Electronic Supplementary Information (ESI)

Dipotassium 1,2,4-diazaphospholide dianion radical as an organometallic building block: The first 1,2-diaza-4-phosphine ruthenocene

Xiang Zhang,[a] Qiang Guo,[a] Yunchen Zhang,[a] Yaona Zhang,[a] and Wenjun Zheng[a,b,*]

[a]*Institute of Organic Chemistry & College of Chemical and Materials Science, Shanxi Normal Univeristy, Gongyuan Street 1, Linfen, Shanxi Province 041004, China*

[b]*Key Laboratory of Magnetic Molecules and Magnetic Information Materials, Ministry of Education, Gongyuan Street 1, Linfen, Shanxi Province, 041004, China*

Email: wjzheng_sxnu@qq.com

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S1 Preparation and characterization data for **2** and **4**

General Information

All manipulations were carried out in a nitrogen atmosphere under anaerobic conditions using standard Schlenk, vacuum line and glove box techniques. The solvents were thoroughly dried, deoxygenated and distilled in a nitrogen atmosphere prior to use. $CDCl_3$ was dried with CaH_2 before use. The ^1H NMR, $^{13}C\{^1H\}$ NMR and $^{31}P\{^1H\}$ NMR spectra were recorded with a Bruker DRX-600 spectrometer. IR measurements were carried out on a NICOLET 360 FT-IR spectrometer from Nujol mulls prepared in a dry box. Elemental analysis was performed on an Elementar vario MACRO cube (Germany). Melting points were measured in sealed argon-filled capillaries without temperature correction with an apparatus XT4-100A (Electronic and Optical Instruments, Beijing). $RuCl_3 \bullet xH_2O$ were purchased from Aldrich and used as received. 1*H*-3,5-di-phenyl-1,2,4-diazaphosphole (H[3,5-Ph_2dp]) was prepared according to the literature.[1]

[1] L. Wan, I. Alkorta, J. Elguero, J. Sun, W. J. Zheng, *Tetrahedron* 2007, **63**, 9129–9133.

Preparation of K_2[3,5-Ph_2dp] (2): To a mixture of 1*H*-3,5-di-phenyl-1,2,4-diazaphosphole (H[3,5-Ph_2dp]) (0.33 g, 1.0 mmol) and metallic potassium (0.08 g, 2.0 mmol) was added THF (20 mL) via syringe at room temperature. After the evolution of gas ceased the solution was refluxed for 12 h. The colorless solution turned to jujube red, and finally to black. The black solution was filtered on a coarse glass frit. The volatile components of the filtration were removed under reduced pressure to give **2** as very air- and moisture-sensitive black pure crystalline (0.39 g, 95%). M.p. > 190°C, decomp..

Preparation of [{$CpMe_5$(μ_2(*P*)-(3,5-Ph_2dp))}Ru-Ru{$CpMe_5$(μ_2(*P*)-(3,5-Ph_2dp))}] (4): To a mixture of $[CpMe_5RuCl]_4$ (0.54 g, 0.5 mmol) and K_2[3,5-Ph_2dp] (**2**, 0.41 g, 1.0 mmol) was added 30 mL tetrahydrofuran (THF) via syringe. The black solution was stirred for 24 h at room temperature and then filtered through Celite. The black-brown filtration was concentrated under the reduced pressure to afford a group of black blocks suitable for single crystal analysis at room temperature (0.18 g, 35%). Mp: > 250°C, decomp.. ^1H NMR (600 MHz, $CDCl_3$, 23°C): δ = 1.32 (s, 30 H, –CH_3), 1.87, 3.77 (2m, 8 H, one solvated THF molecule in the lattice), 7.37, 7.46, 8.38 (m, 20 H, Ph) ppm; $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, 23°C): δ = 10.29 (s, –*C*H_3), 25.62 (s, –*C*H_2, THF), 67.99 (s, –O*C*H_2, THF), 89.58 (s, –*C*CH_3), 128.21–130.13 (3m, –*C* for phenyl rings) ppm, the resonances for P*C*N were not observed. $^{31}P\{^1H\}$ NMR (243 MHz,THF-d_8, 23°C): 179.9(s) ppm; IR (KBr, Nujol mull, cm^{-1}): 2963(s), 1700(s), 1653(s), 1457(m), 1260(vs), 1094(s), 1020(s), 799(s); Anal. calcd for $C_{48}H_{50}N_4P_2Ru_2(C_4H_8O)$: C 61.28, H 5.74, N 5.50; Found: C 61.36, H 5.81, N 5.38.

S2 Crystal data and structure refinement for **4**

Table 1 Crystal data and structure refinement for **4**.

Compound	**4**
Identification code	20161011
Empirical formula	$C_{52}H_{58}N_4P_2Ru_2O$
Formula weight	1019.10
Temperature/K	293(2)
Crystal system	*monoclinic*
Space group	$P2_1/c$
a/Å	11.3240(2)
b/Å	15.3663(2)
c/Å	15.3059(3)
α/°	90.00
β/°	105.0606(19)
γ/°	90.00
Volume/Å^3	2571.86(8)
Z	2
ρ_{calc}g/cm^3	1.316
μ/mm^{-1}	0.688
F(000)	1048.0
Crystal size/mm^3	0.21 × 0.13 × 0.08
Radiation	Mo Kα (λ = 0.71073 Å)
2Θ range for data collection/°	5.8 to 51.3
Index ranges	-13 ⩽ h ⩽ 13, -18 ⩽ k ⩽ 18, -18 ⩽ l ⩽ 18
Reflections collected	59056
Independent reflections	4880 [R_{int} = 0.0383, R_{sigma} = 0.0178]
Data/restraints/parameters	4880/33/303
Goodness-of-fit on F^2	1.181
Final *R* indexes [$I>=2\sigma(I)$]	R_1 = 0.0417, wR_2 = 0.1340
Final *R* indexes [all data]	R_1 = 0.0511, wR_2 = 0.1440
Largest diff. peak/hole / e Å^{-3}	1.04/-0.28

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	4225(6)	5741(4)	2527(4)	64.6(14)
C2	3393(6)	6161(4)	1839(4)	73.4(15)
C3	3270(6)	5938(4)	961(4)	73.2(15)
C4	4000(6)	5295(5)	759(4)	78.6(17)
C5	4852(5)	4881(4)	1433(3)	63.1(13)
C6	4962(4)	5081(3)	2339(3)	45.7(10)
C7	5816(4)	4583(3)	3052(3)	45.8(10)
C8	7044(4)	3701(3)	4332(3)	43.7(9)
C9	7675(4)	3185(3)	5120(3)	45.1(9)
C10	8805(4)	2811(4)	5165(4)	63.0(13)
C11	9341(5)	2271(4)	5888(5)	80.7(18)
C12	8768(6)	2084(4)	6545(4)	80.0(17)
C13	7634(7)	2440(4)	6506(4)	78.1(17)
C14	7106(5)	3003(3)	5804(4)	63.6(13)
C15	4056(10)	2424(6)	5787(8)	182(6)
C16	3458(6)	3094(4)	5076(5)	78.2(18)
C17	3562(5)	3108(3)	4185(5)	70.0(16)
C18	4293(8)	2478(5)	3795(8)	150(5)
C19	2754(5)	3732(4)	3692(3)	58.0(12)
C20	2473(8)	3878(6)	2680(4)	117(3)
C21	2141(4)	4120(3)	4285(4)	56.7(12)
C22	1113(5)	4750(5)	4053(7)	116(3)
C23	2600(5)	3715(4)	5149(4)	70.8(16)
C24	2116(9)	3865(8)	5973(5)	143(4)
C25	990(20)	3595(13)	8047(15)	154(4)
C26	1590(20)	4451(12)	8301(16)	153(4)
C27	870(20)	4673(12)	8955(14)	154(4)
C28	1000(20)	3787(12)	9407(15)	157(4)
N1	7358(4)	3610(3)	3575(3)	62.8(11)
N2	6644(4)	4108(3)	2847(3)	64.0(11)
O1	625(16)	3254(10)	8719(11)	160(4)
P1	5802.4(10)	4485.4(6)	4242.4(7)	35.8(2)
Ru1	4142.8(3)	4398.65(18)	4790.85(19)	32.89(14)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\cdots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	82(4)	65(3)	51(3)	6(2)	25(3)	19(3)
C2	83(4)	70(4)	64(3)	8(3)	14(3)	19(3)
C3	79(4)	74(4)	60(3)	15(3)	8(3)	1(3)
C4	96(5)	95(4)	42(3)	1(3)	13(3)	0(4)
C5	78(3)	70(3)	45(3)	-5(2)	22(2)	5(3)
C6	56(2)	45(2)	40(2)	1.4(18)	21.2(19)	-1.7(19)
C7	57(3)	49(2)	38(2)	-3.1(18)	25(2)	4(2)
C8	47(2)	40(2)	50(2)	-1.7(18)	23.2(19)	6.0(18)
C9	50(2)	35(2)	50(2)	-3.4(18)	14.1(19)	5.7(18)
C10	51(3)	65(3)	74(3)	-1(3)	17(2)	9(2)
C11	55(3)	73(4)	102(5)	2(3)	-2(3)	21(3)
C12	95(4)	65(4)	70(4)	10(3)	1(3)	21(3)
C13	105(5)	68(4)	67(3)	17(3)	33(3)	18(3)
C14	74(3)	58(3)	64(3)	13(2)	27(3)	20(3)
C15	154(9)	121(7)	214(11)	118(8)	-52(8)	-68(7)
C16	69(4)	55(3)	97(5)	23(3)	-4(3)	-26(3)
C17	51(3)	46(3)	112(5)	-31(3)	18(3)	-10(2)
C18	87(5)	94(6)	270(13)	-114(7)	50(7)	-9(4)
C19	58(3)	67(3)	48(3)	-14(2)	10(2)	-23(2)
C20	120(6)	172(8)	54(4)	-21(4)	11(4)	-78(6)
C21	36(2)	52(3)	80(3)	-9(3)	12(2)	-6(2)
C22	43(3)	87(5)	203(9)	-31(6)	7(4)	-1(3)
C23	69(3)	85(4)	67(3)	-14(3)	33(3)	-42(3)
C24	132(7)	225(11)	96(5)	-53(6)	74(5)	-117(8)
C25	205(10)	134(8)	148(9)	-21(6)	91(8)	-40(7)
C26	203(10)	133(8)	149(9)	-15(6)	91(8)	-45(7)
C27	205(10)	132(8)	149(9)	-25(7)	90(8)	-39(8)
C28	208(10)	140(8)	147(9)	-17(6)	91(8)	-39(8)
N1	76(3)	65(3)	58(2)	5(2)	36(2)	29(2)
N2	80(3)	72(3)	51(2)	3(2)	37(2)	26(2)
O1	210(10)	136(8)	156(9)	-16(6)	88(8)	-39(7)
P1	42.2(6)	34.5(5)	35.6(5)	-1.0(4)	19.2(4)	4.6(4)
Ru1	36.1(2)	30.6(2)	35.0(2)	-1.49(11)	14.65(14)	0.01(11)

Table 4 Bond Lengths for **4**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.378(8)	C17	C18	1.495(8)
C1	C6	1.391(7)	C17	C19	1.402(8)
C2	C3	1.358(8)	C17	Ru1	2.215(5)
C3	C4	1.374(9)	C19	C20	1.515(8)
C4	C5	1.373(8)	C19	C21	1.410(7)
C5	C6	1.394(6)	C19	Ru1	2.231(4)
C6	C7	1.470(6)	C21	C22	1.485(8)
C7	N2	1.289(6)	C21	C23	1.430(8)
C7	P1	1.832(4)	C21	Ru1	2.238(4)
C8	C9	1.465(6)	C23	C24	1.519(8)
C8	N1	1.305(5)	C23	Ru1	2.225(5)
C8	P1	1.829(4)	C25	C26	1.485(10)
C9	C10	1.388(6)	C25	O1	1.31(2)
C9	C14	1.393(7)	C26	C27	1.480(10)
C10	C11	1.391(8)	C27	C28	1.516(10)
C11	C12	1.361(9)	C28	O1	1.31(2)
C12	C13	1.383(9)	N1	N2	1.420(6)
C13	C14	1.388(7)	P1	Ru1	2.2526(11)
C15	C16	1.523(9)	P1	Ru1A	2.2552(10)
C16	C17	1.399(9)	Ru1	P1A	2.2552(10)
C16	C23	1.387(9)	Ru1	Ru1A	2.6360(6)
C16	Ru1	2.233(5)			

Symmetry transformations used to generate equivalent atoms: A = 1-X,1-Y,1-Z

Table 5 Bond Angles for **4**.

Atom	Atom	Atom	Angle/	Atom	Atom	Atom	Angle/
C2	C1	C6	120.7(5)	C16	C23	C24	125.6(8)
C3	C2	C1	120.9(6)	C16	C23	Ru1	72.2(3)
C2	C3	C4	119.4(5)	C21	C23	C24	125.4(7)
C5	C4	C3	120.7(5)	C21	C23	Ru1	71.8(3)
C4	C5	C6	120.7(5)	C24	C23	Ru1	127.5(4)
C1	C6	C5	117.6(5)	O1	C25	C26	111.2(17)
C1	C6	C7	122.7(4)	C27	C26	C25	95.2(16)
C5	C6	C7	119.7(4)	C26	C27	C28	95.8(16)
C6	C7	P1	127.4(3)	O1	C28	C27	102.8(18)
N2	C7	C6	119.6(4)	C8	N1	N2	114.0(4)
N2	C7	P1	112.9(4)	C7	N2	N1	114.6(4)
C9	C8	P1	128.3(3)	C25	O1	C28	106.2(16)

N1	C8	C9	119.0(4)	C7	P1	Ru1A	125.76(15)
N1	C8	P1	112.7(3)	C7	P1	Ru1	126.77(16)
C10	C9	C8	120.8(4)	C8	P1	C7	85.6(2)
C10	C9	C14	118.7(4)	C8	P1	Ru1	129.23(14)
C14	C9	C8	120.4(4)	C8	P1	Ru1A	124.19(15)
C9	C10	C11	119.5(5)	Ru1	P1	Ru1A	71.57(3)
C12	C11	C10	121.4(5)	C16	Ru1	C21	61.6(2)
C11	C12	C13	120.0(5)	C16	Ru1	P1	119.4(2)
C12	C13	C14	119.3(6)	C16	Ru1	P1A	120.4(2)
C13	C14	C9	121.1(5)	C16	Ru1	Ru1A	148.56(15)
C15	C16	Ru1	129.3(4)	C17	Ru1	C16	36.7(2)
C17	C16	C15	124.9(8)	C17	Ru1	C19	36.8(2)
C17	C16	Ru1	71.0(3)	C17	Ru1	C21	61.33(19)
C23	C16	C15	126.8(8)	C17	Ru1	C23	60.9(2)
C23	C16	C17	107.8(5)	C17	Ru1	P1	94.74(15)
C23	C16	Ru1	71.6(3)	C17	Ru1	P1A	155.49(17)
C16	C17	C18	125.0(7)	C17	Ru1	Ru1A	148.10(14)
C16	C17	C19	109.0(5)	C19	Ru1	C16	61.5(2)
C16	C17	Ru1	72.4(3)	C19	Ru1	C21	36.79(19)
C18	C17	Ru1	127.7(4)	C19	Ru1	P1A	137.52(15)
C19	C17	C18	125.4(7)	C19	Ru1	P1	103.85(13)
C19	C17	Ru1	72.2(3)	C19	Ru1	Ru1A	146.68(13)
C17	C19	C20	125.8(6)	C21	Ru1	P1A	103.00(14)
C17	C19	C21	107.7(5)	C21	Ru1	P1	138.65(15)
C17	C19	Ru1	71.0(3)	C21	Ru1	Ru1A	146.50(13)
C20	C19	Ru1	128.5(4)	C23	Ru1	C16	36.3(2)
C21	C19	C20	126.0(6)	C23	Ru1	C19	61.56(19)
C21	C19	Ru1	71.9(3)	C23	Ru1	C21	37.4(2)
C19	C21	C22	127.5(6)	C23	Ru1	P1A	94.98(16)
C19	C21	C23	106.8(5)	C23	Ru1	P1	154.69(17)
C19	C21	Ru1	71.3(3)	C23	Ru1	Ru1A	147.87(14)
C22	C21	Ru1	128.2(4)	P1	Ru1	P1A	108.43(3)
C23	C21	C22	125.3(6)	P1A	Ru1	Ru1A	54.17(3)
C23	C21	Ru1	70.8(3)	P1	Ru1	Ru1A	54.26(3)
C16	C23	C21	108.6(5)				

Symmetry transformations used to generate equivalent atoms: A = 1-X,1-Y,1-Z

Table 6 Torsion Angles for **4**.

A	B	C	D	Angle/	A	B	C	D	Angle/
C1	C2	C3	C4	-1.1(10)	C19	C17	Ru1	C23	80.4(3)
C1	C6	C7	N2	-166.0(5)	C19	C17	Ru1	P1A	92.0(5)
C1	C6	C7	P1	18.4(7)	C19	C17	Ru1	P1	-106.9(3)
C2	C1	C6	C5	1.8(8)	C19	C17	Ru1	Ru1A	-119.4(3)
C2	C1	C6	C7	-176.7(5)	C19	C21	C23	C16	-0.5(5)
C2	C3	C4	C5	-0.3(11)	C19	C21	C23	C24	-173.7(5)
C3	C4	C5	C6	2.5(10)	C19	C21	C23	Ru1	62.7(3)
C4	C5	C6	C1	-3.2(8)	C19	C21	Ru1	C16	-79.4(4)
C4	C5	C6	C7	175.3(5)	C19	C21	Ru1	C17	-37.5(3)
C5	C6	C7	N2	15.6(7)	C19	C21	Ru1	C23	-116.1(5)
C5	C6	C7	P1	-160.1(4)	C19	C21	Ru1	P1	23.9(4)
C6	C1	C2	C3	0.3(10)	C19	C21	Ru1	P1A	162.8(3)
C6	C7	N2	N1	-175.8(4)	C19	C21	Ru1	Ru1A	120.5(3)
C6	C7	P1	C8	174.5(4)	C20	C19	C21	C22	-0.5(9)
C6	C7	P1	Ru1	37.2(5)	C20	C19	C21	C23	172.8(5)
C6	C7	P1	Ru1A	-55.7(5)	C20	C19	C21	Ru1	-124.8(5)
C7	P1	Ru1	C16	95.5(3)	C20	C19	Ru1	C16	-158.2(8)
C7	P1	Ru1	C17	66.8(3)	C20	C19	Ru1	C17	-121.1(8)
C7	P1	Ru1	C19	30.7(2)	C20	C19	Ru1	C21	122.0(8)
C7	P1	Ru1	C21	16.2(3)	C20	C19	Ru1	C23	160.3(7)
C7	P1	Ru1	C23	81.9(4)	C20	C19	Ru1	P1	-42.0(7)
C7	P1	Ru1	P1A	-121.33(19)	C20	C19	Ru1	P1A	96.7(7)
C7	P1	Ru1	Ru1A	-121.33(19)	C20	C19	Ru1	Ru1A	2.0(8)
C8	C9	C10	C11	-175.2(5)	C21	C19	Ru1	C16	79.8(4)
C8	C9	C14	C13	173.1(5)	C21	C19	Ru1	C17	116.9(5)
C8	N1	N2	C7	1.2(7)	C21	C19	Ru1	C23	38.3(3)
C8	P1	Ru1	C16	-23.7(3)	C21	C19	Ru1	P1	-164.0(3)
C8	P1	Ru1	C17	-52.4(3)	C21	C19	Ru1	P1A	-25.3(4)
C8	P1	Ru1	C19	-88.5(2)	C21	C19	Ru1	Ru1A	-120.0(3)
C8	P1	Ru1	C21	-103.0(3)	C21	C23	Ru1	C16	-117.3(5)
C8	P1	Ru1	C23	-37.2(4)	C21	C23	Ru1	C17	-79.8(3)
C8	P1	Ru1	P1A	119.52(19)	C21	C23	Ru1	C19	-37.7(3)
C8	P1	Ru1	Ru1A	119.52(19)	C21	C23	Ru1	P1	-97.2(5)
C9	C8	N1	N2	176.9(4)	C21	C23	Ru1	P1A	104.9(3)
C9	C8	P1	C7	-177.0(4)	C21	C23	Ru1	Ru1A	119.9(3)
C9	C8	P1	Ru1A	51.9(5)	C22	C21	C23	C16	172.9(5)
C9	C8	P1	Ru1	-41.6(5)	C22	C21	C23	C24	-0.3(9)
C9	C10	C11	C12	1.4(9)	C22	C21	C23	Ru1	-123.8(5)

C10	C9	C14	C13	-2.0(8)
C10	C11	C12	C13	-0.5(10)
C11	C12	C13	C14	-1.6(10)
C12	C13	C14	C9	2.8(9)
C14	C9	C10	C11	-0.1(8)
C15	C16	C17	C18	-1.1(9)
C15	C16	C17	C19	171.4(6)
C15	C16	C17	Ru1	-125.2(6)
C15	C16	C23	C21	-171.2(6)
C15	C16	C23	C24	2.0(9)
C15	C16	C23	Ru1	125.8(6)
C15	C16	Ru1	C17	120.0(11)
C15	C16	Ru1	C19	157.2(10)
C15	C16	Ru1	C21	-160.7(10)
C15	C16	Ru1	C23	-122.9(11)
C15	C16	Ru1	P1	66.9(10)
C15	C16	Ru1	P1A	-71.9(9)
C15	C16	Ru1	Ru1A	-1.9(12)
C16	C17	C19	C20	-172.3(5)
C16	C17	C19	C21	0.5(5)
C16	C17	C19	Ru1	63.4(3)
C16	C17	Ru1	C19	-117.5(5)
C16	C17	Ru1	C21	-80.0(4)
C16	C17	Ru1	C23	-37.0(3)
C16	C17	Ru1	P1	135.6(3)
C16	C17	Ru1	P1A	-25.5(6)
C16	C17	Ru1	Ru1A	123.1(4)
C16	C23	Ru1	C17	37.5(3)
C16	C23	Ru1	C19	79.6(4)
C16	C23	Ru1	C21	117.3(5)
C16	C23	Ru1	P1A	-137.8(4)
C16	C23	Ru1	P1	20.1(6)
C16	C23	Ru1	Ru1A	-122.8(4)
C17	C16	C23	C21	0.8(6)
C17	C16	C23	C24	174.1(5)
C17	C16	C23	Ru1	-62.1(4)
C17	C16	Ru1	C19	37.2(3)
C17	C16	Ru1	C21	79.3(3)
C17	C16	Ru1	C23	117.1(5)
C17	C16	Ru1	P1	-53.2(4)
C17	C16	Ru1	P1A	168.0(3)
C22	C21	Ru1	C16	157.1(7)
C22	C21	Ru1	C17	-160.9(7)
C22	C21	Ru1	C19	-123.5(8)
C22	C21	Ru1	C23	120.4(8)
C22	C21	Ru1	P1	-99.5(6)
C22	C21	Ru1	P1A	39.3(7)
C22	C21	Ru1	Ru1A	-3.0(8)
C23	C16	C17	C18	-173.4(5)
C23	C16	C17	C19	-0.9(6)
C23	C16	C17	Ru1	62.5(4)
C23	C16	Ru1	C17	-117.1(5)
C23	C16	Ru1	C19	-79.9(4)
C23	C16	Ru1	C21	-37.8(3)
C23	C16	Ru1	P1	-170.3(3)
C23	C16	Ru1	P1A	50.9(4)
C23	C16	Ru1	Ru1A	121.0(4)
C23	C21	Ru1	C16	36.7(4)
C23	C21	Ru1	C17	78.7(4)
C23	C21	Ru1	C19	116.1(5)
C23	C21	Ru1	P1	140.1(3)
C23	C21	Ru1	P1A	-81.1(3)
C23	C21	Ru1	Ru1A	-123.4(3)
C24	C23	Ru1	C16	121.6(10)
C24	C23	Ru1	C17	159.1(9)
C24	C23	Ru1	C19	-158.8(9)
C24	C23	Ru1	C21	-121.1(9)
C24	C23	Ru1	P1	141.8(7)
C24	C23	Ru1	P1A	-16.1(8)
C24	C23	Ru1	Ru1A	-1.2(10)
C25	C26	C27	C28	45(2)
C26	C25	O1	C28	-4(3)
C26	C27	C28	O1	-53(2)
C27	C28	O1	C25	35(3)
N1	C8	C9	C10	19.4(7)
N1	C8	C9	C14	-155.5(5)
N1	C8	P1	C7	2.0(4)
N1	C8	P1	Ru1A	-129.0(3)
N1	C8	P1	Ru1	137.5(3)
N2	C7	P1	C8	-1.4(4)
N2	C7	P1	Ru1	-138.6(4)
N2	C7	P1	Ru1A	128.4(4)

C17 C16 Ru1 Ru1A	-121.9(3)	O1	C25 C26 C27	-29(3)
C17 C19 C21 C22	-173.3(5)	P1	C7 N2 N1	0.5(6)
C17 C19 C21 C23	0.0(5)	P1	C8 C9 C10	-161.6(4)
C17 C19 C21 Ru1	62.3(3)	P1	C8 C9 C14	23.5(7)
C17 C19 Ru1 C16	-37.1(4)	P1	C8 N1 N2	-2.3(6)
C17 C19 Ru1 C21	-116.9(5)	Ru1	C16 C17 C18	124.1(6)
C17 C19 Ru1 C23	-78.6(4)	Ru1	C16 C17 C19	-63.4(3)
C17 C19 Ru1 P1A	-142.1(3)	Ru1	C16 C23 C21	62.9(3)
C17 C19 Ru1 P1	79.2(3)	Ru1	C16 C23 C24	-123.8(6)
C17 C19 Ru1 Ru1A	123.1(3)	Ru1	C17 C19 C20	124.3(5)
C18 C17 C19 C20	0.2(9)	Ru1	C17 C19 C21	-62.9(3)
C18 C17 C19 C21	173.0(5)	Ru1	C19 C21 C22	124.4(6)
C18 C17 C19 Ru1	-124.1(6)	Ru1	C19 C21 C23	-62.4(3)
C18 C17 Ru1 C16	-121.1(9)	Ru1	C21 C23 C16	-63.2(4)
C18 C17 Ru1 C19	121.5(9)	Ru1	C21 C23 C24	123.6(6)
C18 C17 Ru1 C21	159.0(9)	Ru1A	P1 Ru1 C16	-143.21(19)
C18 C17 Ru1 C23	-158.1(9)	Ru1A	P1 Ru1 C17	-171.87(18)
C18 C17 Ru1 P1A	-146.6(7)	Ru1A	P1 Ru1 C19	151.99(15)
C18 C17 Ru1 P1	14.6(8)	Ru1A	P1 Ru1 C21	137.5(2)
C18 C17 Ru1 Ru1A	2.0(10)	Ru1A	P1 Ru1 C23	-156.7(4)
C19 C17 Ru1 C16	117.5(5)	Ru1A	P1 Ru1 P1A	0.0
C19 C17 Ru1 C21	37.5(3)			

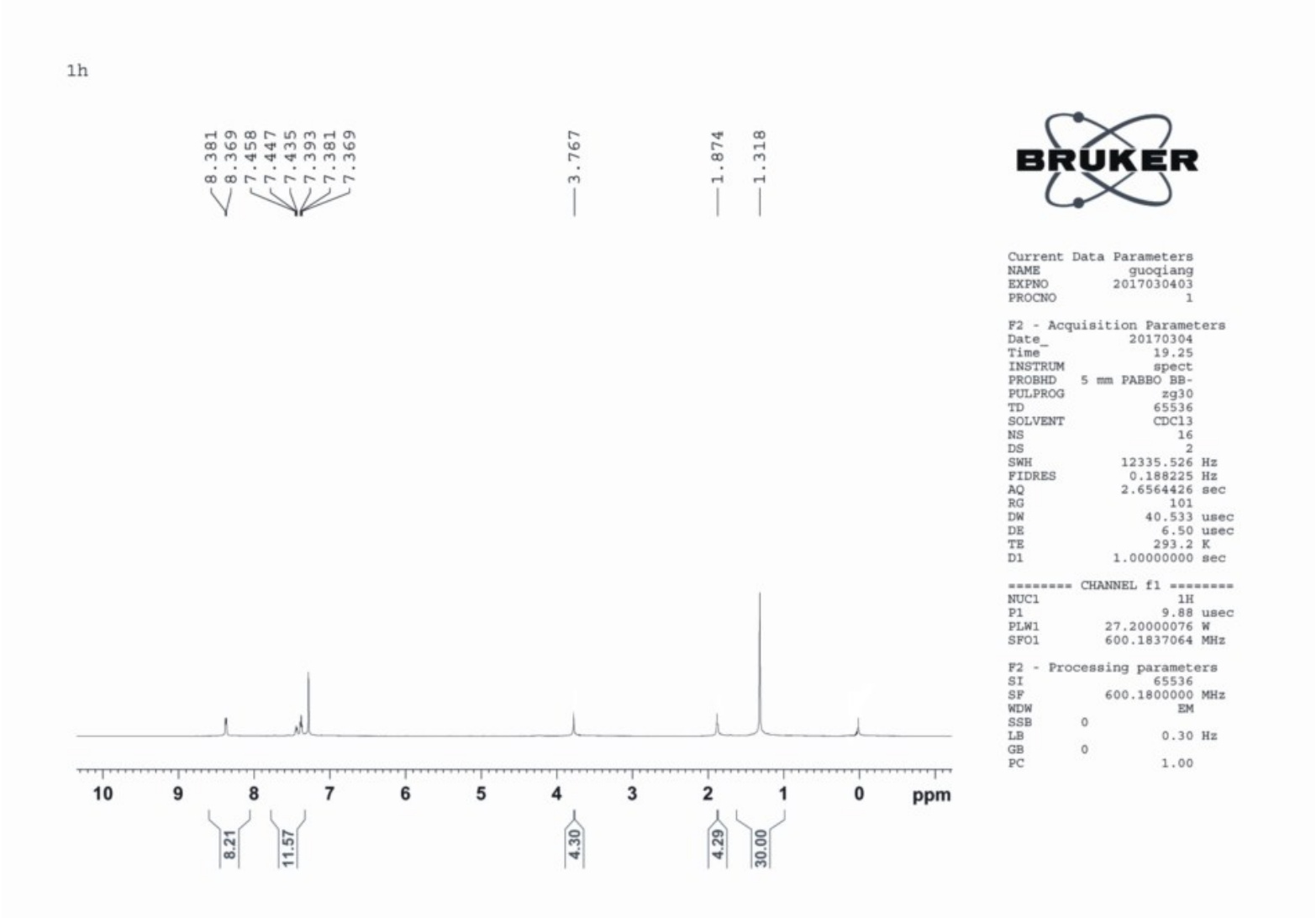
Symmetry transformations used to generate equivalent atoms: A = 1-X,1-Y,1-Z

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4**.

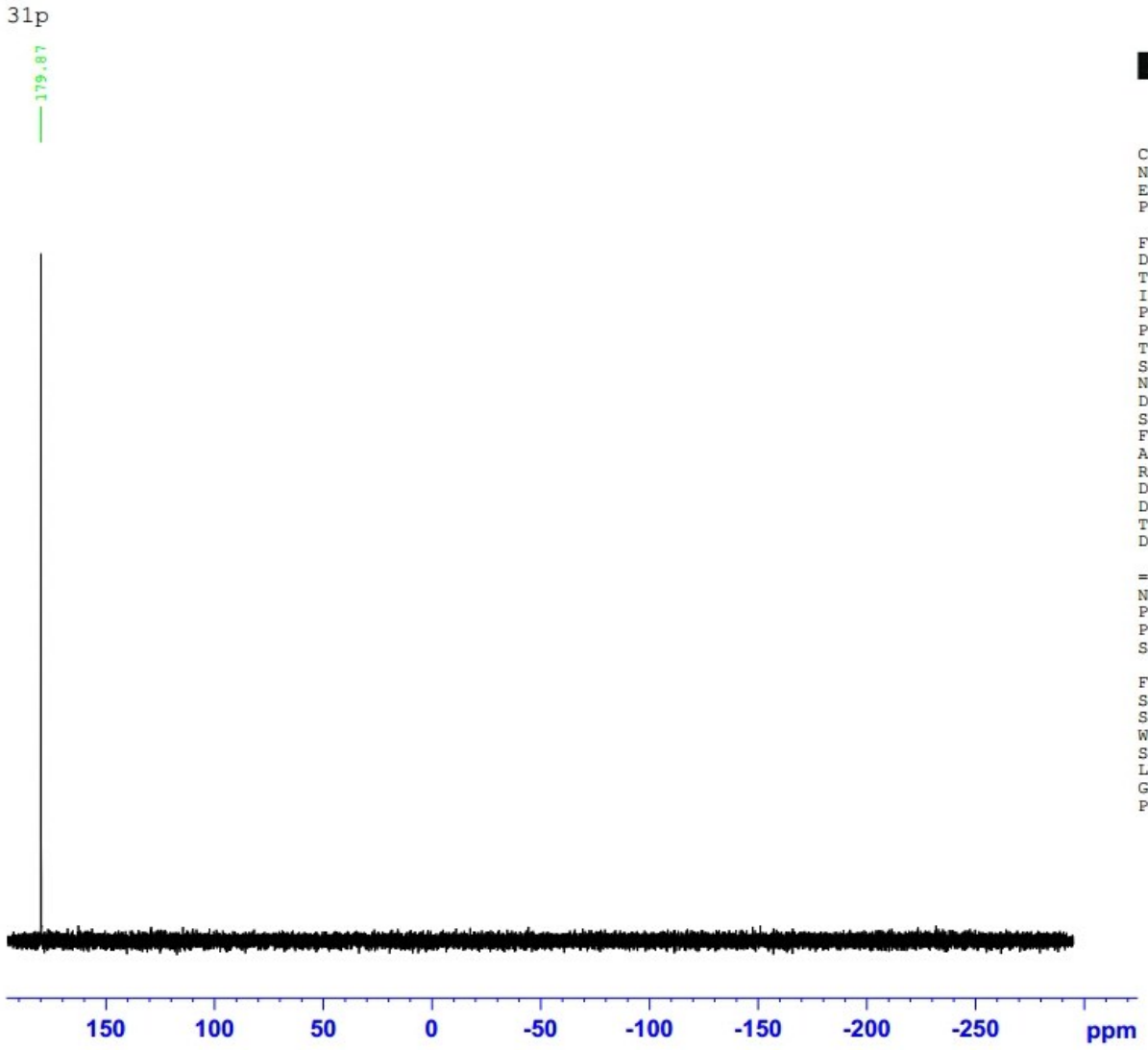
Atom	*x*	*y*	*z*	U(eq)
H1	4294	5901	3125	77
H2	2911	6603	1977	88
H3	2697	6218	501	88
H4	3915	5139	158	94
H5	5362	4464	1284	76
H10	9202	2922	4716	76
H11	10107	2032	5924	97
H12	9139	1717	7020	96
H13	7230	2303	6945	94
H14	6360	3264	5791	76
H15A	4372	2709	6358	273
H15B	4713	2143	5607	273
H15C	3460	1998	5844	273
H18A	5001	2301	4257	224
H18B	4547	2752	3310	224
H18C	3801	1978	3568	224
H20A	3153	3686	2464	176
H20B	2332	4486	2552	176
H20C	1756	3554	2384	176
H22A	1223	5134	3586	173
H22B	1095	5084	4580	173
H22C	356	4440	3844	173
H24A	1497	3440	5984	214
H24B	1771	4438	5946	214
H24C	2773	3810	6512	214
H25A	294	3667	7528	185
H25B	1563	3202	7876	185
H26A	2457	4401	8584	184
H26B	1446	4854	7796	184
H27A	31	4820	8661	185
H27B	1249	5133	9368	185
H28A	1837	3670	9732	188
H28B	482	3744	9823	188

S3 The NMR data for complex **4**

S3-1 The ^{1}H NMR spectrum for complex **4**



S3-2 The $^{31}P\{^{1}H\}$ NMR spectrum for complex **4**

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Current Data Parameters
NAME                 guoqiang
EXPNO             2017041101
PROCNO                    1

F2 - Acquisition Parameters
Date_               20170511
Time                   11.18
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDC13
NS                      160
DS                        4
SWH              119047.617 Hz
FIDRES             1.816522 Hz
AQ                 0.2753012 sec
RG                      2050
DW                     4.200 usec
DE                     6.50 usec
TE                     293.4 K
D1               2.00000000 sec

======== CHANNEL f1 ========
NUC1                     31P
P1                    11.70 usec
PLW1            53.50000000 W
SFO1           242.9451695 MHz

F2 - Processing parameters
SI                       32768
SF              242.9573170 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
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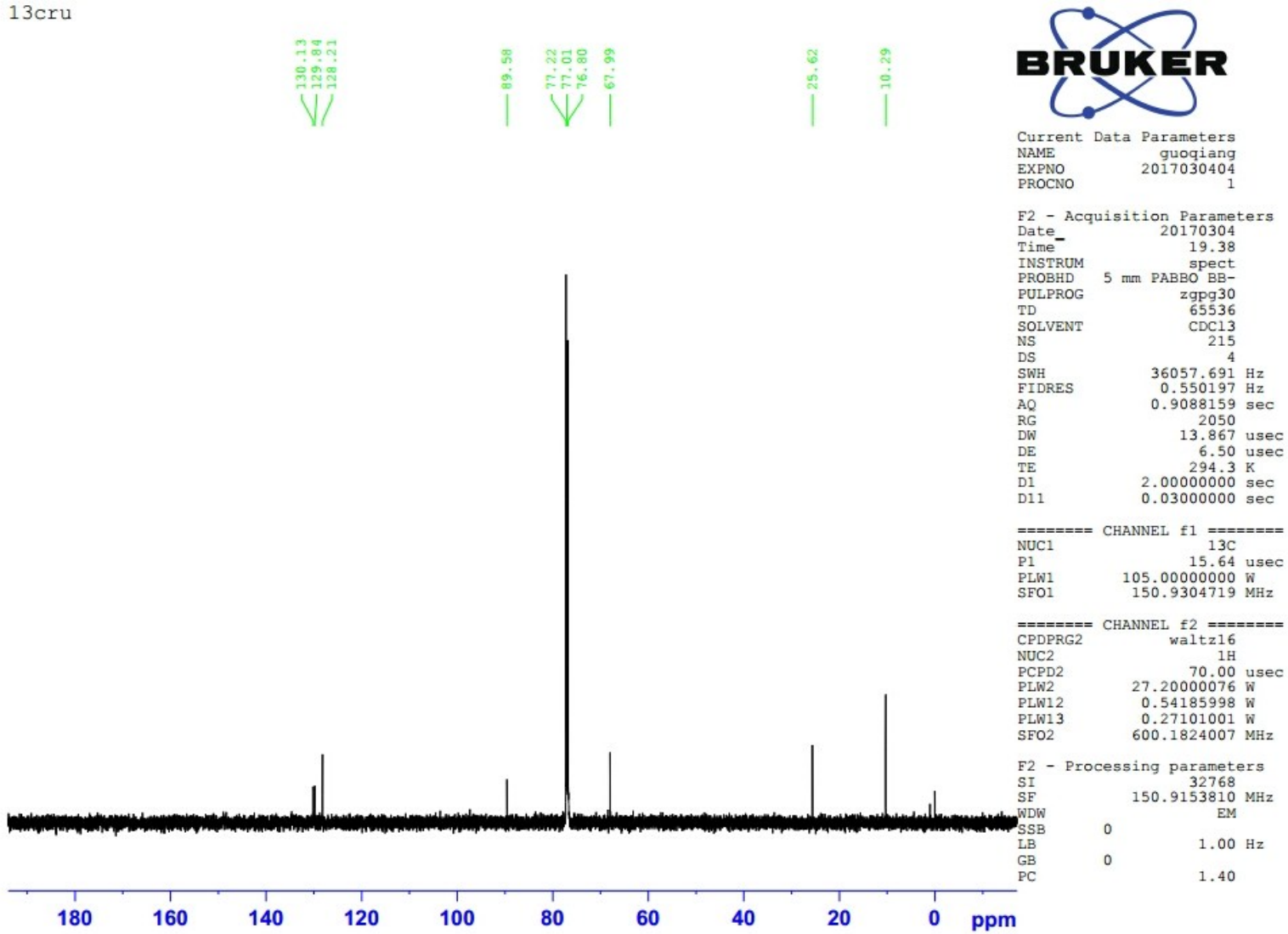
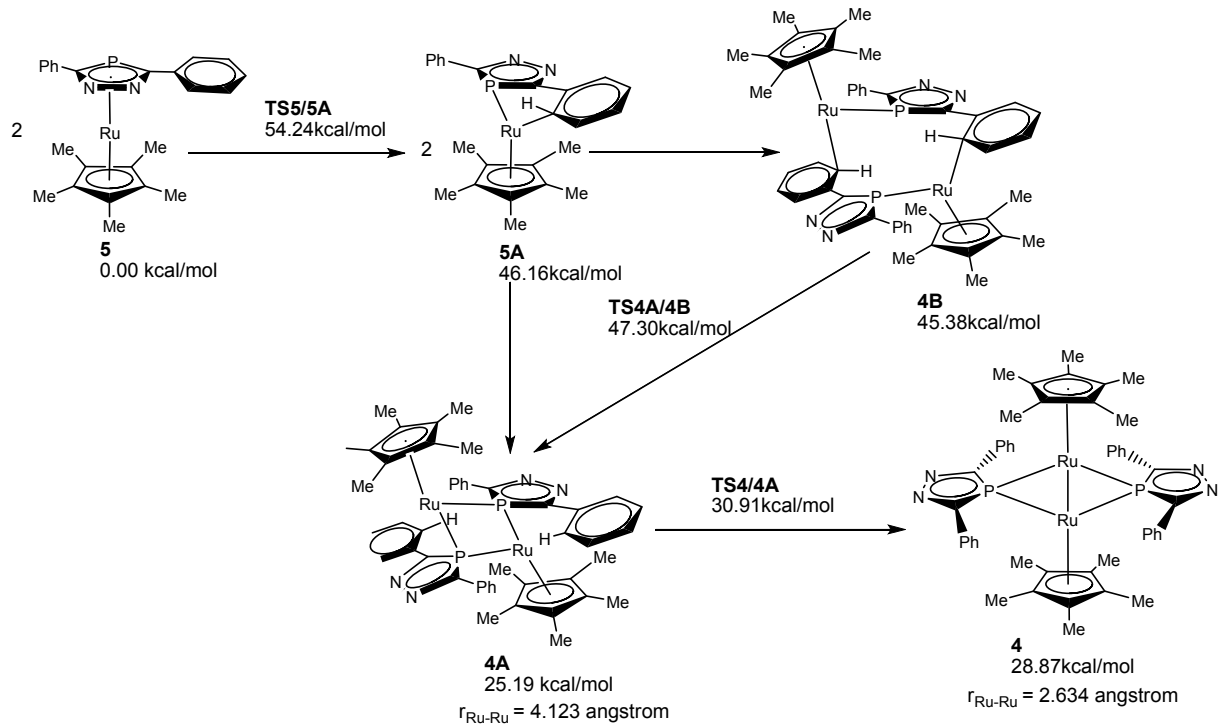
S3-3 The $^{13}C\{^{1}H\}$ NMR spectrum for complex **4**



S4 Conversion mechanism between **4** and **5**

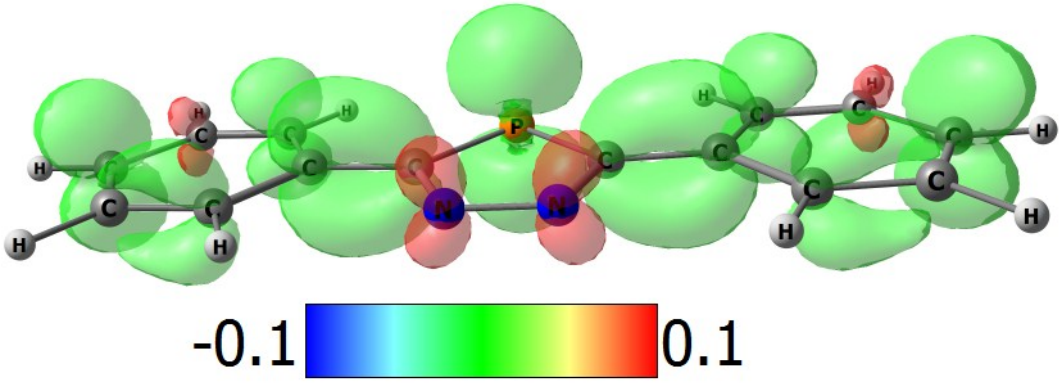


Conversion mechanism between **4** and **5**. Transition states for the dimerization of **5A** to afford **4A** and **4B** have not been confirmed.

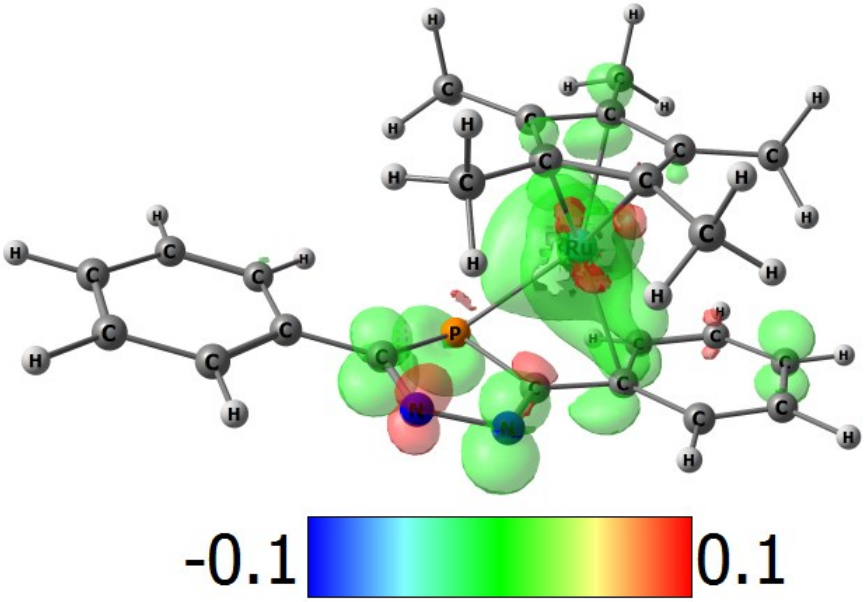
* A transition state was located, seemed to link **4A** and **5A** judged by the imaginary mode, but could not be confirmed due to the very small value of imaginary frequency.

Before the dimerization, complex **5** needs to overcome a barrier height of 54.24 kcal/mol at **TS5/5A** to afford **5A**, which is located 46.16 kcal/mol higher than **5**. Dimerization of **5A** may afford **4A** and **4B**, which relative free energies were 25.19 and 45.38 kcal/mol, respectively. Unfortunately, the transition states from **5A** to **4A** and **4B** were not confirmed for the time being, but it seemed that the barrier heights for the two dimerization channels should be small.[23] **4B** readily transforms to **4A** by surmounting a small barrier of 1.92 kcal/mol. Conversion of **4A** to **4** needs to overcome a barrier height of 5.72 kcal/mol.

S5 Spin density diagrams of $[(3,5\text{-}Ph_2dp)]^-$ and $[\mathbf{5A'}]^-$ (isovalue=0.002)

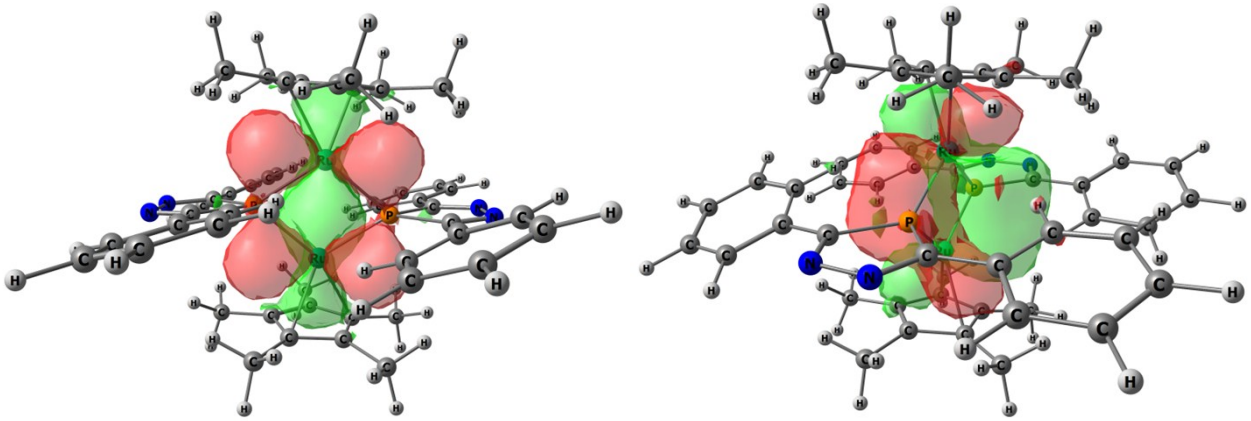


Spin density diagram of $[(3,5\text{-}Ph_2dp)]^-$



Spin density diagram of $[\mathbf{5A'}]^-$

S6 Two AdNDP orbitals between two Ru atoms (isovalue=0.01)



d-d σ-bond **d-d π-bond**

S7 Optimized coordinates of the stationary points in the conversion mechanism between **4** and **5:**

5:

Ru	0.000099000	0.381620000	-0.080923000
P	0.000142000	-1.962913000	0.758040000
N	0.676079000	-1.037225000	-1.645372000
N	-0.675700000	-1.037238000	-1.645397000
C	1.209231000	-1.481249000	-0.468482000
C	-1.208914000	-1.481270000	-0.468540000
C	0.000996000	1.717424000	1.591597000
C	1.164690000	1.954750000	0.781940000
C	0.717200000	2.345107000	-0.527430000
C	-0.719903000	2.344316000	-0.526087000
C	-1.164478000	1.953468000	0.784118000
C	0.002434000	1.325140000	3.038674000
C	2.592734000	1.813653000	1.215146000
C	1.603536000	2.676205000	-1.689537000
C	-1.608848000	2.674908000	-1.686334000
C	-2.591567000	1.810834000	1.219987000
H	0.001376000	2.214186000	3.679818000
H	0.885421000	0.730325000	3.284679000
H	-0.878353000	0.727479000	3.285658000
H	3.001367000	2.775442000	1.545749000
H	3.218693000	1.437760000	0.399408000
H	2.683274000	1.103781000	2.041771000
H	1.848497000	3.744459000	-1.705132000
H	1.120050000	2.422582000	-2.636174000
H	2.539463000	2.113304000	-1.635088000
H	-2.544302000	2.111394000	-1.630033000
H	-1.127151000	2.421810000	-2.634025000
H	-1.854566000	3.742999000	-1.701212000
H	-2.679707000	1.101329000	2.047188000
H	-3.218552000	1.433787000	0.405570000
H	-3.000752000	2.772305000	1.550845000
C	2.679287000	-1.442032000	-0.306555000
C	3.488962000	-0.970842000	-1.348403000
C	3.277617000	-1.815491000	0.901046000
C	4.865232000	-0.869364000	-1.175698000
C	4.654421000	-1.711472000	1.070357000
C	5.453672000	-1.235193000	0.033889000
H	3.021905000	-0.684622000	-2.284709000
H	2.660283000	-2.184040000	1.716725000
H	5.482004000	-0.503542000	-1.990986000
H	5.103194000	-2.003556000	2.014642000
H	6.527782000	-1.153095000	0.166367000
C	-2.678970000	-1.442232000	-0.306703000
C	-3.277409000	-1.817145000	0.900387000

C	-3.488523000	-0.969589000	-1.347993000
C	-4.654207000	-1.713132000	1.069764000
C	-4.864787000	-0.868134000	-1.175233000
C	-5.453335000	-1.235415000	0.033866000
H	-2.660166000	-2.186854000	1.715604000
H	-3.021384000	-0.682195000	-2.283900000
H	-5.103074000	-2.006338000	2.013656000
H	-5.481461000	-0.501184000	-1.990088000
H	-6.527437000	-1.153324000	0.166410000

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Sum of electronic and thermal Energies= -1474.369653
Sum of electronic and thermal Enthalpies= -1474.368709
Sum of electronic and thermal Free Energies= -1474.456966

5A:

C	-1.604242000	-0.035350000	2.757483000
H	-0.847993000	-0.826273000	2.758636000
H	-2.583368000	-0.504231000	2.631926000
H	-1.585925000	0.464732000	3.732810000
C	-1.332615000	0.947807000	1.660380000
C	-2.305723000	1.588993000	0.815092000
C	-3.786205000	1.375609000	0.873674000
H	-4.022927000	0.335242000	1.115884000
H	-4.257467000	1.603234000	-0.086020000
H	-4.241637000	2.017290000	1.636593000
C	-1.595924000	2.427153000	-0.104679000
C	-2.202541000	3.271423000	-1.183182000
H	-3.141402000	2.840968000	-1.541187000
H	-1.527508000	3.360459000	-2.038382000
H	-2.412639000	4.281931000	-0.814202000
C	-0.183240000	2.338322000	0.195711000
C	0.915449000	3.065033000	-0.517615000
H	0.675787000	3.197395000	-1.576212000
H	1.853995000	2.507288000	-0.457443000
H	1.076020000	4.056762000	-0.079424000
C	-0.020868000	1.435853000	1.298213000
C	1.255893000	1.061453000	1.983032000
H	1.348868000	1.613766000	2.925544000
H	2.126821000	1.291390000	1.364123000
H	1.289971000	-0.009503000	2.205177000
Ru	-0.912621000	0.442589000	-0.315465000
C	-2.233250000	-1.315394000	-1.579770000
H	-1.662928000	-0.935035000	-2.428259000
C	-3.635985000	-1.278199000	-1.627846000

H	-4.125711000	-0.786978000	-2.463048000
C	-4.382491000	-1.883582000	-0.632922000
H	-5.466851000	-1.860278000	-0.669969000
C	-3.727551000	-2.542043000	0.422053000
H	-4.313196000	-3.029087000	1.196279000
C	-2.348711000	-2.572010000	0.491963000
H	-1.830094000	-3.062067000	1.309016000
C	-1.567069000	-1.958277000	-0.514197000
C	-0.103492000	-1.874922000	-0.381844000
C	2.203753000	-1.240331000	-0.206857000
C	3.589457000	-0.742553000	-0.197093000
C	4.458874000	-1.095137000	0.845222000
H	4.093957000	-1.763611000	1.617373000
C	5.754317000	-0.593987000	0.881383000
C	6.207502000	0.267937000	-0.116711000
H	7.220393000	0.657089000	-0.085466000
C	5.351021000	0.625265000	-1.155213000
H	5.693946000	1.293416000	-1.939365000
C	4.053768000	0.124913000	-1.194461000
H	3.393251000	0.403455000	-2.012657000
N	1.782334000	-2.033570000	0.777525000
N	0.496117000	-2.360623000	0.709518000
P	0.965054000	-0.891477000	-1.426376000
H	6.416256000	-0.877608000	1.694181000

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TS5/5A

Ru	-0.586711000	0.413601000	-0.002879000
P	0.647275000	-1.825459000	-1.022082000
N	1.271493000	-1.283119000	1.492231000
N	-0.073247000	-1.497503000	1.509988000
C	1.805518000	-1.392154000	0.292999000
C	-0.549390000	-1.852796000	0.297639000
C	-0.743700000	2.150465000	1.146530000
C	0.495665000	2.128219000	0.403064000
C	0.167188000	2.078114000	-1.001786000
C	-1.262408000	2.035001000	-1.123147000
C	-1.824611000	2.079909000	0.209163000
C	-0.850239000	2.163863000	2.640227000
C	1.871740000	2.145716000	0.995227000
C	1.158956000	2.029369000	-2.123073000
C	-2.053573000	1.955995000	-2.392432000

C	-3.286926000	2.004994000	0.524934000
H	-0.825960000	3.190894000	3.022046000
H	-0.023769000	1.608225000	3.090067000
H	-1.780346000	1.696750000	2.972799000
H	1.919123000	1.509677000	1.883777000
H	2.157472000	3.165736000	1.276711000
H	2.612011000	1.764276000	0.286787000
H	1.452527000	3.041990000	-2.422491000
H	0.739823000	1.521242000	-2.994797000
H	2.059592000	1.485811000	-1.823002000
H	-2.953965000	1.351394000	-2.251668000
H	-1.467325000	1.498870000	-3.193210000
H	-2.362250000	2.954813000	-2.722240000
H	-3.449848000	1.698495000	1.560754000
H	-3.786383000	1.270533000	-0.115384000
H	-3.769388000	2.977481000	0.374076000
C	3.236477000	-1.084295000	0.109345000
C	3.784092000	-0.951265000	-1.172271000
C	4.062358000	-0.869915000	1.222143000
C	5.122896000	-0.608729000	-1.340603000
C	5.398173000	-0.529439000	1.051064000
C	5.934491000	-0.395809000	-0.229768000
H	3.155508000	-1.115794000	-2.044291000
H	3.632847000	-0.974757000	2.212669000
H	5.531216000	-0.509589000	-2.341612000
H	6.027126000	-0.368587000	1.921439000
H	6.978823000	-0.129697000	-0.359680000
C	-2.027879000	-1.916427000	0.136149000
C	-2.864739000	-1.745776000	1.252165000
C	-2.611266000	-2.069570000	-1.131210000
C	-4.245392000	-1.718852000	1.096023000
C	-3.993427000	-2.039688000	-1.281082000
C	-4.814865000	-1.858642000	-0.169417000
H	-2.405209000	-1.632588000	2.228324000
H	-1.973156000	-2.206978000	-2.000208000
H	-4.881485000	-1.586845000	1.965952000
H	-4.429717000	-2.158934000	-2.267837000
H	-5.893666000	-1.834328000	-0.287918000

Sum of electronic and zero-point Energies= -1474.354319

Sum of electronic and thermal Energies= -1474.327078

Sum of electronic and thermal Enthalpies= -1474.326134

Sum of electronic and thermal Free Energies= -1474.413750

4A

C	-2.227533000	-0.384341000	1.995565000
H	-1.606439000	0.449278000	1.680899000

C	-3.556801000	-0.145115000	2.377593000
H	-3.964001000	0.855347000	2.274616000
C	-4.331489000	-1.167117000	2.896083000
C	-3.770777000	-2.444257000	3.062787000
C	-2.463596000	-2.690872000	2.694335000
H	-2.009387000	-3.663166000	2.844627000
C	-1.663551000	-1.662988000	2.140388000
C	-0.268020000	-1.953036000	1.773296000
C	2.059210000	-2.246266000	1.143185000
C	3.464690000	-2.288233000	0.710223000
C	4.026640000	-3.490781000	0.258994000
H	3.408591000	-4.383010000	0.254927000
C	5.349752000	-3.532988000	-0.167882000
C	6.138037000	-2.381592000	-0.144825000
H	7.170531000	-2.420055000	-0.477802000
C	5.590055000	-1.184834000	0.310311000
H	6.189408000	-0.278520000	0.325002000
C	4.264989000	-1.140780000	0.729861000
H	3.826402000	-0.199962000	1.048932000
C	4.316282000	2.508474000	0.967618000
H	4.399179000	2.211075000	-0.084699000
H	4.835462000	1.763206000	1.575496000
H	4.839398000	3.463432000	1.090873000
C	2.881267000	2.646774000	1.383734000
C	2.222566000	1.956551000	2.447998000
C	2.833414000	1.021329000	3.448210000
H	3.713174000	0.507876000	3.054286000
H	2.119020000	0.255289000	3.761052000
H	3.140896000	1.581586000	4.338897000
C	0.845389000	2.391284000	2.465911000
C	-0.172010000	1.991325000	3.490400000
H	-0.125679000	0.919266000	3.704631000
H	-1.186139000	2.224219000	3.156032000
H	0.003493000	2.533232000	4.427366000
C	0.685032000	3.393659000	1.441128000
C	-0.559645000	4.170580000	1.147331000
H	-1.458876000	3.595142000	1.384859000
H	-0.614613000	4.445152000	0.090297000
H	-0.572689000	5.089449000	1.745505000
C	1.934901000	3.551032000	0.772148000
C	2.232709000	4.547074000	-0.306413000
H	2.318568000	5.551421000	0.124880000
H	1.441795000	4.559613000	-1.062804000
H	3.178112000	4.311497000	-0.801719000
N	1.473387000	-3.350693000	1.611231000
N	0.207186000	-3.198198000	1.958658000

P	0.966941000	-0.875474000	1.105633000
Ru	1.245737000	1.509789000	0.600347000
C	2.214848000	-0.035192000	-1.886413000
H	1.503459000	-0.784748000	-1.553890000
C	3.527507000	-0.413521000	-2.185187000
H	3.838017000	-1.442017000	-2.024056000
C	4.425560000	0.520617000	-2.678380000
H	5.446059000	0.226029000	-2.903260000
C	4.003690000	1.838201000	-2.903333000
H	4.696894000	2.565555000	-3.315806000
C	2.703630000	2.217331000	-2.620159000
H	2.353421000	3.222364000	-2.823594000
C	1.784197000	1.285560000	-2.090510000
C	0.396262000	1.707293000	-1.827042000
C	-1.904054000	2.257657000	-1.250080000
C	-3.303565000	2.480253000	-0.850117000
C	-3.859167000	3.766312000	-0.929142000
H	-3.234718000	4.577562000	-1.287837000
C	-5.182327000	3.986244000	-0.567053000
C	-5.978664000	2.933005000	-0.116125000
H	-7.011742000	3.109767000	0.166188000
C	-5.436077000	1.653718000	-0.032458000
H	-6.040315000	0.821966000	0.321081000
C	-4.111128000	1.430630000	-0.397722000
H	-3.694098000	0.428870000	-0.328938000
C	-4.400458000	-2.487076000	-0.699916000
H	-4.392841000	-2.569972000	0.391775000
H	-4.868115000	-1.534800000	-0.964939000
H	-5.027042000	-3.293405000	-1.098460000
C	-3.012453000	-2.579649000	-1.256214000
C	-2.458867000	-1.756106000	-2.289184000
C	-3.172619000	-0.722160000	-3.106541000
H	-3.966912000	-0.227959000	-2.542048000
H	-2.483505000	0.053210000	-3.452271000
H	-3.624884000	-1.191647000	-3.988052000
C	-1.091335000	-2.168903000	-2.489733000
C	-0.192518000	-1.661550000	-3.576959000
H	0.837612000	-1.996162000	-3.436976000
H	-0.538537000	-2.043315000	-4.544749000
H	-0.188894000	-0.568670000	-3.626514000
C	-0.823623000	-3.259406000	-1.588892000
C	0.471104000	-4.000820000	-1.465879000
H	1.324342000	-3.350555000	-1.685698000
H	0.608206000	-4.389735000	-0.453314000
H	0.492965000	-4.841787000	-2.169020000
C	-2.013044000	-3.533262000	-0.841784000

C	-2.198890000	-4.665411000	0.121027000
H	-2.302986000	-5.608539000	-0.428260000
H	-1.344559000	-4.748727000	0.799746000
H	-3.102084000	-4.524512000	0.719879000
N	-1.268127000	3.196779000	-1.939149000
N	-0.006033000	2.909679000	-2.249075000
P	-0.874967000	0.859734000	-0.909978000
Ru	-1.343915000	-1.504714000	-0.496653000
H	-5.356375000	-0.977125000	3.199460000
H	-4.364785000	-3.242501000	3.498396000
H	-5.596834000	4.987556000	-0.634912000
H	5.770260000	-4.470101000	-0.520239000

Sum of electronic and zero-point Energies= -2948.785339
Sum of electronic and thermal Energies= -2948.729795
Sum of electronic and thermal Enthalpies= -2948.728851
Sum of electronic and thermal Free Energies= -2948.873785

4B

C	5.090169000	-0.916788000	0.559867000
H	4.412630000	-0.066059000	0.624588000
C	6.359536000	-0.827846000	1.121279000
H	6.659511000	0.081301000	1.635255000
C	7.244853000	-1.898501000	1.019486000
C	6.846403000	-3.054739000	0.350056000
C	5.577246000	-3.145967000	-0.209348000
H	5.256106000	-4.039766000	-0.733050000
C	4.677362000	-2.076475000	-0.109827000
C	3.335952000	-2.182159000	-0.709524000
C	1.089201000	-2.119539000	-1.600152000
C	-0.309977000	-1.983295000	-2.014028000
C	-0.940060000	-2.974131000	-2.781175000
H	-0.353373000	-3.835969000	-3.082686000
C	-2.279918000	-2.849152000	-3.139064000
C	-3.032071000	-1.743311000	-2.741544000
H	-4.075218000	-1.646614000	-3.026130000
C	-2.415943000	-0.732929000	-2.000711000
H	-2.959791000	0.174881000	-1.748649000
C	-1.064826000	-0.852237000	-1.645836000
H	-0.565680000	-0.013102000	-1.157168000
C	-0.312791000	2.841955000	-2.099650000
H	-0.881534000	3.145197000	-1.215189000
H	-0.746939000	1.918976000	-2.493629000
H	-0.439041000	3.620908000	-2.861447000
C	1.141858000	2.671554000	-1.786968000
C	2.038904000	1.725539000	-2.397563000
C	1.703066000	0.773851000	-3.504406000

H	0.675840000	0.408075000	-3.422022000
H	2.364901000	-0.095377000	-3.498138000
H	1.804954000	1.280565000	-4.471078000
C	3.332749000	1.905214000	-1.802625000
C	4.580195000	1.163334000	-2.173521000
H	4.369447000	0.110108000	-2.379003000
H	5.322277000	1.199179000	-1.372457000
H	5.028596000	1.606776000	-3.070319000
C	3.226372000	2.986524000	-0.847071000
C	4.347875000	3.490343000	0.007947000
H	4.999500000	2.668747000	0.321376000
H	3.964997000	3.978603000	0.907328000
H	4.958760000	4.213244000	-0.544734000
C	1.888935000	3.487620000	-0.866091000
C	1.357082000	4.690808000	-0.152676000
H	1.384888000	5.553531000	-0.829321000
H	1.961217000	4.935134000	0.724199000
H	0.321430000	4.548019000	0.173658000
N	1.778726000	-3.204897000	-1.948657000
N	3.017376000	-3.237389000	-1.462409000
P	1.991822000	-1.069749000	-0.522689000
Ru	1.945826000	1.385836000	-0.321953000
C	-5.218298000	0.784360000	-0.443845000
H	-4.721058000	-0.065582000	0.020351000
C	-6.428822000	0.597657000	-1.103513000
H	-6.868525000	-0.394807000	-1.151647000
C	-7.078742000	1.680832000	-1.690042000
H	-8.024267000	1.539111000	-2.203930000
C	-6.505803000	2.949482000	-1.607341000
H	-7.007274000	3.799981000	-2.059366000
C	-5.295245000	3.137481000	-0.951216000
H	-4.840517000	4.119459000	-0.880283000
C	-4.631031000	2.053942000	-0.360396000
C	-3.337420000	2.260261000	0.314524000
C	-1.198105000	2.343322000	1.437597000
C	0.141511000	2.257967000	2.030722000
C	0.728480000	3.368451000	2.658732000
H	0.143843000	4.278661000	2.741794000
C	2.031837000	3.303537000	3.135883000
C	2.789390000	2.136932000	3.001353000
H	3.809587000	2.096257000	3.369917000
C	2.209544000	1.010463000	2.418173000
H	2.756757000	0.071478000	2.361099000
C	0.887771000	1.068774000	1.950611000
H	0.410868000	0.166990000	1.569803000
C	0.172784000	-2.197571000	2.909851000

H	0.985531000	-2.116590000	2.179975000
H	0.145065000	-1.278234000	3.499942000
H	0.409789000	-3.027799000	3.585737000
C	-1.136767000	-2.455964000	2.231539000
C	-2.417278000	-1.938692000	2.620526000
C	-2.685170000	-1.018875000	3.771862000
H	-1.858181000	-0.318993000	3.921097000
H	-3.585789000	-0.424048000	3.603749000
H	-2.818409000	-1.596677000	4.693457000
C	-3.393267000	-2.489736000	1.720112000
C	-4.870447000	-2.248117000	1.760215000
H	-5.100093000	-1.245173000	2.129606000
H	-5.313190000	-2.349933000	0.764841000
H	-5.358779000	-2.974942000	2.419942000
C	-2.713557000	-3.403830000	0.826550000
C	-3.377082000	-4.246850000	-0.216794000
H	-4.180163000	-3.701721000	-0.720506000
H	-2.661808000	-4.566434000	-0.977423000
H	-3.810809000	-5.141550000	0.244821000
C	-1.328437000	-3.385994000	1.140765000
C	-0.251633000	-4.229710000	0.532286000
H	-0.183455000	-5.180041000	1.075126000
H	-0.446080000	-4.451336000	-0.519543000
H	0.724094000	-3.739688000	0.583472000
N	-1.689412000	3.541883000	1.115618000
N	-2.869076000	3.495452000	0.499851000
P	-2.284261000	1.038897000	1.006696000
Ru	-1.998011000	-1.387511000	0.630685000
H	8.236795000	-1.831694000	1.455147000
H	7.530909000	-3.893321000	0.264184000
H	2.468976000	4.175685000	3.614108000
H	-2.746185000	-3.631083000	-3.732047000

Sum of electronic and zero-point Energies= -2948.750501
Sum of electronic and thermal Energies= -2948.694595
Sum of electronic and thermal Enthalpies= -2948.693651
Sum of electronic and thermal Free Energies= -2948.841618

TS4A/4B

C	-4.894445000	0.943758000	0.467416000
H	-4.251865000	0.064705000	0.473842000
C	-6.151554000	0.881038000	1.059551000
H	-6.476139000	-0.038400000	1.539474000
C	-6.993405000	1.990513000	1.029691000
C	-6.564133000	3.158446000	0.400616000
C	-5.306189000	3.223957000	-0.187253000
H	-4.961476000	4.127102000	-0.679004000

C	-4.449173000	2.115638000	-0.158284000
C	-3.115715000	2.195775000	-0.780011000
C	-0.882554000	2.102111000	-1.699210000
C	0.522576000	1.960570000	-2.096216000
C	1.187258000	2.969354000	-2.809484000
H	0.623061000	3.851538000	-3.094934000
C	2.531901000	2.830098000	-3.140023000
C	3.257454000	1.700898000	-2.755111000
H	4.307722000	1.601046000	-3.010707000
C	2.607852000	0.677720000	-2.065519000
H	3.133850000	-0.239401000	-1.811628000
C	1.246430000	0.800786000	-1.755838000
H	0.716042000	-0.054134000	-1.337243000
C	0.394821000	-2.983687000	-2.111785000
H	0.925344000	-3.314394000	-1.213725000
H	0.885900000	-2.083508000	-2.492079000
H	0.499573000	-3.766692000	-2.872689000
C	-1.056085000	-2.738266000	-1.833193000
C	-1.889401000	-1.750636000	-2.465507000
C	-1.489008000	-0.830209000	-3.577203000
H	-0.443542000	-0.522349000	-3.489643000
H	-2.101527000	0.074374000	-3.586733000
H	-1.610260000	-1.340795000	-4.539654000
C	-3.200479000	-1.854432000	-1.889677000
C	-4.400665000	-1.056212000	-2.298058000
H	-4.139305000	-0.011015000	-2.485655000
H	-5.174573000	-1.069435000	-1.527308000
H	-4.830595000	-1.473657000	-3.216099000
C	-3.171046000	-2.934434000	-0.927696000
C	-4.334424000	-3.376190000	-0.095236000
H	-4.956679000	-2.522848000	0.191632000
H	-3.996781000	-3.867889000	0.820113000
H	-4.961874000	-4.079307000	-0.654945000
C	-1.862865000	-3.507930000	-0.922468000
C	-1.408532000	-4.733673000	-0.194162000
H	-1.421822000	-5.587847000	-0.881897000
H	-2.070925000	-4.968226000	0.642228000
H	-0.390432000	-4.622081000	0.193543000
N	-1.559086000	3.197662000	-2.037263000
N	-2.791536000	3.247595000	-1.535465000
P	-1.787865000	1.057804000	-0.617880000
Ru	-1.809729000	-1.404559000	-0.388101000
C	5.107524000	-0.851136000	-0.226125000
H	4.602537000	0.010654000	0.205113000
C	6.353865000	-0.693762000	-0.823705000
H	6.816703000	0.288906000	-0.853417000

C	7.009665000	-1.794004000	-1.370764000
H	7.983221000	-1.675482000	-1.835866000
C	6.405983000	-3.049639000	-1.311649000
H	6.911523000	-3.913280000	-1.733169000
C	5.159075000	-3.207789000	-0.718543000
H	4.680993000	-4.179756000	-0.665632000
C	4.488616000	-2.106583000	-0.168796000
C	3.159533000	-2.282274000	0.443036000
C	0.970164000	-2.330938000	1.471864000
C	-0.385369000	-2.230404000	2.030670000
C	-1.011291000	-3.347466000	2.614777000
H	-0.450715000	-4.274064000	2.675295000
C	-2.310195000	-3.258042000	3.093211000
C	-3.031409000	-2.062155000	2.999704000
H	-4.051199000	-2.003993000	3.367009000
C	-2.414846000	-0.935515000	2.464872000
H	-2.933940000	0.019812000	2.436040000
C	-1.089750000	-1.012373000	2.004909000
H	-0.573603000	-0.105378000	1.701807000
C	-0.352607000	2.291561000	2.875807000
H	-1.155188000	2.216826000	2.134744000
H	-0.362101000	1.388594000	3.491101000
H	-0.574263000	3.145516000	3.526844000
C	0.976390000	2.496157000	2.215617000
C	2.231254000	1.939334000	2.630476000
C	2.446973000	1.012302000	3.786930000
H	1.595018000	0.339786000	3.920854000
H	3.330670000	0.388145000	3.635891000
H	2.581666000	1.586369000	4.710693000
C	3.243812000	2.461160000	1.751789000
C	4.713912000	2.190440000	1.833400000
H	4.915397000	1.191287000	2.228227000
H	5.183334000	2.265441000	0.847849000
H	5.198564000	2.921010000	2.491838000
C	2.611935000	3.395220000	0.845146000
C	3.327585000	4.224789000	-0.173586000
H	4.111952000	3.652773000	-0.676825000
H	2.639010000	4.591142000	-0.937223000
H	3.794605000	5.089486000	0.312262000
C	1.219649000	3.415809000	1.126459000
C	0.180392000	4.280809000	0.483741000
H	0.126398000	5.240088000	1.012433000
H	0.403161000	4.480907000	-0.566706000
H	-0.809978000	3.818332000	0.518285000
N	1.483163000	-3.538322000	1.226310000
N	2.688221000	-3.511232000	0.663378000

P	2.062242000	-1.038337000	1.015748000
Ru	1.838666000	1.401211000	0.632298000
H	-7.975863000	1.944819000	1.488938000
H	-7.215107000	4.027054000	0.370129000
H	-2.774119000	-4.131312000	3.543554000
H	3.026546000	3.621936000	-3.695852000

Sum of electronic and zero-point Energies= -2948.749828
Sum of electronic and thermal Energies= -2948.694916
Sum of electronic and thermal Enthalpies= -2948.693972
Sum of electronic and thermal Free Energies= -2948.838549

4

C	-3.082381000	1.944880000	-0.948921000
H	-2.498923000	1.060220000	-1.192177000
C	-4.471922000	1.919819000	-1.037175000
H	-4.968669000	1.015777000	-1.376114000
C	-5.217686000	3.047271000	-0.700418000
C	-4.567782000	4.209721000	-0.284979000
C	-3.180462000	4.249125000	-0.219823000
H	-2.657628000	5.150534000	0.083341000
C	-2.423739000	3.117026000	-0.555381000
C	-0.953454000	3.183234000	-0.492487000
C	1.510583000	3.032385000	-0.279442000
C	2.963064000	2.804281000	-0.161942000
C	3.817315000	3.894543000	0.058696000
H	3.380430000	4.881384000	0.167177000
C	5.191883000	3.707205000	0.120848000
C	5.735889000	2.434294000	-0.052016000
H	6.811829000	2.292918000	-0.020690000
C	4.893771000	1.346832000	-0.269808000
H	5.307620000	0.354547000	-0.422431000
C	3.512039000	1.523427000	-0.306824000
H	2.854802000	0.671238000	-0.468257000
C	3.056493000	-1.096807000	-2.784299000
H	3.241108000	-1.810174000	-1.974034000
H	3.630769000	-0.191171000	-2.571773000
H	3.448972000	-1.530629000	-3.712063000
C	1.595647000	-0.788941000	-2.924597000
C	1.011779000	0.482097000	-3.213119000
C	1.752598000	1.760570000	-3.470738000
H	2.663825000	1.827670000	-2.870529000
H	1.135774000	2.633708000	-3.237223000
H	2.038599000	1.824524000	-4.527274000
C	-0.415347000	0.305961000	-3.363088000
C	-1.376186000	1.368016000	-3.805261000

H	-1.185646000	2.324689000	-3.309347000
H	-2.410200000	1.085610000	-3.594332000
H	-1.287218000	1.527033000	-4.886627000
C	-0.713236000	-1.067279000	-3.141644000
C	-2.061462000	-1.715610000	-3.238429000
H	-2.851466000	-1.047422000	-2.882188000
H	-2.106056000	-2.623388000	-2.630317000
H	-2.289916000	-1.990903000	-4.275098000
C	0.532140000	-1.745324000	-2.870208000
C	0.709635000	-3.228407000	-2.738108000
H	0.775751000	-3.679485000	-3.735421000
H	-0.124833000	-3.702032000	-2.212458000
H	1.628783000	-3.472961000	-2.198672000
N	1.051097000	4.235939000	-0.372193000
N	-0.349451000	4.323265000	-0.498439000
P	0.184387000	1.762329000	-0.287067000
Ru	0.158876000	-0.222460000	-1.288115000
C	3.082357000	-1.945079000	0.948789000
H	2.498928000	-1.060418000	1.192133000
C	4.471901000	-1.920045000	1.036962000
H	4.968679000	-1.016016000	1.375891000
C	5.217615000	-3.047517000	0.700169000
H	6.301136000	-3.023318000	0.764077000
C	4.567656000	-4.209958000	0.284784000
H	5.144823000	-5.089912000	0.018565000
C	3.180332000	-4.249332000	0.219695000
H	2.657460000	-5.150725000	-0.083442000
C	2.423663000	-3.117207000	0.555278000
C	0.953368000	-3.183311000	0.492454000
C	-1.510665000	-3.032308000	0.279431000
C	-2.963140000	-2.804119000	0.161978000
C	-3.817450000	-3.894325000	-0.058698000
H	-3.380622000	-4.881180000	-0.167293000
C	-5.192016000	-3.706925000	-0.120727000
C	-5.735959000	-2.434009000	0.052308000
H	-6.811898000	-2.292594000	0.021099000
C	-4.893781000	-1.346600000	0.270131000
H	-5.307565000	-0.354302000	0.422865000
C	-3.512051000	-1.523254000	0.307007000
H	-2.854779000	-0.671091000	0.468449000
C	-3.056469000	1.096518000	2.784468000
H	-3.241235000	1.809620000	1.973997000
H	-3.630706000	0.190771000	2.572303000
H	-3.448867000	1.530608000	3.712139000
C	-1.595585000	0.788800000	2.924690000
C	-1.011555000	-0.482170000	3.213192000

C	-1.752223000	-1.760725000	3.470846000
H	-2.663443000	-1.827946000	2.870642000
H	-1.135296000	-2.633796000	3.237351000
H	-2.038217000	-1.824689000	4.527385000
C	0.415558000	-0.305880000	3.363073000
C	1.376511000	-1.367843000	3.805216000
H	1.186155000	-2.324494000	3.309194000
H	2.410502000	-1.085261000	3.594413000
H	1.287466000	-1.526986000	4.886558000
C	0.713293000	1.067378000	3.141564000
C	2.061436000	1.715880000	3.238361000
H	2.851527000	1.047801000	2.882103000
H	2.105917000	2.623675000	2.630263000
H	2.289842000	1.991176000	4.275039000
C	-0.532189000	1.745287000	2.870211000
C	-0.709842000	3.228350000	2.738101000
H	-0.775919000	3.679444000	3.735410000
H	0.124533000	3.702052000	2.212373000
H	-1.629063000	3.472793000	2.198736000
N	-1.051262000	-4.235890000	0.372162000
N	0.349291000	-4.323298000	0.498380000
P	-0.184390000	-1.762320000	0.287066000
Ru	-0.158832000	0.222467000	1.288099000
H	-6.301203000	3.023040000	-0.764404000
H	-5.144984000	5.089658000	-0.018764000
H	-5.843920000	-4.557559000	-0.293649000
H	5.843740000	4.557882000	0.293736000

Sum of electronic and zero-point Energies= -2948.778255
Sum of electronic and thermal Energies= -2948.722890
Sum of electronic and thermal Enthalpies= -2948.721946
Sum of electronic and thermal Free Energies= -2948.865746

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C	2.573612000	-2.412720000	-1.193472000
H	2.066215000	-1.516744000	-1.546808000
C	3.951098000	-2.534693000	-1.348031000
H	4.508487000	-1.732584000	-1.823123000
C	4.604789000	-3.686758000	-0.915638000
C	3.865695000	-4.723486000	-0.345352000
C	2.487119000	-4.610265000	-0.203521000
H	1.897928000	-5.413516000	0.228096000
C	1.822832000	-3.445671000	-0.616021000
C	0.372946000	-3.328164000	-0.417211000
C	-2.009513000	-2.842660000	-0.154123000
C	-3.410508000	-2.420568000	0.008476000
C	-4.428080000	-3.384435000	-0.034213000

H	-4.144908000	-4.425292000	-0.145621000
C	-5.762784000	-3.006312000	0.048082000
C	-6.110322000	-1.661032000	0.158729000
H	-7.153933000	-1.366488000	0.205819000
C	-5.106772000	-0.695786000	0.205356000
H	-5.363576000	0.357023000	0.275216000
C	-3.767321000	-1.072001000	0.147399000
H	-2.991088000	-0.307993000	0.187752000
C	-3.048492000	1.619461000	-2.291775000
H	-2.942398000	2.479408000	-1.625841000
H	-3.647153000	0.862558000	-1.778995000
H	-3.604319000	1.942641000	-3.180456000
C	-1.718680000	1.069884000	-2.705817000
C	-1.465149000	-0.289729000	-3.110429000
C	-2.478761000	-1.386521000	-3.217521000
H	-3.286475000	-1.262591000	-2.492520000
H	-2.027413000	-2.368113000	-3.050493000
H	-2.919358000	-1.379808000	-4.221508000
C	-0.093249000	-0.379756000	-3.506555000
C	0.587289000	-1.609267000	-4.028758000
H	0.262481000	-2.505142000	-3.492124000
H	1.673382000	-1.537573000	-3.933481000
H	0.353332000	-1.742005000	-5.091478000
C	0.498583000	0.927374000	-3.357791000
C	1.927475000	1.285705000	-3.631043000
H	2.596492000	0.452193000	-3.395573000
H	2.237718000	2.140865000	-3.024473000
H	2.067097000	1.542145000	-4.687777000
C	-0.515744000	1.830644000	-2.903235000
C	-0.361532000	3.313347000	-2.755954000
H	-0.393003000	3.780441000	-3.747211000
H	0.585555000	3.586636000	-2.280860000
H	-1.168491000	3.739084000	-2.156011000
N	-1.703986000	-4.128614000	-0.186413000
N	-0.397510000	-4.398370000	-0.385797000
P	-0.556223000	-1.830429000	-0.262856000
Ru	-0.156189000	0.231956000	-1.477068000
C	-2.573260000	2.413005000	1.193400000
H	-2.065965000	1.516972000	1.546731000
C	-3.950738000	2.535115000	1.347924000
H	-4.508221000	1.733060000	1.823001000
C	-4.604297000	3.687264000	0.915559000
H	-5.678962000	3.783381000	1.033998000
C	-3.865074000	4.723942000	0.345348000
H	-4.366323000	5.627797000	0.012913000
C	-2.486504000	4.610585000	0.203558000

H	-1.897216000	5.413796000	-0.228003000
C	-1.822352000	3.445898000	0.616012000
C	-0.372475000	3.328232000	0.417217000
C	2.009926000	2.842433000	0.154115000
C	3.410868000	2.420168000	-0.008532000
C	4.428505000	3.384007000	0.033181000
H	4.145428000	4.424963000	0.143904000
C	5.763165000	3.005741000	-0.049189000
C	6.110593000	1.660359000	-0.158935000
H	7.154175000	1.365721000	-0.206079000
C	5.106975000	0.695137000	-0.204581000
H	5.363684000	-0.357743000	-0.273732000
C	3.767563000	1.071479000	-0.146555000
H	2.991282000	0.307478000	-0.186120000
C	3.048144000	-1.619300000	2.292426000
H	2.942179000	-2.478643000	1.625686000
H	3.647316000	-0.862127000	1.780652000
H	3.603365000	-1.943424000	3.181142000
C	1.718244000	-1.069719000	2.706178000
C	1.464539000	0.289874000	3.110752000
C	2.478016000	1.386778000	3.218003000
H	3.285780000	1.263025000	2.493026000
H	2.026543000	2.368322000	3.051029000
H	2.918567000	1.380041000	4.222009000
C	0.092546000	0.379814000	3.506573000
C	-0.588128000	1.609290000	4.028686000
H	-0.263485000	2.505157000	3.491935000
H	-1.674218000	1.537442000	3.933508000
H	-0.354099000	1.742172000	5.091372000
C	-0.499184000	-0.927349000	3.357626000
C	-1.928142000	-1.285805000	3.630384000
H	-2.597056000	-0.452013000	3.395615000
H	-2.238389000	-2.140359000	3.022952000
H	-2.067923000	-1.543233000	4.686856000
C	0.515305000	-1.830550000	2.903309000
C	0.361261000	-3.313265000	2.755995000
H	0.392655000	-3.780353000	3.747259000
H	-0.585744000	-3.586652000	2.280794000
H	1.168344000	-3.738919000	2.156157000
N	1.704559000	4.128420000	0.186457000
N	0.398112000	4.398338000	0.385853000
P	0.556496000	1.830382000	0.262736000
Ru	0.156014000	-0.231875000	1.477083000
H	5.679461000	-3.782768000	-1.034111000
H	4.367050000	-5.627272000	-0.012888000
H	6.538213000	3.765270000	-0.013545000

H	-6.537777000	-3.765861000	0.011666000

Sum of electronic and zero-point Energies= -2948.773415
Sum of electronic and thermal Energies= -2948.717805
Sum of electronic and thermal Enthalpies= -2948.716860
Sum of electronic and thermal Free Energies= -2948.864679

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6	3.869886000	1.394476000	0.704246000
1	4.162306000	0.378728000	0.988374000
1	4.268344000	1.572235000	-0.299139000
1	4.356164000	2.097940000	1.393280000
6	2.379870000	1.547838000	0.728524000
6	1.597930000	2.371687000	-0.152401000
6	2.129841000	3.266807000	-1.231514000
1	3.037626000	2.849244000	-1.677150000
1	1.397477000	3.389194000	-2.034701000
1	2.374943000	4.266840000	-0.846449000
6	0.222078000	2.237589000	0.237260000
6	-0.949707000	2.946985000	-0.374340000
1	-0.775975000	3.141941000	-1.437051000
1	-1.854798000	2.336247000	-0.301021000
1	-1.146383000	3.908721000	0.118851000
6	0.168724000	1.357795000	1.380483000
6	-1.058526000	0.968959000	2.149113000
1	-1.968797000	1.199970000	1.589248000
1	-1.078757000	-0.106814000	2.351396000
1	-1.101518000	1.505224000	3.106282000
6	1.499774000	0.949842000	1.693102000
6	1.883674000	0.024266000	2.806299000
1	2.036343000	0.562857000	3.751327000
1	1.101145000	-0.726361000	2.961659000
1	2.807843000	-0.511925000	2.568395000
44	0.949349000	0.302680000	-0.362979000
6	2.115152000	-1.277323000	-1.621608000
1	1.551900000	-1.119730000	-2.537776000
6	3.536700000	-1.255156000	-1.688388000
1	4.006290000	-0.819138000	-2.567452000
6	4.308529000	-1.791226000	-0.690765000
1	5.392679000	-1.761118000	-0.753660000
6	3.677643000	-2.415692000	0.424741000
1	4.290776000	-2.866300000	1.201840000
6	2.315156000	-2.457558000	0.528392000
1	1.818591000	-2.927460000	1.371515000
6	1.480672000	-1.877096000	-0.484913000
6	0.038220000	-1.822974000	-0.346796000
6	-2.259919000	-1.155731000	-0.182165000
6	-3.634916000	-0.651786000	-0.173246000
6	-4.540587000	-1.042284000	0.831100000
1	-4.188539000	-1.736449000	1.586586000
6	-5.839097000	-0.551504000	0.853760000
6	-6.282026000	0.342948000	-0.122206000

1	-7.298627000	0.725283000	-0.101207000
6	-5.395908000	0.741398000	-1.120585000
1	-5.719236000	1.441525000	-1.886883000
6	-4.092421000	0.256433000	-1.143639000
1	-3.407455000	0.582603000	-1.922820000
7	-1.845719000	-1.930669000	0.827538000
7	-0.584266000	-2.306067000	0.763107000
15	-1.022100000	-0.855071000	-1.430396000
1	-6.516770000	-0.870097000	1.642350000

Sum of electronic and zero-point Energies = -1474.409089
Sum of electronic and thermal Energies = -1474.381471
Sum of electronic and thermal Enthalpies = -1474.380527
Sum of electronic and thermal Free Energies = -1474.467143