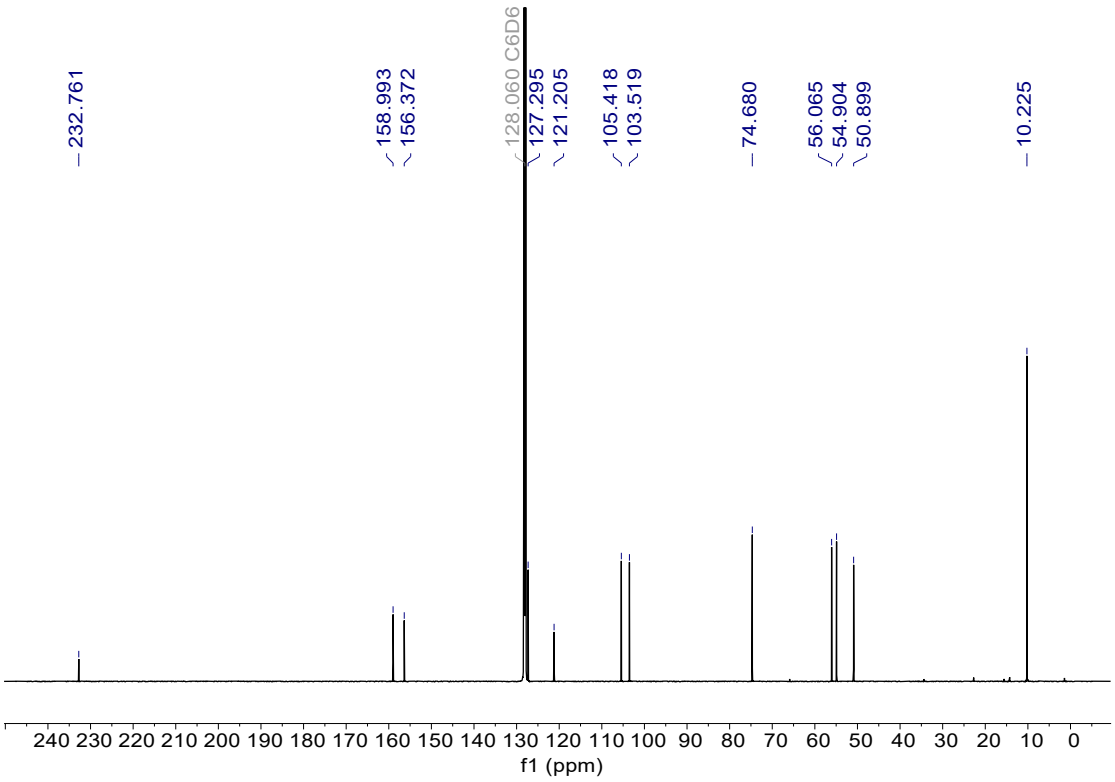


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 (298 K).

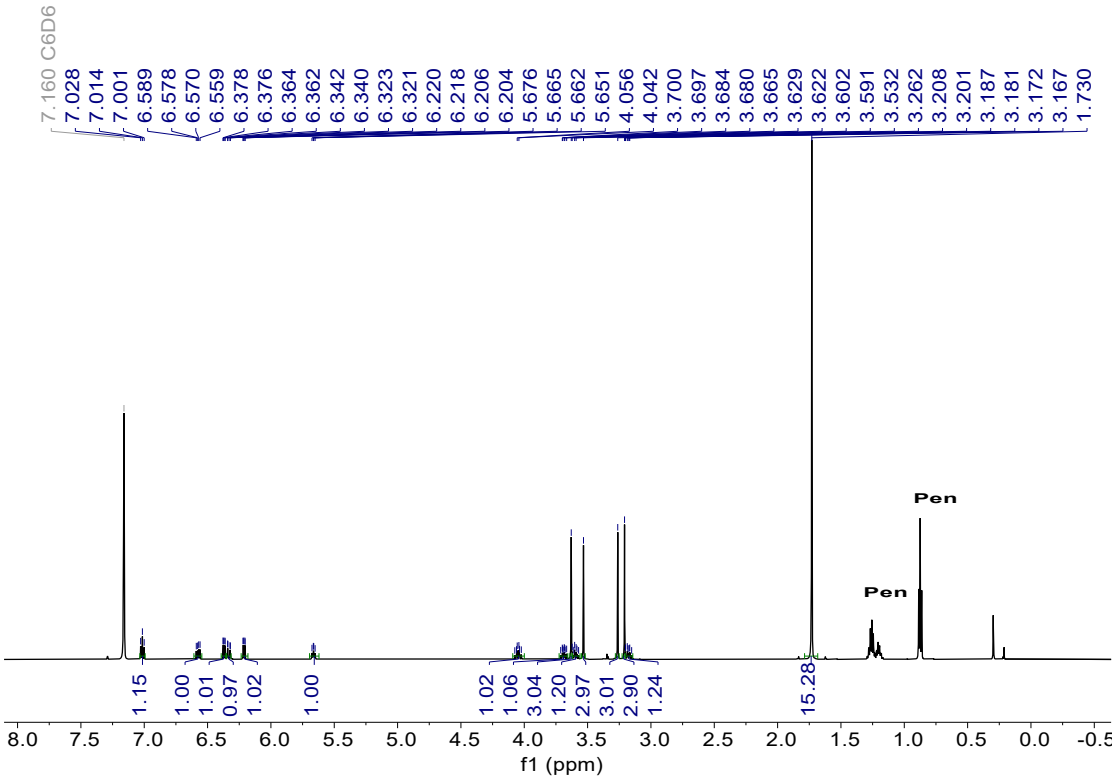


Figure S5. ^{1}H NMR spectrum of **3** in C_6D_6 (298 K).

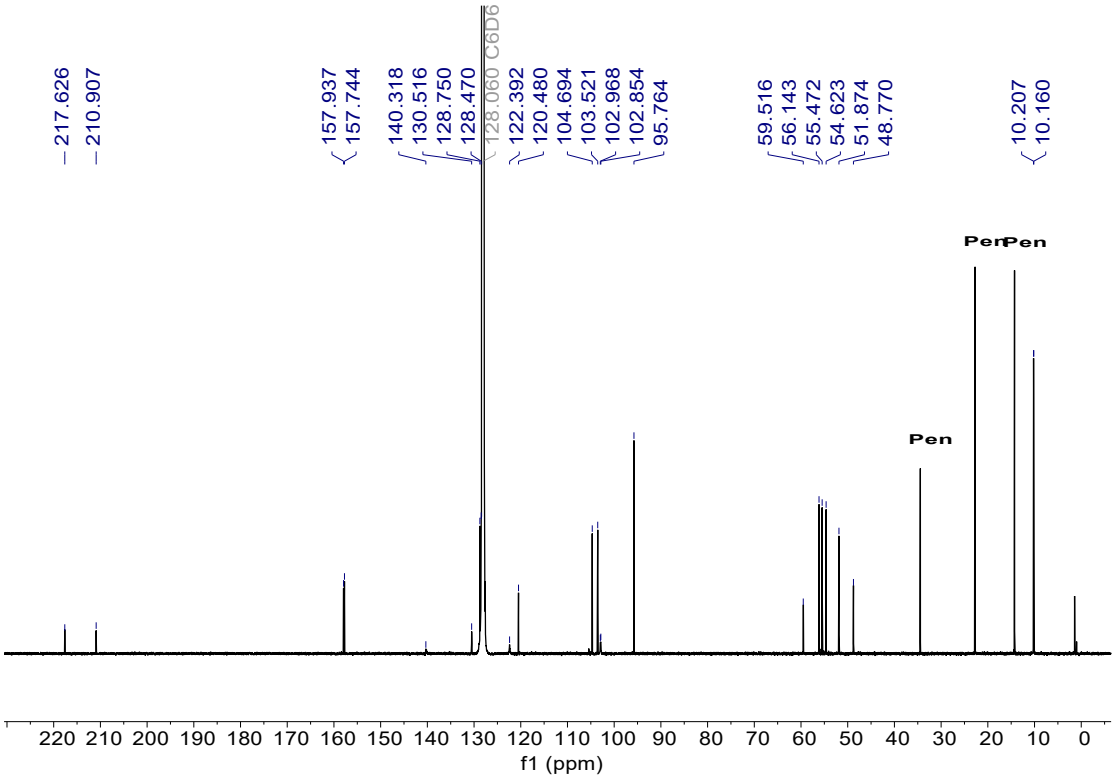


Figure S6. ^{13}C{^{1}H} NMR spectrum of **3** in C_6D_6 (298 K).

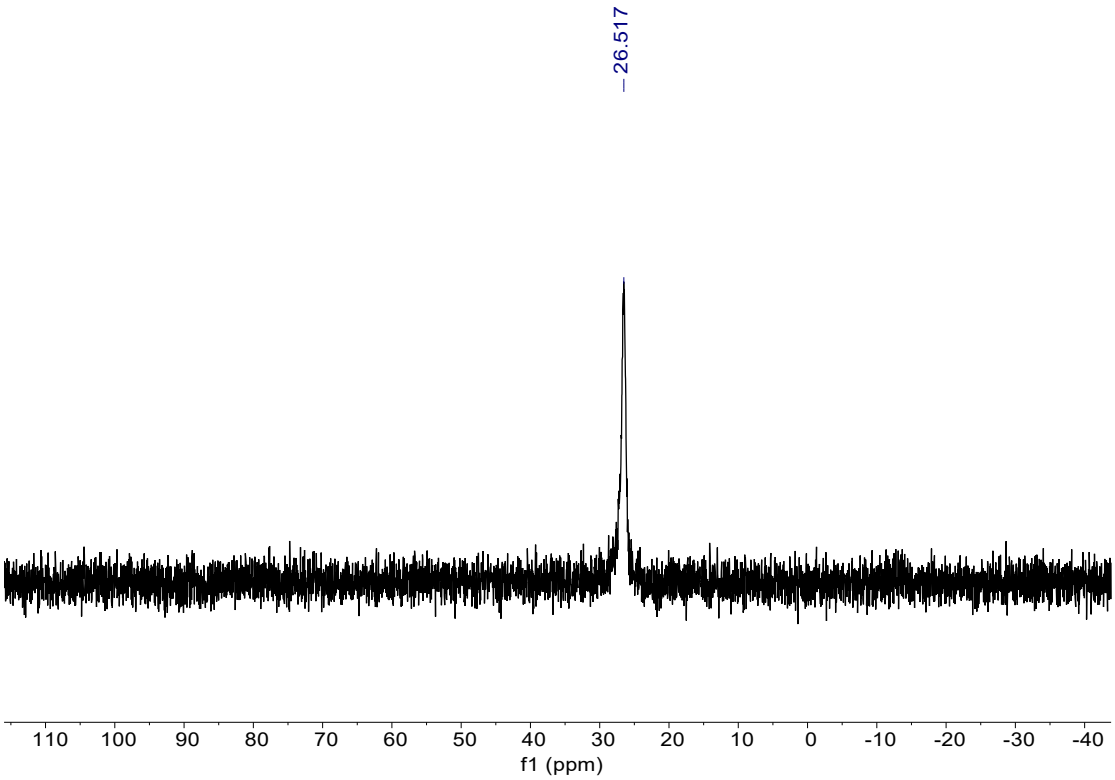


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in C_6D_6 (298 K).

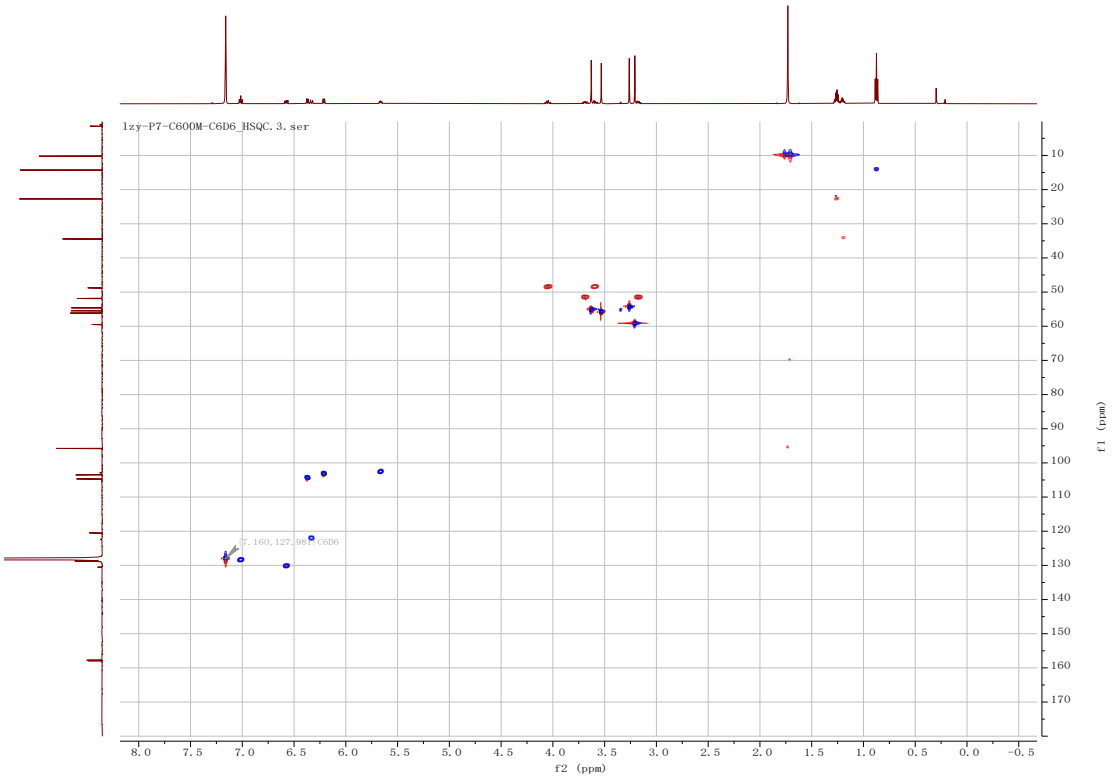


Figure S8. ^{1}H-^{13}C HSQC spectrum of **3** in C_6D_6 (298 K).

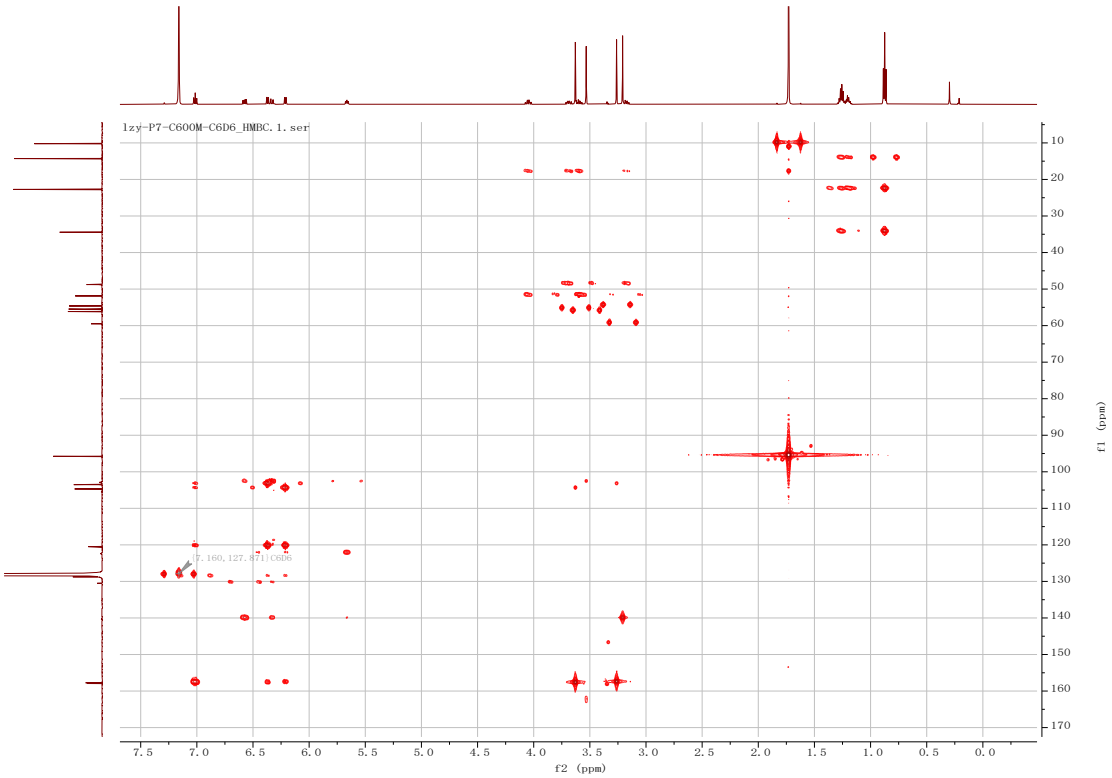


Figure S9. ^{1}H-^{13}C HMBC spectrum of **3** in C_6D_6 (298 K).

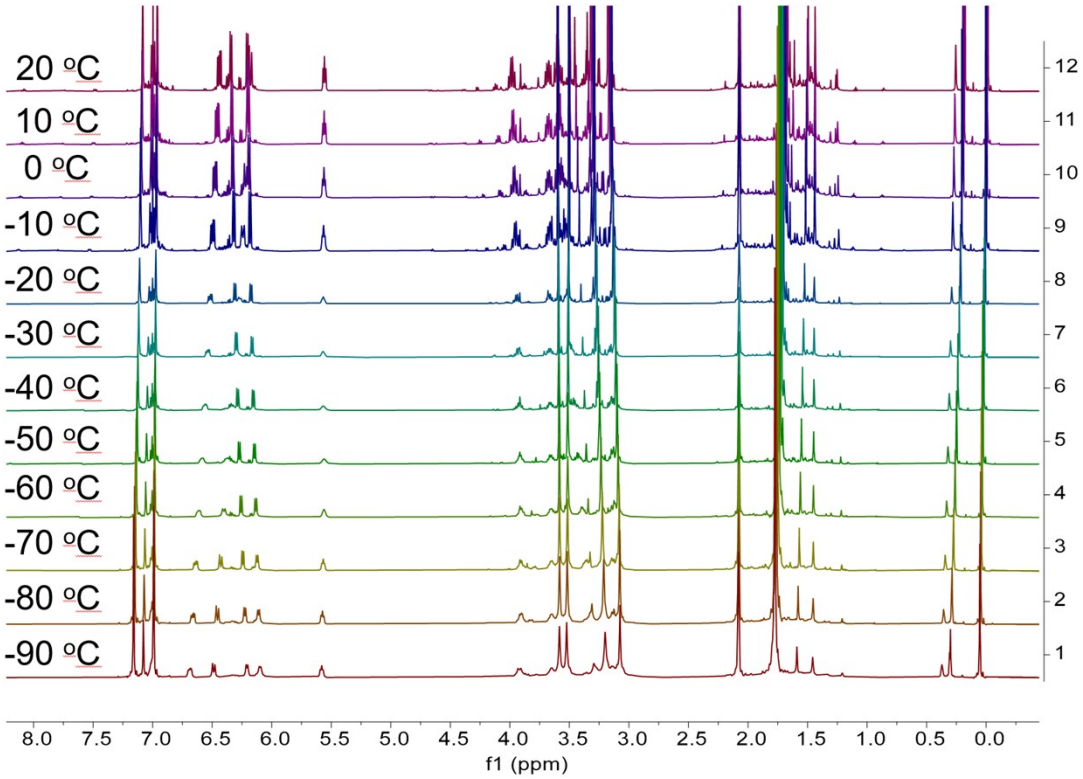


Figure S10. ^{1}H NMR spectrum of **3** in toluene-d_8 (from -90 °C to 20 °C).

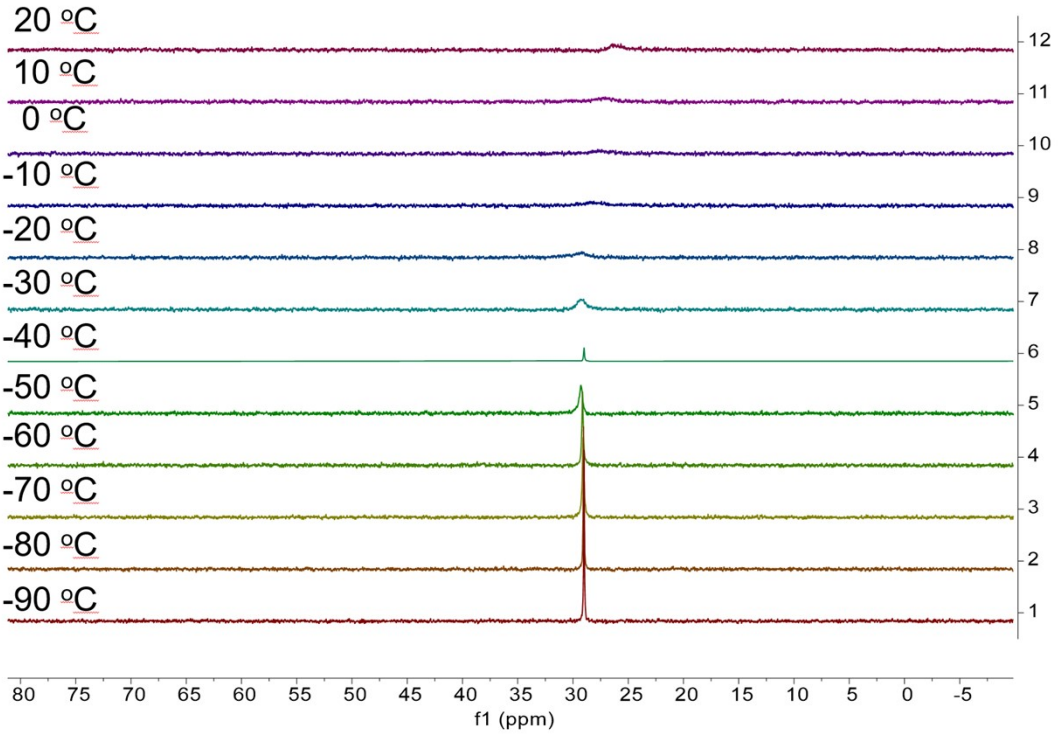


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in toluene-d_8 (from -90 °C to 20 °C).

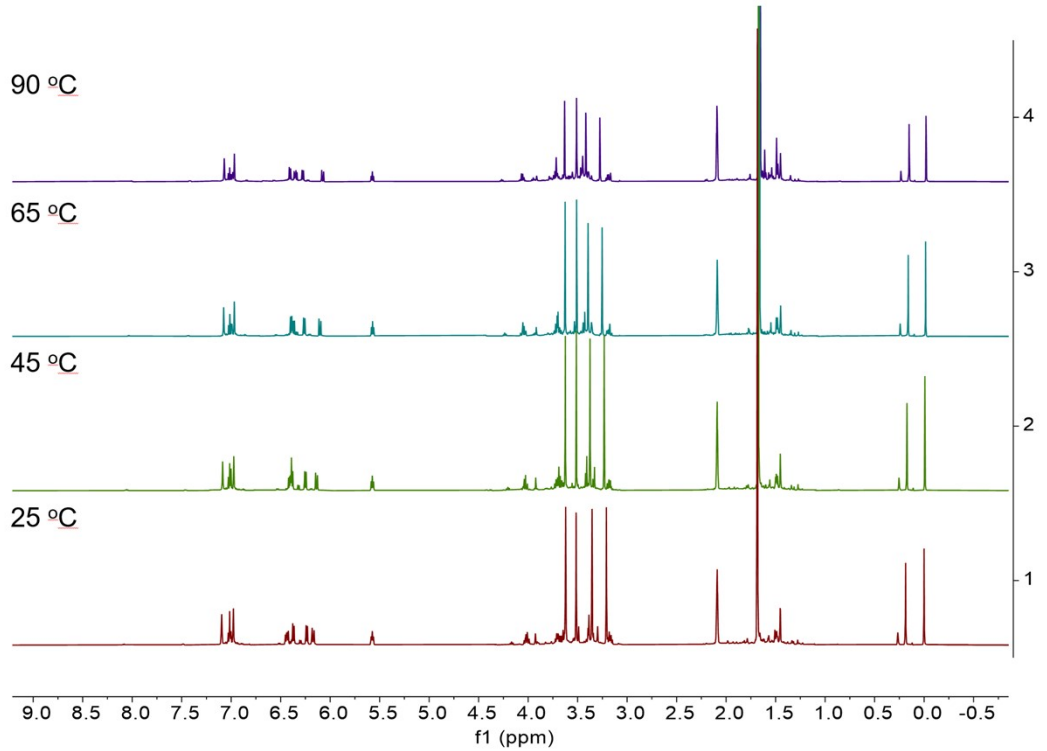


Figure S12. ^{1}H NMR spectrum of **3** in toluene-d_8 (from 20 °C to 90 °C).

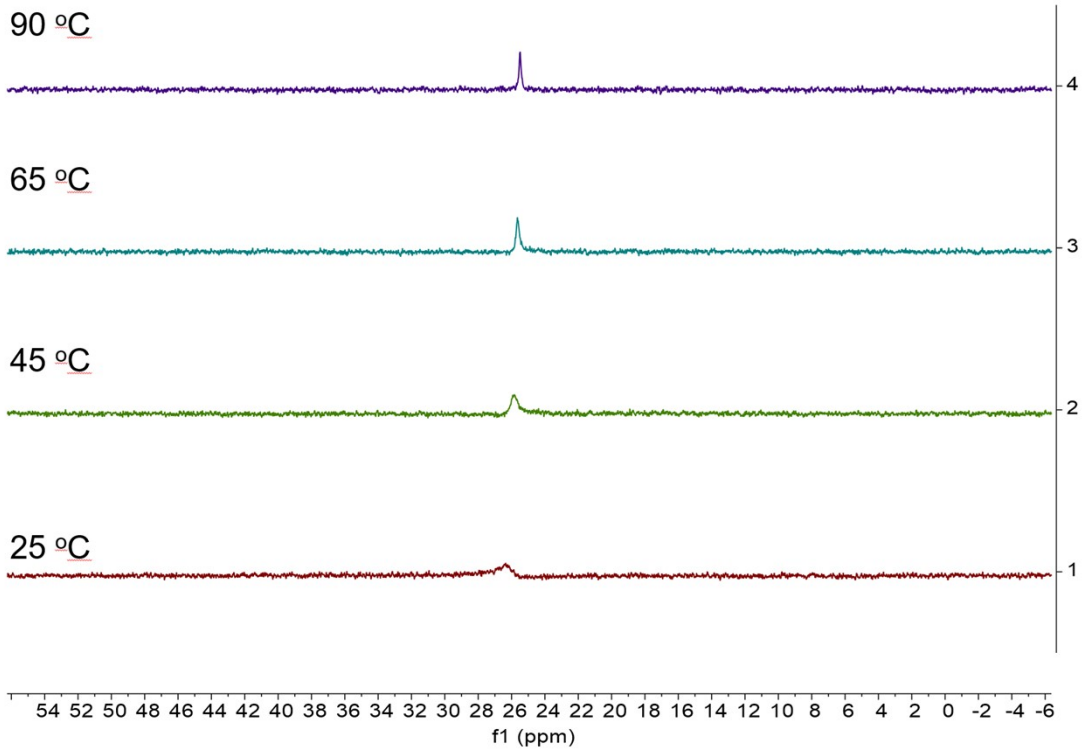


Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in toluene-d_8 (from 20 °C to 90 °C).

Details of Computational Results

Computational details. All density functional theory (DFT) calculations were performed using Orca 5.0.3 program.[2-6] Geometry optimizations of all structures were carried out using the PBE0 functional with the D4 empirical dispersion correction to account for van der Waals interactions.[7-11] The ZORA-def2-SVP basis set was used for C, H, N, O, and ZORA-def2-TZVP basis set for P, and SARC-ZORA-TZVP basis set for Ru.[12, 13] The ZORA Hamiltonian was employed to account for scalar relativistic effects for all atoms.[14] The resolution-of-identity (RI) approximation was employed to accelerate the calculations. For the RI-J approximation, the automatically generated AutoAux auxiliary basis sets were used for light atoms (C, H, N, O, P).[15, 16] For the ruthenium atom, the SARC/J auxiliary basis set was employed in conjunction with the SARC-ZORA-TZVP primary basis set.[13, 17-19] The solvation effects in benzene were evaluated using the conductor-like polarizable continuum model (CPCM) with a self-consistent reaction field (SCRF).[20, 21] The molecular cavity was defined using the United Atom Topological Model (UFF) atomic radii. Frequency analysis was performed at the same level of theory as geometry optimization to confirm whether optimized stationary points were either local minimum or transition state, as well as to evaluate zero-point vibrational energies and thermal corrections for enthalpies and free energies at 298.15 K. Single-point energies were computed on the optimized structures using the PBE0-D4 functional and the larger ZORA-def2-TZVPP basis set for C, H, O, N, P and SARC-ZORA-TZVPP for Ru.[12, 22, 23] The resolution-of-identity (RI) approximation was employed with the matching def2-TZVPP/C and SARC/J auxiliary basis sets.[3-5, 24] All other settings (ZORA, CPCM(benzene)) remained unchanged. The electron spin density distribution diagram and orbital diagrams were generated and visualized from Multiwfn and VMD.[25-27]

Table S2. Selected orbital composition analysis of ground state of **3** with Mullikenpartition.

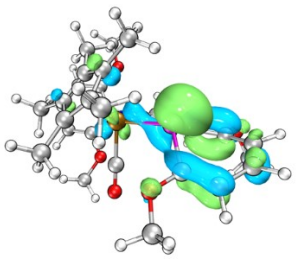
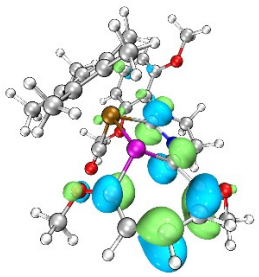
Orbital		
	HOMO	LUMO
Ru	8.5%	2.5%
P	29.1%	2.4%

Table S3. Selected orbital composition analysis of triplet state of **3** with Mullikenpartition. (The phenyl group exhibits a notable contribution to the delocalized character of HOMO, LUMO and LUMO+1.)

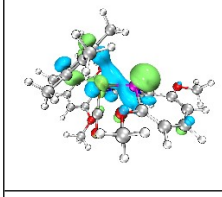
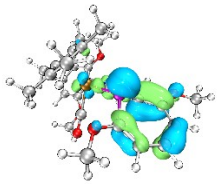
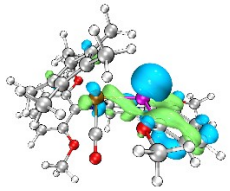
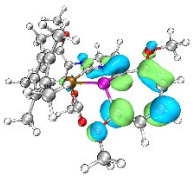
Orbital				
	SOMO-3	SOMO-2	SOMO-1	SOMO
P	15.1%	24.6%	26.0%	3.9%

Table S4. Selected atomic spin densities for triplet state of **3**.

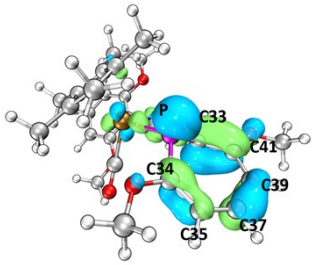
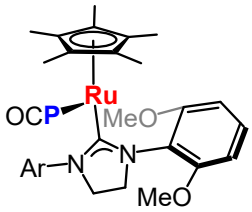
	P	C33	C41	C39	C37	C35	C34
Spin density	0.15	0.58	0.15	~0	0.48	~0	0.40

Table S5. UNO occupation numbers (HONO and LUNO) and broken-symmetry ⟨S^2⟩ expectation values for the open-shell singlet intermediates and transition states along the stepwise pathway.

Transition state /Intermediate	orbital	occupation	<S^2>
TS1	HONO (165)	1.41	0.8512
	LUNO (166)	0.59	
IM2	HONO (165)	1.21	0.9693
	LUNO (166)	0.79	
TS2	HONO (165)	1.09	1.0310
	LUNO (166)	0.91	
IM3	HONO (165)	1.03	1.0444
	LUNO (166)	0.97	
TS3	HONO (165)	1.51	1.0406
	LUNO (166)	0.49	

Coordinates for calculated structures

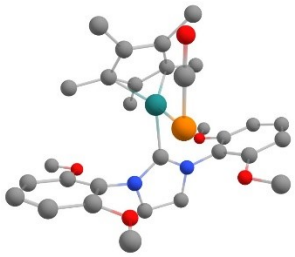


IM1

Gibbs free energy = -6571.7839043733

Electronic energy = -6572.3448591033

Imaginary frequency = NO

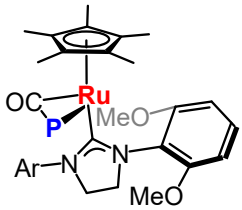


$RuC_{30}PN_2H_{37}O_5$

Ru	1.363865000	-4.867096000	5.520377000
P	-0.903732000	-5.139331000	4.781405000
N	2.273162000	-4.318747000	2.657622000
N	2.504982000	-6.412558000	3.148793000
C	2.680742000	-5.633165000	7.012462000
C	3.227713000	-7.006864000	7.199230000
C	1.495055000	-5.127992000	7.682524000
C	0.622370000	-5.946130000	8.573770000
C	1.384954000	-3.745219000	7.394887000
C	0.378353000	-2.778140000	7.922220000
C	2.496287000	-3.377952000	6.535681000
C	2.813482000	-1.979679000	6.129663000
C	3.328888000	-4.534313000	6.355506000
C	4.632744000	-4.583861000	5.630730000
C	2.042226000	-5.233893000	3.625611000
C	1.867907000	-2.972163000	2.672697000
C	0.530488000	-2.641940000	2.383749000
C	0.126506000	-1.300767000	2.393671000
H	-0.910233000	-1.031054000	2.213931000
C	1.078075000	-0.307356000	2.606201000
H	0.764059000	0.735650000	2.605812000
C	2.423629000	-0.609525000	2.797552000
H	3.146408000	0.189044000	2.938645000

C	2.819372000	-1.951477000	2.822676000
C	-1.630612000	-3.418944000	1.819042000
H	-2.087234000	-4.388340000	1.606610000
H	-2.129525000	-2.981100000	2.693765000
H	-1.756400000	-2.758016000	0.949560000
C	5.114200000	-1.388440000	3.037472000
H	6.057363000	-1.933916000	3.122419000
H	5.131257000	-0.776872000	2.124755000
H	5.004863000	-0.728635000	3.909803000
C	2.341275000	-7.674937000	3.747065000
C	1.084463000	-8.307927000	3.719317000
C	0.928196000	-9.573170000	4.300575000
H	-0.043487000	-10.058126000	4.322650000
C	2.043867000	-10.223324000	4.820523000
H	1.923289000	-11.211951000	5.261627000
C	3.313100000	-9.653213000	4.772978000
H	4.168397000	-10.193690000	5.168375000
C	3.459964000	-8.372513000	4.228438000
C	-1.183483000	-8.192136000	3.060121000
H	-1.807857000	-7.482501000	2.512844000
H	-1.194287000	-9.163270000	2.544769000
H	-1.590277000	-8.306015000	4.073511000
C	5.814940000	-8.391361000	4.524592000
H	6.641471000	-7.705472000	4.322393000
H	5.804188000	-8.630693000	5.597467000
H	5.964611000	-9.316902000	3.951604000
H	3.658351000	-7.110005000	8.206593000
H	4.015583000	-7.218452000	6.473809000
H	2.451904000	-7.772500000	7.088734000
H	4.656205000	-3.847764000	4.820578000
H	4.790318000	-5.570276000	5.182587000
H	5.471338000	-4.374836000	6.310864000
H	3.200501000	-1.412212000	6.989423000
H	1.927714000	-1.454744000	5.755873000
H	3.572381000	-1.961985000	5.345321000
H	0.113547000	-2.033761000	7.162593000
H	0.784532000	-2.237299000	8.789464000
H	-0.543097000	-3.274878000	8.237890000
H	-0.371088000	-5.504145000	8.690317000

H	1.071472000	-6.037593000	9.573535000
H	0.493154000	-6.959133000	8.175368000
C	-1.629345000	-4.898974000	6.245698000
O	-2.201815000	-4.741485000	7.256983000
O	4.639546000	-7.726471000	4.129719000
O	0.111324000	-7.642928000	3.086861000
O	-0.270695000	-3.669093000	2.077986000
O	4.095223000	-2.357487000	2.987446000
C	3.013453000	-6.346033000	1.779503000
H	2.379352000	-6.951388000	1.117775000
H	4.037060000	-6.735954000	1.733929000
C	2.930291000	-4.854684000	1.467086000
H	3.916248000	-4.389843000	1.339769000
H	2.327989000	-4.642610000	0.575171000



TS1

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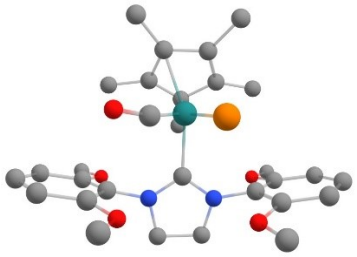
Electronic energy = -6572.3183112167

Imaginary frequency = -299.5

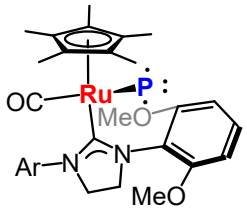


$RuC_{30}PN_2H_{37}O_5$

Ru	-0.647029000	-0.064714000	1.161973000
P	-2.307003000	-1.584794000	1.125060000
N	-0.159348000	0.907351000	-1.699012000
N	0.483189000	-1.143430000	-1.464790000
C	0.046523000	-0.422418000	3.279845000
C	-0.514401000	-1.417090000	4.241039000
C	-0.383278000	0.941755000	3.120531000
C	-1.475056000	1.615035000	3.887661000

C	0.508237000	1.593370000	2.202776000
C	0.525558000	3.056534000	1.908236000
C	1.450503000	0.608492000	1.762955000
C	2.589746000	0.862240000	0.828103000
C	1.198319000	-0.623880000	2.460043000
C	2.043845000	-1.853126000	2.454919000
C	-0.128931000	-0.121634000	-0.830843000
C	-0.844246000	2.126618000	-1.545788000
C	-2.240767000	2.154990000	-1.701530000
C	-2.926431000	3.371302000	-1.604907000
H	-4.009520000	3.405795000	-1.678548000
C	-2.200113000	4.543010000	-1.416841000
H	-2.733537000	5.489648000	-1.340712000
C	-0.808749000	4.543532000	-1.339247000
H	-0.270453000	5.478977000	-1.215559000
C	-0.126623000	3.325161000	-1.421783000
C	-4.217805000	0.899540000	-2.053926000
H	-4.457189000	-0.150898000	-2.236474000
H	-4.692362000	1.217400000	-1.117608000
H	-4.592472000	1.507814000	-2.889258000
C	2.000061000	4.374795000	-1.391521000
H	3.042911000	4.049767000	-1.428537000
H	1.786255000	5.007991000	-2.263594000
H	1.841206000	4.959861000	-0.474670000
C	0.583540000	-2.479535000	-1.034116000
C	-0.539587000	-3.320793000	-1.135292000
C	-0.442508000	-4.662322000	-0.748360000
H	-1.310680000	-5.314461000	-0.779251000
C	0.791805000	-5.161289000	-0.341430000
H	0.868394000	-6.206298000	-0.044002000
C	1.936385000	-4.368390000	-0.329179000
H	2.891753000	-4.795467000	-0.037880000
C	1.831647000	-3.021611000	-0.695555000
C	-2.815576000	-3.523689000	-1.755942000
H	-3.575076000	-2.863343000	-2.181012000
H	-2.667516000	-4.385990000	-2.421361000
H	-3.160160000	-3.870309000	-0.772298000
C	4.177902000	-2.687379000	-0.583087000
H	4.864929000	-1.852189000	-0.741281000

H	4.321929000	-3.078570000	0.433940000
H	4.400052000	-3.482330000	-1.308321000
H	0.013806000	-1.364426000	5.204180000
H	-0.415886000	-2.438276000	3.857459000
H	-1.578056000	-1.238828000	4.429919000
H	2.749728000	-1.837178000	1.622159000
H	1.441508000	-2.764816000	2.366655000
H	2.626028000	-1.929314000	3.385580000
H	3.476714000	1.203079000	1.381263000
H	2.326892000	1.631401000	0.094838000
H	2.857239000	-0.046094000	0.279533000
H	1.108502000	3.265898000	1.008922000
H	0.978431000	3.618429000	2.739173000
H	-0.483378000	3.453415000	1.750144000
H	-1.955258000	2.400793000	3.294575000
H	-1.077118000	2.080568000	4.800605000
H	-2.252090000	0.903709000	4.186431000
C	-2.407472000	0.526272000	0.912068000
O	-3.353257000	1.227079000	0.935046000
O	2.879779000	-2.175577000	-0.765795000
O	-1.641668000	-2.755777000	-1.644563000
O	-2.815248000	0.972610000	-1.955494000
O	1.217044000	3.205751000	-1.402637000
C	0.904879000	-0.829367000	-2.830300000
H	0.453788000	-1.540007000	-3.533281000
H	1.996301000	-0.905784000	-2.909192000
C	0.389403000	0.592931000	-3.017768000
H	1.179021000	1.307829000	-3.275373000
H	-0.403937000	0.659831000	-3.773722000



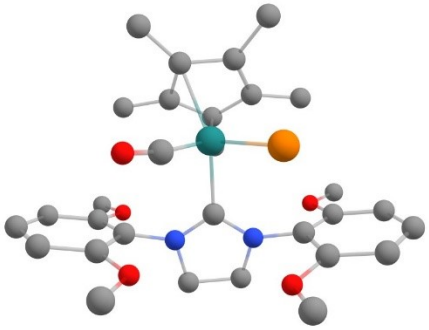
OSS

IM2

Gibbs free energy = -6571.7771396502

Electronic energy = -6572.3378604602

Imaginary frequency = NO

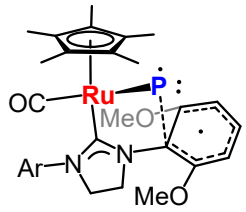


$RuC_{30}PN_2H_{37}O_5$

Ru	-0.617011000	-0.088114000	1.210834000
P	-1.545764000	-2.172652000	1.324647000
N	-0.177947000	0.874904000	-1.644434000
N	0.558152000	-1.145814000	-1.425236000
C	0.095675000	-0.327442000	3.351973000
C	-0.410789000	-1.272307000	4.388546000
C	-0.330694000	1.020391000	3.144534000
C	-1.398605000	1.738117000	3.905302000
C	0.546239000	1.629979000	2.182405000
C	0.569609000	3.084852000	1.850790000
C	1.489215000	0.634433000	1.770509000
C	2.617555000	0.850073000	0.814334000
C	1.225282000	-0.571839000	2.496462000
C	2.040025000	-1.821121000	2.515247000
C	-0.113709000	-0.164400000	-0.782673000
C	-0.891743000	2.077551000	-1.495758000
C	-2.288867000	2.079249000	-1.656122000
C	-2.998510000	3.282502000	-1.564920000
H	-4.082006000	3.295924000	-1.639921000
C	-2.295423000	4.470835000	-1.390842000
H	-2.847429000	5.407234000	-1.321049000
C	-0.904163000	4.499761000	-1.326520000
H	-0.383116000	5.447235000	-1.221837000
C	-0.198567000	3.294039000	-1.400044000
C	-4.240010000	0.799657000	-2.052695000
H	-4.463943000	-0.251370000	-2.249849000
H	-4.750213000	1.106805000	-1.131527000
H	-4.594678000	1.409340000	-2.895608000
C	1.905994000	4.389032000	-1.430569000
H	2.954265000	4.084350000	-1.482726000

H	1.661814000	5.000767000	-2.309888000
H	1.753703000	4.988209000	-0.521823000
C	0.616064000	-2.508886000	-1.081637000
C	-0.516436000	-3.309700000	-1.320190000
C	-0.472674000	-4.679938000	-1.035181000
H	-1.350973000	-5.304622000	-1.169744000
C	0.717057000	-5.234409000	-0.575094000
H	0.751406000	-6.298891000	-0.346993000
C	1.873147000	-4.472362000	-0.418451000
H	2.794531000	-4.944037000	-0.088965000
C	1.826459000	-3.101973000	-0.697623000
C	-2.796512000	-3.349517000	-1.947013000
H	-3.512306000	-2.632227000	-2.355869000
H	-2.741710000	-4.222037000	-2.613372000
H	-3.132068000	-3.660968000	-0.948026000
C	4.163753000	-2.839514000	-0.395441000
H	4.879987000	-2.015342000	-0.446498000
H	4.220587000	-3.299245000	0.601357000
H	4.422664000	-3.592495000	-1.152723000
H	0.243466000	-1.254269000	5.272259000
H	-0.441899000	-2.298858000	4.004697000
H	-1.423239000	-1.010588000	4.712775000
H	2.761000000	-1.826741000	1.695760000
H	1.405396000	-2.711261000	2.413230000
H	2.595271000	-1.911030000	3.460185000
H	3.509714000	1.212383000	1.344890000
H	2.348876000	1.590071000	0.053348000
H	2.878599000	-0.081432000	0.302786000
H	1.151694000	3.268883000	0.946396000
H	1.028980000	3.660325000	2.668656000
H	-0.436899000	3.485817000	1.688976000
H	-1.884366000	2.502352000	3.288943000
H	-0.973282000	2.242298000	4.784784000
H	-2.174119000	1.050536000	4.258015000
C	-2.322513000	0.517479000	0.955036000
O	-3.410383000	0.922920000	0.952830000
O	2.895720000	-2.281655000	-0.641123000
O	-1.563296000	-2.677934000	-1.869136000
O	-2.842532000	0.886356000	-1.909637000

O	1.147122000	3.204056000	-1.403364000
C	1.008600000	-0.778521000	-2.768342000
H	0.653379000	-1.515772000	-3.497343000
H	2.105517000	-0.759430000	-2.800161000
C	0.380269000	0.592668000	-2.965949000
H	1.108185000	1.364219000	-3.239155000
H	-0.424826000	0.588203000	-3.713282000



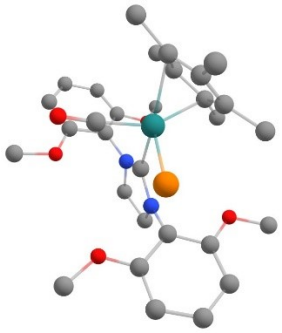
OSS

TS2

Gibbs free energy = -6571.7607172715

Electronic energy = -6572.3207949115

Imaginary frequency = -377.5

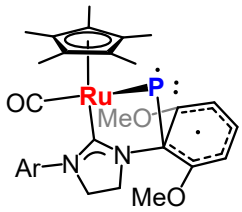


$RuC_{30}PN_2H_{37}O_5$

Ru	-0.481152000	-0.136534000	1.309616000
P	-0.652311000	-2.403165000	1.236730000
N	-0.104929000	0.840324000	-1.554352000
N	0.300467000	-1.280583000	-1.393396000
C	0.138710000	-0.124483000	3.469740000
C	-0.343190000	-1.053195000	4.534789000
C	-0.401459000	1.159498000	3.139983000
C	-1.575593000	1.816195000	3.792625000
C	0.453561000	1.781403000	2.170487000
C	0.382203000	3.213789000	1.758744000
C	1.511093000	0.855070000	1.876571000
C	2.649689000	1.097509000	0.939196000
C	1.338490000	-0.302990000	2.692076000

C	2.280823000	-1.450909000	2.830614000
C	-0.115890000	-0.209020000	-0.696464000
C	-0.756897000	2.076437000	-1.386604000
C	-2.163398000	2.127794000	-1.413674000
C	-2.819925000	3.361043000	-1.320697000
H	-3.904861000	3.413235000	-1.299403000
C	-2.063209000	4.530002000	-1.297163000
H	-2.573616000	5.490345000	-1.236570000
C	-0.673664000	4.505118000	-1.374265000
H	-0.111768000	5.434733000	-1.380903000
C	-0.019455000	3.268798000	-1.429075000
C	-4.185138000	0.922076000	-1.672848000
H	-4.459892000	-0.124664000	-1.822283000
H	-4.659404000	1.280833000	-0.751124000
H	-4.535010000	1.517690000	-2.527735000
C	2.119116000	4.277390000	-1.640468000
H	3.149601000	3.926861000	-1.738675000
H	1.852258000	4.868492000	-2.527417000
H	2.042282000	4.913954000	-0.747621000
C	0.363764000	-2.644142000	-1.005181000
C	-0.641483000	-3.510461000	-1.542191000
C	-0.466860000	-4.887093000	-1.526924000
H	-1.265614000	-5.552498000	-1.843637000
C	0.754654000	-5.418869000	-1.093803000
H	0.889799000	-6.498861000	-1.075101000
C	1.819861000	-4.588455000	-0.730831000
H	2.773210000	-5.027582000	-0.449051000
C	1.649336000	-3.208341000	-0.749313000
C	-2.868814000	-3.641532000	-2.326033000
H	-3.657505000	-2.934395000	-2.595582000
H	-2.649280000	-4.282783000	-3.191906000
H	-3.217605000	-4.268557000	-1.493558000
C	3.913967000	-2.783679000	-0.222919000
H	4.545582000	-1.903679000	-0.073427000
H	3.950618000	-3.406636000	0.682199000
H	4.300550000	-3.365364000	-1.072151000
H	0.225572000	-0.912873000	5.465565000
H	-0.231864000	-2.099621000	4.226001000
H	-1.401609000	-0.886941000	4.761241000

H	3.022443000	-1.449199000	2.028449000
H	1.750704000	-2.412180000	2.794682000
H	2.814820000	-1.395158000	3.789888000
H	3.491051000	1.578040000	1.458693000
H	2.343824000	1.743007000	0.110085000
H	3.007365000	0.155375000	0.511160000
H	1.035214000	3.406384000	0.905476000
H	0.712027000	3.866279000	2.581412000
H	-0.631915000	3.519131000	1.480131000
H	-2.081071000	2.502940000	3.105000000
H	-1.254419000	2.397389000	4.668631000
H	-2.311175000	1.080121000	4.133029000
C	-2.302799000	-0.050902000	1.117948000
O	-3.462255000	0.001272000	1.132146000
O	2.616328000	-2.309393000	-0.473370000
O	-1.753168000	-2.874309000	-1.952792000
O	-2.781900000	0.951317000	-1.572741000
O	1.317113000	3.127045000	-1.528462000
C	0.703574000	-0.973710000	-2.763487000
H	0.216589000	-1.658412000	-3.466788000
H	1.791623000	-1.090561000	-2.858205000
C	0.246333000	0.467686000	-2.925169000
H	1.028208000	1.129837000	-3.312979000
H	-0.640643000	0.556318000	-3.567669000



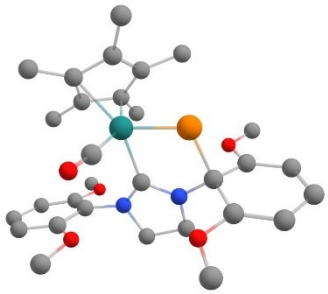
OSS

IM3

Gibbs free energy = -6571.7786008047

Electronic energy = -6572.33798601467

Imaginary frequency = NO

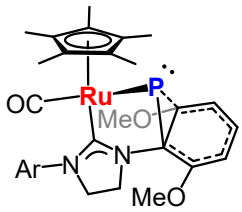


$RuC_{30}PN_2H_{37}O_5$

Ru	-0.444222000	-0.177390000	1.330011000
P	-0.288721000	-2.459292000	1.118900000
N	-0.059102000	0.809041000	-1.564420000
N	0.238261000	-1.322696000	-1.321243000
C	0.081815000	-0.117802000	3.506443000
C	-0.394714000	-1.067505000	4.556823000
C	-0.521199000	1.130099000	3.137269000
C	-1.758977000	1.719245000	3.734006000
C	0.329080000	1.789794000	2.189207000
C	0.184148000	3.204847000	1.736359000
C	1.458095000	0.929087000	1.956614000
C	2.620102000	1.232215000	1.067147000
C	1.323709000	-0.223994000	2.784638000
C	2.336283000	-1.303983000	2.970243000
C	-0.099866000	-0.205109000	-0.667083000
C	-0.660413000	2.074060000	-1.428593000
C	-2.063643000	2.179259000	-1.401397000
C	-2.669266000	3.439946000	-1.324092000
H	-3.750032000	3.534851000	-1.267140000
C	-1.868965000	4.578947000	-1.363004000
H	-2.340808000	5.559575000	-1.316219000
C	-0.484460000	4.497996000	-1.479808000
H	0.111948000	5.404606000	-1.526110000
C	0.120801000	3.236016000	-1.515735000
C	-4.139211000	1.045587000	-1.531004000
H	-4.459319000	0.006069000	-1.628991000
H	-4.561866000	1.454280000	-0.604311000
H	-4.503569000	1.625307000	-2.390766000
C	2.296413000	4.158359000	-1.730678000
H	3.313615000	3.767909000	-1.815485000
H	2.065178000	4.758412000	-2.621716000

H	2.231880000	4.798374000	-0.839384000
C	0.276194000	-2.635965000	-0.733665000
C	-0.711346000	-3.550538000	-1.389886000
C	-0.430631000	-4.864616000	-1.673593000
H	-1.206542000	-5.520034000	-2.062876000
C	0.872529000	-5.374776000	-1.475044000
H	1.084441000	-6.417909000	-1.697920000
C	1.914431000	-4.524121000	-1.039365000
H	2.923707000	-4.920020000	-0.952684000
C	1.658714000	-3.207202000	-0.746749000
C	-2.969829000	-3.694644000	-2.073731000
H	-3.820702000	-3.013311000	-2.155156000
H	-2.751263000	-4.120851000	-3.063889000
H	-3.225793000	-4.511048000	-1.383304000
C	3.925595000	-2.688552000	-0.325560000
H	4.503782000	-1.801541000	-0.052404000
H	4.074545000	-3.465026000	0.438622000
H	4.283012000	-3.069303000	-1.293569000
H	0.092940000	-0.870366000	5.522775000
H	-0.177803000	-2.106246000	4.281227000
H	-1.476378000	-0.985467000	4.706521000
H	2.945331000	-1.438653000	2.072044000
H	1.859253000	-2.265887000	3.188677000
H	3.005509000	-1.058799000	3.807493000
H	3.370229000	1.840587000	1.592682000
H	2.301598000	1.778165000	0.173667000
H	3.107980000	0.309851000	0.735236000
H	0.884872000	3.428736000	0.928859000
H	0.401201000	3.897692000	2.563210000
H	-0.824329000	3.427882000	1.371201000
H	-2.269791000	2.376888000	3.022308000
H	-1.511606000	2.316796000	4.622961000
H	-2.467249000	0.943235000	4.042654000
C	-2.261777000	-0.287467000	1.098725000
O	-3.418979000	-0.365594000	1.057598000
O	2.582141000	-2.289544000	-0.396537000
O	-1.892034000	-2.937554000	-1.590106000
O	-2.733126000	1.023720000	-1.491116000
O	1.448729000	3.040532000	-1.627912000

C	0.617224000	-1.112055000	-2.709008000
H	0.078937000	-1.801933000	-3.370161000
H	1.695022000	-1.288584000	-2.831209000
C	0.231613000	0.347866000	-2.925348000
H	1.034932000	0.946049000	-3.369271000
H	-0.668266000	0.453498000	-3.546881000

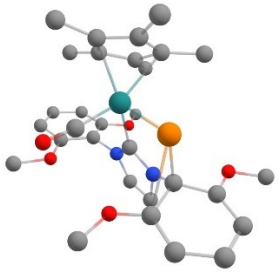


TS3

Gibbs free energy = -6571.7775483520

Electronic energy = -6572.3372435220

Imaginary frequency = -175.5

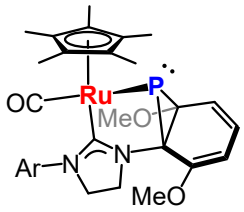


$RuC_{30}PN_2H_{37}O_5$

Ru	-0.431228000	-0.275791000	1.163867000
P	0.152412000	-2.501564000	1.070939000
N	0.114823000	0.701496000	-1.716986000
N	0.594989000	-1.385618000	-1.394014000
C	0.076131000	-0.246888000	3.342631000
C	-0.005495000	-1.400874000	4.286204000
C	-0.934810000	0.732127000	3.094991000
C	-2.291704000	0.772245000	3.721485000
C	-0.386134000	1.750907000	2.233807000
C	-1.058359000	3.032011000	1.866930000
C	0.964062000	1.381785000	1.948212000
C	1.966939000	2.198174000	1.202108000
C	1.257423000	0.152345000	2.614702000
C	2.586525000	-0.525951000	2.664550000
C	0.121668000	-0.281169000	-0.788465000
C	-0.390548000	2.007641000	-1.589694000

C	-1.780204000	2.231169000	-1.545331000
C	-2.275889000	3.540881000	-1.482700000
H	-3.344295000	3.726768000	-1.422364000
C	-1.386721000	4.609700000	-1.521354000
H	-1.775365000	5.626077000	-1.474382000
C	-0.013136000	4.412748000	-1.636404000
H	0.656597000	5.266151000	-1.690589000
C	0.483618000	3.104491000	-1.691019000
C	-3.952459000	1.295969000	-1.585883000
H	-4.373608000	0.290188000	-1.636061000
H	-4.296661000	1.773287000	-0.658508000
H	-4.298291000	1.883982000	-2.447860000
C	2.719373000	3.847955000	-1.954410000
H	3.697039000	3.378379000	-2.087018000
H	2.511395000	4.495277000	-2.817774000
H	2.738573000	4.460412000	-1.041822000
C	0.530052000	-2.681799000	-0.789434000
C	-0.721793000	-3.424993000	-1.144104000
C	-0.730425000	-4.811016000	-1.296600000
H	-1.669615000	-5.332541000	-1.467193000
C	0.465897000	-5.526503000	-1.281296000
H	0.451687000	-6.608568000	-1.391851000
C	1.718715000	-4.851086000	-1.178145000
H	2.638601000	-5.428120000	-1.235090000
C	1.760575000	-3.496395000	-1.009177000
C	-3.036497000	-3.183984000	-1.557393000
H	-3.734662000	-2.355116000	-1.693962000
H	-3.089088000	-3.851747000	-2.429682000
H	-3.320727000	-3.743706000	-0.655025000
C	4.116786000	-3.374466000	-1.044633000
H	4.875873000	-2.591754000	-0.970489000
H	4.275650000	-4.110042000	-0.243349000
H	4.210632000	-3.881747000	-2.015858000
H	0.440967000	-1.143744000	5.257345000
H	0.530086000	-2.274734000	3.894724000
H	-1.043460000	-1.702064000	4.462170000
H	3.194656000	-0.268766000	1.790485000
H	2.473998000	-1.617171000	2.672720000
H	3.148345000	-0.237144000	3.564928000

H	2.761733000	2.531349000	1.883735000
H	1.505442000	3.089049000	0.768678000
H	2.436132000	1.637343000	0.387841000
H	-0.656323000	3.447564000	0.938359000
H	-0.927883000	3.786921000	2.657241000
H	-2.134998000	2.893258000	1.720676000
H	-3.026630000	1.239898000	3.057282000
H	-2.272266000	1.351807000	4.655293000
H	-2.652329000	-0.233437000	3.960942000
C	-2.172571000	-0.640735000	0.706518000
O	-3.302219000	-0.856187000	0.548959000
O	2.868786000	-2.742651000	-0.918258000
O	-1.761696000	-2.615443000	-1.420374000
O	-2.554820000	1.141750000	-1.598908000
O	1.784470000	2.802555000	-1.855157000
C	0.757483000	-1.243267000	-2.832486000
H	-0.041555000	-1.791390000	-3.352762000
H	1.724827000	-1.641698000	-3.157719000
C	0.643128000	0.266344000	-3.013937000
H	1.611734000	0.745670000	-3.201987000
H	-0.046980000	0.548905000	-3.816939000

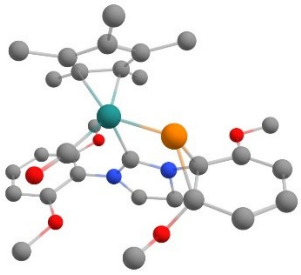


4

Gibbs free energy = -6571.8032078731

Electronic energy = -6572.3652531931

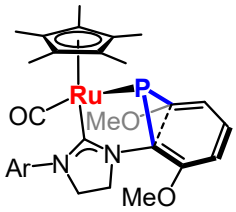
Imaginary frequency = NO



$RuC_{30}PN_2H_{37}O_5$

Ru	-0.521016000	-0.219961000	1.216566000
P	-0.263184000	-2.535087000	0.934466000
N	-0.101639000	0.794228000	-1.672223000
N	0.720198000	-1.172825000	-1.266831000
C	-0.022468000	-0.302605000	3.399345000
C	-0.483456000	-1.312560000	4.398316000
C	-0.636987000	0.955030000	3.098003000
C	-1.880484000	1.502019000	3.721832000
C	0.211936000	1.677149000	2.188832000
C	0.038898000	3.107103000	1.796244000
C	1.359183000	0.848921000	1.927956000
C	2.532560000	1.210961000	1.076911000
C	1.226209000	-0.355256000	2.675530000
C	2.243047000	-1.441625000	2.787058000
C	0.023553000	-0.155631000	-0.727345000
C	-0.760593000	2.032338000	-1.558547000
C	-2.163436000	2.096095000	-1.648746000
C	-2.809825000	3.337098000	-1.566055000
H	-3.893527000	3.401261000	-1.599885000
C	-2.048091000	4.498156000	-1.473398000
H	-2.554314000	5.461214000	-1.421525000
C	-0.657098000	4.461561000	-1.462597000
H	-0.087236000	5.384560000	-1.405620000
C	-0.013506000	3.220002000	-1.506724000
C	-4.199206000	0.936206000	-1.948328000
H	-4.499970000	-0.100675000	-2.111722000
H	-4.669796000	1.295694000	-1.024747000
H	-4.532991000	1.547932000	-2.798155000
C	2.142684000	4.214249000	-1.499356000
H	3.175499000	3.857197000	-1.515440000
H	1.960633000	4.835254000	-2.387114000
H	1.987833000	4.821482000	-0.596462000
C	0.721472000	-2.466556000	-0.676929000
C	-0.611039000	-3.199497000	-0.793972000
C	-0.487178000	-4.664501000	-0.924563000
H	-1.407765000	-5.241606000	-1.009375000
C	0.713146000	-5.285826000	-0.953053000
H	0.747522000	-6.372525000	-1.032336000
C	1.974751000	-4.577075000	-0.909259000

H	2.901657000	-5.142297000	-0.951307000
C	1.975184000	-3.221499000	-0.825198000
C	-2.868016000	-2.805399000	-1.307218000
H	-3.472102000	-2.166046000	-1.957266000
H	-3.175279000	-3.850976000	-1.463890000
H	-3.058180000	-2.532861000	-0.259495000
C	4.322590000	-3.028320000	-0.965588000
H	5.058500000	-2.220544000	-0.981916000
H	4.530684000	-3.691814000	-0.114285000
H	4.397488000	-3.609834000	-1.895513000
H	0.035152000	-1.181835000	5.359315000
H	-0.286900000	-2.334198000	4.051870000
H	-1.558920000	-1.226399000	4.584879000
H	2.895907000	-1.473528000	1.908496000
H	1.769096000	-2.426163000	2.879033000
H	2.872130000	-1.285949000	3.675055000
H	3.299350000	1.726596000	1.672563000
H	2.236141000	1.868267000	0.254790000
H	2.992598000	0.318340000	0.639448000
H	0.723173000	3.374267000	0.987949000
H	0.255119000	3.771719000	2.646180000
H	-0.978700000	3.323601000	1.454164000
H	-2.404248000	2.180136000	3.039554000
H	-1.636142000	2.067992000	4.631990000
H	-2.577072000	0.705334000	4.002833000
C	-2.326463000	-0.182301000	0.897311000
O	-3.486581000	-0.135790000	0.834080000
O	3.059199000	-2.424066000	-0.842355000
O	-1.524207000	-2.594602000	-1.647497000
O	-2.796184000	0.932744000	-1.840668000
O	1.325841000	3.068148000	-1.498029000
C	0.931425000	-1.025174000	-2.703234000
H	0.265278000	-1.715626000	-3.237590000
H	1.970038000	-1.247350000	-2.970147000
C	0.556828000	0.437215000	-2.931346000
H	1.432977000	1.079979000	-3.085195000
H	-0.131686000	0.576336000	-3.772526000

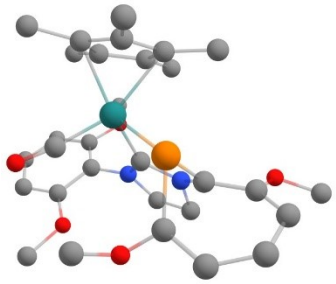


TS4

Gibbs free energy = -6571.7813819619

Electronic energy = -6572.3420474519

Imaginary frequency = -238.2

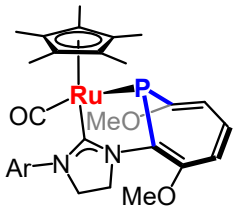


$RuC_{30}PN_2H_{37}O_5$

Ru	-0.483044000	-0.113330000	1.215362000
P	-0.254416000	-2.444837000	0.909352000
N	0.141708000	0.877483000	-1.630942000
N	0.922097000	-1.098066000	-1.151169000
C	0.014417000	-0.355350000	3.393661000
C	-0.400938000	-1.459820000	4.306915000
C	-0.639684000	0.897786000	3.200859000
C	-1.895126000	1.352893000	3.871814000
C	0.181991000	1.717358000	2.342522000
C	-0.056043000	3.159185000	2.035062000
C	1.351070000	0.954316000	2.013693000
C	2.511474000	1.425415000	1.200379000
C	1.254304000	-0.321339000	2.646847000
C	2.301527000	-1.385634000	2.664601000
C	0.192976000	-0.062443000	-0.671740000
C	-0.657213000	2.037217000	-1.628001000
C	-2.016333000	1.924763000	-1.972819000
C	-2.830953000	3.063167000	-1.989145000
H	-3.891127000	2.985963000	-2.212455000
C	-2.259290000	4.305222000	-1.730096000
H	-2.890676000	5.192653000	-1.745478000
C	-0.898512000	4.447784000	-1.471608000
H	-0.477942000	5.434233000	-1.298502000

C	-0.089885000	3.305753000	-1.435544000
C	-3.770957000	0.493545000	-2.657119000
H	-3.859302000	-0.560171000	-2.931170000
H	-4.442177000	0.708034000	-1.815406000
H	-4.051201000	1.113033000	-3.520643000
C	1.890780000	4.578643000	-1.133822000
H	2.956476000	4.363342000	-1.022820000
H	1.734775000	5.179497000	-2.040124000
H	1.548941000	5.149688000	-0.259140000
C	0.900720000	-2.329939000	-0.497354000
C	-0.994116000	-3.210681000	-0.577896000
C	-0.742598000	-4.564811000	-0.876012000
H	-1.568644000	-5.099238000	-1.352153000
C	0.453757000	-5.240717000	-0.680433000
H	0.434805000	-6.327923000	-0.767299000
C	1.724927000	-4.641340000	-0.601174000
H	2.587657000	-5.304008000	-0.631497000
C	1.927536000	-3.271141000	-0.735387000
C	-3.216158000	-2.563743000	-0.554497000
H	-3.892329000	-1.873147000	-1.063180000
H	-3.677819000	-3.561701000	-0.515201000
H	-3.051461000	-2.209024000	0.471066000
C	4.085482000	-3.575682000	-1.703134000
H	4.861100000	-2.931676000	-2.128635000
H	4.545253000	-4.214503000	-0.935128000
H	3.671187000	-4.219242000	-2.493089000
H	0.158144000	-1.414180000	5.252511000
H	-0.209113000	-2.439568000	3.852499000
H	-1.468103000	-1.403503000	4.544884000
H	2.975131000	-1.304917000	1.804811000
H	1.854036000	-2.387398000	2.636292000
H	2.908878000	-1.316511000	3.578212000
H	3.245501000	1.936195000	1.839528000
H	2.192078000	2.118778000	0.417959000
H	3.021024000	0.585731000	0.715953000
H	0.535194000	3.476658000	1.173168000
H	0.227031000	3.793522000	2.888195000
H	-1.108207000	3.359225000	1.806100000
H	-2.459724000	2.045906000	3.239068000

H	-1.661167000	1.875609000	4.810043000
H	-2.551727000	0.511112000	4.114359000
C	-2.226450000	0.207868000	0.730640000
O	-3.335829000	0.498690000	0.540897000
O	3.106883000	-2.727788000	-1.160901000
O	-2.003154000	-2.611187000	-1.277803000
O	-2.426781000	0.692672000	-2.294675000
O	1.240816000	3.333208000	-1.227542000
C	1.259834000	-0.948372000	-2.565683000
H	0.664672000	-1.661843000	-3.152638000
H	2.319144000	-1.155829000	-2.734346000
C	0.876895000	0.504421000	-2.839986000
H	1.750505000	1.158387000	-2.959491000
H	0.235503000	0.615317000	-3.721562000

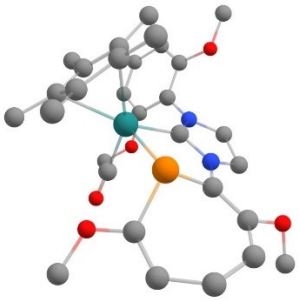


3

Gibbs free energy = -6571.8015908906

Electronic energy = -6572.3618458906

Imaginary frequency = NO

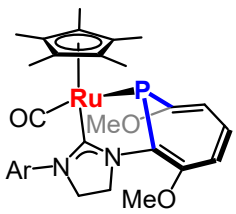


$RuC_{30}PN_2H_{37}O_5$

Ru	2.157575000	3.216342000	10.176483000
P	2.950975000	3.919503000	12.238285000
N	2.169089000	5.856383000	8.601085000
N	3.138474000	6.001748000	10.547022000
C	1.091863000	1.509599000	11.152217000
C	1.509506000	0.798009000	12.397657000

C	1.418966000	1.143034000	9.811664000
C	2.277595000	-0.011815000	9.405382000
C	0.682770000	1.995803000	8.910866000
C	0.591954000	1.820344000	7.431696000
C	-0.090978000	2.891293000	9.711686000
C	-1.130312000	3.845855000	9.223501000
C	0.160504000	2.609964000	11.088823000
C	-0.529940000	3.232995000	12.256273000
C	2.463674000	5.158671000	9.714815000
C	1.611797000	5.379492000	7.400161000
C	2.397652000	4.632998000	6.503889000
C	1.871173000	4.256393000	5.261105000
H	2.459364000	3.664550000	4.565610000
C	0.584167000	4.657788000	4.918231000
H	0.175856000	4.362890000	3.952414000
C	-0.193508000	5.436140000	5.772471000
H	-1.188949000	5.748173000	5.469324000
C	0.333972000	5.816754000	7.012728000
C	4.460698000	3.547515000	6.098139000
H	5.388964000	3.401400000	6.653388000
H	4.001330000	2.566698000	5.912515000
H	4.675547000	4.034670000	5.136499000
C	-1.600063000	7.057925000	7.591861000
H	-1.919525000	7.672308000	8.437068000
H	-1.610445000	7.669261000	6.678716000
H	-2.301477000	6.220184000	7.473049000
C	3.571059000	5.587964000	11.805451000
C	4.567582000	3.113392000	12.621351000
C	5.386462000	3.553651000	13.614862000
H	6.222862000	2.925731000	13.925606000
C	5.189273000	4.753502000	14.393503000
H	5.558133000	4.701183000	15.421183000
C	4.682926000	5.952987000	14.007739000
H	4.691917000	6.759621000	14.745653000
C	4.232719000	6.378657000	12.696743000
C	5.969719000	1.258497000	12.133878000
H	5.955669000	0.430533000	11.419865000
H	6.840866000	1.898184000	11.934405000
H	6.049767000	0.855478000	13.153980000

C	5.806219000	8.097413000	12.357305000
H	5.830756000	9.181762000	12.209311000
H	6.353785000	7.850231000	13.278077000
H	6.313527000	7.606964000	11.511213000
H	0.788653000	0.008117000	12.653908000
H	1.564332000	1.488099000	13.247490000
H	2.495425000	0.337032000	12.282711000
H	-0.958353000	4.205522000	11.990416000
H	0.166475000	3.394219000	13.088744000
H	-1.347937000	2.593669000	12.619119000
H	-2.131001000	3.462483000	9.468350000
H	-1.079653000	3.970058000	8.138858000
H	-1.030825000	4.834768000	9.681226000
H	0.252870000	2.735856000	6.939288000
H	-0.116674000	1.018347000	7.174574000
H	1.560712000	1.555056000	6.994187000
H	2.783597000	0.180074000	8.452905000
H	1.673928000	-0.922524000	9.283887000
H	3.046487000	-0.217247000	10.157454000
C	3.848034000	2.938145000	9.533262000
O	4.911074000	2.726227000	9.118774000
O	4.453163000	7.713661000	12.431053000
O	4.770070000	1.966344000	11.951554000
O	3.639797000	4.350807000	6.910418000
O	-0.303722000	6.604332000	7.896165000
C	3.381661000	7.320526000	9.958654000
H	4.458025000	7.474765000	9.814355000
H	3.016063000	8.109559000	10.617608000
C	2.622565000	7.244735000	8.639241000
H	1.760333000	7.922092000	8.605460000
H	3.261024000	7.451160000	7.771789000

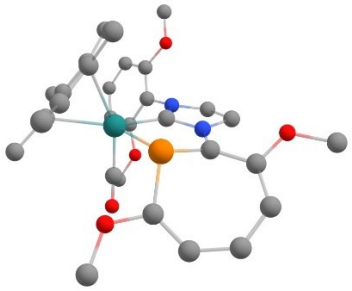


3 (triplet state)

Gibbs free energy = -6571.7605135804

Electronic energy = -6572.3182635004

Imaginary frequency = NO



$RuC_{30}PN_2H_{37}O_5$

Ru	2.208446000	3.156245000	10.122709000
P	3.268286000	3.821093000	12.060266000
N	2.159720000	5.833482000	8.567356000
N	3.189062000	5.937762000	10.490912000
C	1.069318000	1.544974000	11.178376000
C	1.466556000	0.820192000	12.421880000
C	1.317709000	1.130970000	9.835556000
C	2.067708000	-0.094618000	9.422106000
C	0.614277000	2.022722000	8.943234000
C	0.463690000	1.834843000	7.470416000
C	-0.058547000	2.988682000	9.753473000
C	-1.030984000	4.020928000	9.285791000
C	0.227738000	2.715442000	11.126653000
C	-0.362401000	3.415867000	12.305907000
C	2.515301000	5.105221000	9.654208000
C	1.645870000	5.353569000	7.349667000
C	2.445398000	4.578881000	6.488573000
C	1.939995000	4.168951000	5.247338000
H	2.536121000	3.550339000	4.582641000
C	0.666938000	4.576079000	4.862233000
H	0.275863000	4.255053000	3.897693000
C	-0.114684000	5.397997000	5.670824000
H	-1.094866000	5.721049000	5.331837000
C	0.390795000	5.809533000	6.910029000
C	4.529039000	3.521346000	6.116830000
H	5.460440000	3.407110000	6.673904000
H	4.100153000	2.525343000	5.940510000
H	4.730520000	4.006356000	5.151345000

C	-1.528749000	7.111302000	7.394025000
H	-1.852658000	7.769922000	8.203556000
H	-1.511834000	7.679634000	6.453668000
H	-2.242941000	6.281062000	7.300485000
C	3.755488000	5.482116000	11.675034000
C	4.817270000	2.967337000	12.398891000
C	5.987921000	3.498961000	12.926447000
H	6.787659000	2.780210000	13.109999000
C	6.304824000	4.802593000	13.330792000
H	7.281231000	4.891357000	13.808841000
C	5.572907000	6.028662000	13.299630000
H	5.994702000	6.808701000	13.932143000
C	4.458922000	6.372508000	12.572203000
C	5.662060000	0.730843000	12.569477000
H	5.279839000	-0.270983000	12.351936000
H	6.588545000	0.887615000	11.997671000
H	5.891743000	0.802601000	13.643187000
C	4.521894000	8.620314000	13.390215000
H	3.928006000	9.528554000	13.253270000
H	4.556367000	8.376198000	14.462192000
H	5.548350000	8.802795000	13.038436000
H	0.687894000	0.099204000	12.710197000
H	1.607317000	1.514678000	13.257349000
H	2.407110000	0.279233000	12.286803000
H	-0.684379000	4.429809000	12.044785000
H	0.364586000	3.499186000	13.122565000
H	-1.239087000	2.874108000	12.690262000
H	-2.035094000	3.785619000	9.664768000
H	-1.084413000	4.047735000	8.194266000
H	-0.768145000	5.025599000	9.630850000
H	0.179434000	2.767078000	6.974251000
H	-0.310577000	1.085054000	7.247748000
H	1.396310000	1.492505000	7.009018000
H	2.554435000	0.041846000	8.450370000
H	1.389425000	-0.955535000	9.336702000
H	2.843031000	-0.349645000	10.151859000
C	3.854525000	2.764690000	9.416297000
O	4.900016000	2.458610000	9.020274000
O	3.891580000	7.611590000	12.648853000

O	4.657820000	1.631066000	12.188475000
O	3.682644000	4.308407000	6.919564000
O	-0.246862000	6.650472000	7.743510000
C	3.224036000	7.320257000	10.011439000
H	4.238599000	7.725269000	10.071164000
H	2.574937000	7.944595000	10.634066000
C	2.719522000	7.182936000	8.582575000
H	1.952388000	7.922299000	8.329697000
H	3.531572000	7.250121000	7.844129000

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