

SUPPORTING INFORMATIONS

Synthesis, Characterization and Cytotoxicity of Arene-Ruthenium(II) Complexes with Acylpyrazolones Functionalized with Aromatic Groups in the Acyl Moiety

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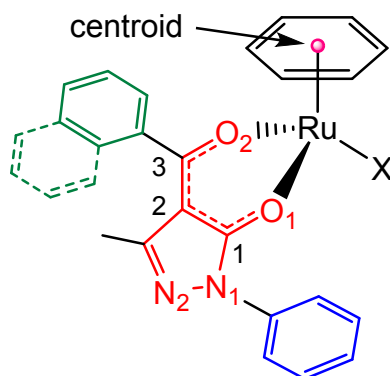
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Supporting Information

Table S1. Geometrical parameters for complexes **1** – **4** and **6**.

	1	2	3	4	6
Distances (Å)					
Ru-O1	2.0885(10)	2.097(5)	2.0951(17)	2.118(7)	2.108(2)
Ru-O2	2.0935(9)	2.114(5)	2.0915(16)	2.124(7)	2.106(3)
Ru-X	2.4087(4)	2.4088(19)	2.4069(7)	2.423(3)	2.3226(11)
N1-N2	1.4042(17)	1.403(8)	1.409(3)	1.435(12)	1.402(4)
C1-O1	1.2698(16)	1.270(9)	1.268(3)	1.278(13)	1.276(4)
C3-O2	1.2673(17)	1.277(8)	1.275(3)	1.275(13)	1.289(4)
C1-C2	1.4314(19)	1.422(10)	1.427(3)	1.448(15)	1.430(5)
C2-C3	1.404(2)	1.426(10)	1.406(4)	1.395(15)	1.404(5)
Ru-centroid	1.65	1.65	1.64	1.65	1.71
Angles (°)					
O1-Ru-O2	89.05(4)	88.99(18)	87.95(7)	87.8(3)	87.95(9)
O1-Ru-X	84.84(3)	83.71(14)	85.45(6)	85.0(2)	87.86(8)
O2-Ru-X	83.93(3)	82.89(14)	84.88(6)	84.9(2)	83.84(8)
Angles between the acylpyrazolone plane and the N_{phenyl}, C_{phenyl} and C_{naphthyl} plane (°)					
N _{ph}	21.04	36.05	20.16	20.85	8.03
C _{ph}	66.17		60.18		61.95
C _{naph}		82.17		83.76	

Table S2: Crystallographic and structure refinement parameters for compounds **1** – **4** and **6**.

	1	2	3	4	6
Chemical formula	C ₂₇ H ₂₇ ClN ₂ O ₂ Ru	C ₃₁ H ₂₉ ClN ₂ O ₂ Ru	C ₂₉ H ₃₁ ClN ₂ O ₂ Ru	C ₃₃ H ₃₃ ClN ₂ O ₂ Ru	C ₃₇ H ₄₁ F ₆ N ₅ O ₂ P ₂ Ru
Formula weight	548.02	598.08	576.08	626.13	864.76
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Triclinic
Space group	<i>P2₁/n</i> (no. 14)	<i>P2₁/c</i> (no. 14)	<i>P2₁/c</i> (no. 14)	<i>Pbca</i> (no. 61)	<i>P</i> -1 (no. 2)
Crystal color and shape	orange block	orange prism	orange block	orange prism	orange prism
Crystal size	0.25 x 0.21 x 0.17	0.35 x 0.21 x 0.18	0.19 x 0.18 x 0.15	0.26 x 0.14 x 0.13	0.47 x 0.21 x 0.18
<i>a</i> (Å)	16.4494(7)	9.9327(18)	8.1807(7)	13.815(2)	10.5733(8)
<i>b</i> (Å)	8.1443(2)	27.560(4)	16.3923(18)	15.2054(13)	11.3341(13)
<i>c</i> (Å)	17.6939(8)	10.059(2)	19.3118(18)	29.897(4)	16.2898(16)
α (°)	90	90	90	90	97.731(9)
β (°)	92.101(3)	106.967(14)	96.340(7)	90	106.620(7)
γ (°)	90	90	90	90	100.180(9)
<i>V</i> (Å ³)	2368.8(2)	2633.8(9)	2573.9(4)	6280.2(14)	1805.3(3)
<i>Z</i>	4	4	4	8	2
<i>D_c</i> (g.cm ⁻³)	1.537	1.508	1.487	1.324	1.591
μ (mm ⁻¹)	0.802	0.729	0.742	0.614	0.596
Scan range (°)	1.66 < θ < 29.23	2.27 < θ < 25.44	1.63 < θ < 29.24	2.41 < θ < 25.21	2.49 < θ < 27.50
Unique reflections	6423 [R _{int} = 0.0423]	4848 [R _{int} = 0.1330]	6987 [R _{int} = 0.0842]	5659 [R _{int} = 0.1384]	8225 [R _{int} = 0.0471]
Final R indices [I > 2 σ (I)]*	0.0217, wR ₂ 0.0499	0.0718, wR ₂ 0.1424	0.0369, wR ₂ 0.0572	0.1083, wR ₂ 0.2212	0.0537, wR ₂ 0.1028
R indices (all data)	0.0291, wR ₂ 0.0517	0.1237, wR ₂ 0.1678	0.0732, wR ₂ 0.0629	0.1419, wR ₂ 0.2338	0.0816, wR ₂ 0.1162
Goodness-of-fit	1.030	1.089	0.877	1.260	1.109
Max, Min $\Delta\rho/e$ (Å ⁻³)	0.359, -0.521	1.702, -2.096	0.601, -0.657	1.444, -1.305	1.545, -0.937

* Structures were refined on F₀²: wR₂ = [Σ[w(F₀² - F_c²)] / Σw(F₀²)^{1/2}, where w⁻¹ = [Σ(F₀²) + (aP)² + bP] and P = [max(F₀², 0) + 2F_c²]/3

Table S3. Comparison of selected computed and experimental structural parameters for compounds **1** – **4** and **6**.

Bond distances (Å) and angles (°)	1	1c	2	2c	3	3c	4	4c	6	6c
Ru-centroid	1.647	1.739	1.651	1.739	1.643	1.731	1.646	1.731	1.710	1.819
Ru-O	2.089(1) 2.094(1)	2.101 2.103	2.097(5) 2.114(5)	2.098 2.099	2.095(2) 2.092(2)	2.111 2.113	2.118(7) 2.124(7)	2.110 2.111	2.106(3) 2.108(2)	2.103 2.106
Ru-Cl	2.4087(4)	2.434	2.409(2)	2.442	2.4069(7)	2.447	2.423(3)	2.451	-	-
Ru-P	-	-	-	-	-	-	-	-	2.323(1)	2.350
N1-N2	1.404(2)	1.392	1.403(8)	1.394	1.409(3)	1.392	1.435(12)	1.393	1.402(4)	1.394
O1-C (acyl)	1.267(2)	1.277	1.277(8)	1.277	1.275(3)	1.274	1.275(13)	1.276	1.289(4)	1.287
O2-C	1.270(2)	1.277	1.270(9)	1.275	1.268(3)	1.274	1.278(13)	1.275	1.276(4)	1.285
O-Ru-O	89.05(4)	87.8	89.0(2)	88.5	87.95(7)	88.4	87.8(3)	88.3	88.0(1)	88.7
Cl-Ru-O	83.93(3) 84.84(3)	86.0 86.7	82.9(1) 83.7(1)	85.5 86.3	84.88(6) 85.45(6)	85.6 85.9	84.9(2) 85.0(2)	85.7 86.5	-	-
P-Ru-O	-	-	-	-	-	-	-	-	83.84(8) 87.86(8)	83.7 87.0

Table S4. Comparison of selected experimental and calculated IR absorptions of complexes **1-4** (cm⁻¹).

1		2		3		4		Assignment^b
Experimental	Calculated^a	Experimental	Calculated^a	Experimental	Calculated^a	Experimental	Calculated^a	
1599s	1598	1604s	1598	1605s	1599	1604s	1598	ν(C [≡] O) symmetrical (both C [≡] O of Q ^R) + ν(C [≡] C) phenyl
1591m	1583	1592s	1583	1591s	1583	1591v	1583	
1575vs	1562	1577vs	1570	1572vs	1567	1578vs	1569	
1539s	1539	1533m	1542	1539s	1541	1542m	1539	ν(C=N), Q ^R
1476vs	1465	1482vs	1474	1473vs	1467	1483vs	1472	ν(C [≡] C), Q ^R
1456vs		1459s		1458vs	1461	1462m		
1374vs	1365	1373s	1367	1369vs br	1367	1371vs	1368	ν(C [≡] N), Q ^R
1360m		1360m				1360m		
453m	445	443w	435	460m	440	462m	435	ν(Ru-O)
445sh				445m		441w		
279s	267	279s	263	285s	274	287s	277	ν(Ru-Cl)
				280sh				

^a The computed IR spectrum was scaled by a factor of 0.96, according to references 34 and 35 in the manuscript. ^b Due to the absence of symmetry, only the main vibrational modes were included in the assignment.

Table S5. Comparison of selected experimental and calculated IR absorptions of complexes **5-8** (cm⁻¹).

5		6		7		8		Assignment^b	
Experimental	Calculated^a	Experimental	Calculated^a	Experimental	Calculated^a	Experimental	Calculated^a		
1604m	1593	1599w	1594	1592w	1582	1600m	1593	ν(C [≡] O) symmetrical (both C [≡] O of Q ^R) + ν(C=N), Q ^R + ν(C [≡] C) phenyl	
1594m	1583	1591m	1583	1566s	1541	1571s	1547		
1573s	1571	1567s	1548	1531w	1538	1529w	1542		
1542m	1541	1536m	1542						
	1539								
1474s	1480	1479s	1466	1492w	1481 w	1478s	1466	ν(C [≡] C), Q ^R	
1460m	1459	1459m		1471m		1448			1458m
				1457m					
				1440m					
1377s	1391	1392m	1392	1379m	1392	1393w	1394	ν(C [≡] N), Q ^R	
		1374m				1377m			
1359w	1366	1361w	1366	1361w	1367	1359w	1365	ν(C [≡] O) asymmetrical (both C [≡] O of Q ^R)	
481m	460	451m	459	477m	453	455m	455	ν(Ru-P)	
455sh	454	478m	470	453m	448	475m	464	ν(Ru-O)	
449m	441	440w	449		438		442		

^a The computed IR spectrum was scaled by a factor of 0.96, according to references 34 and 35 in the manuscript. ^b Due to the absence of symmetry, only the main vibrational modes were included in the assignment.

Figure S1. Optimized structures of compounds **1c-8c**.

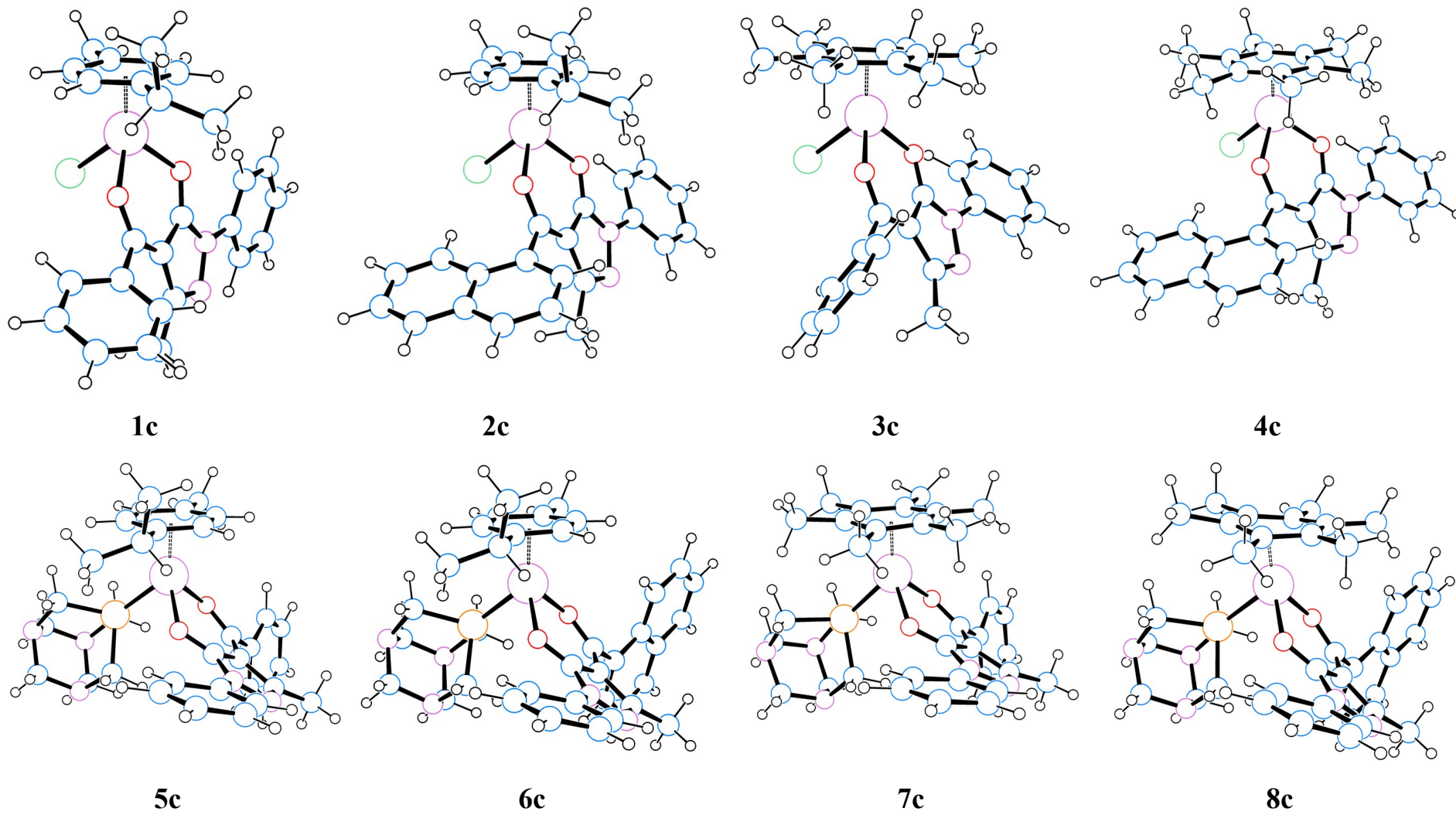
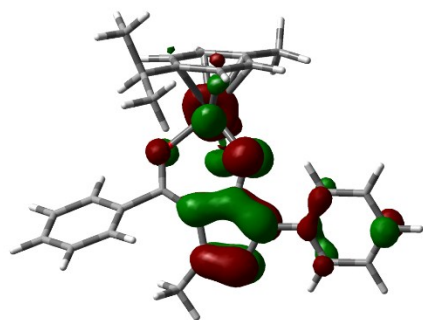
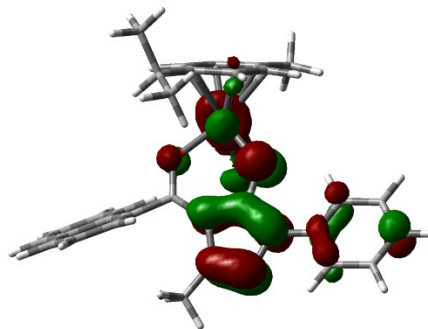


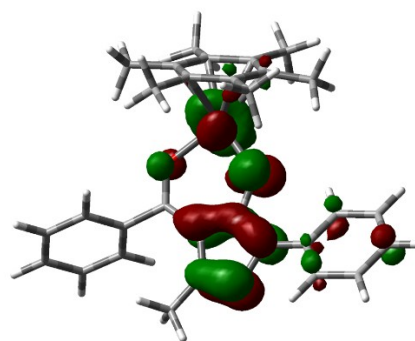
Figure S2. HOMOs of **1c-8c** (Isovalue = 0.04).



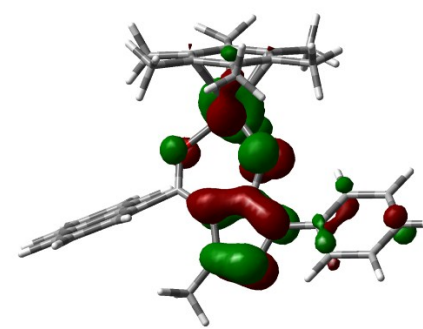
1c



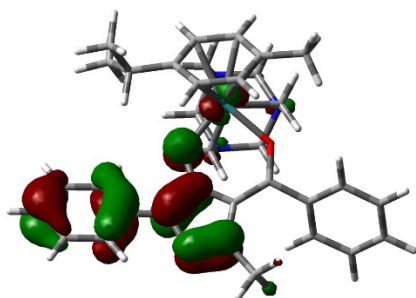
2c



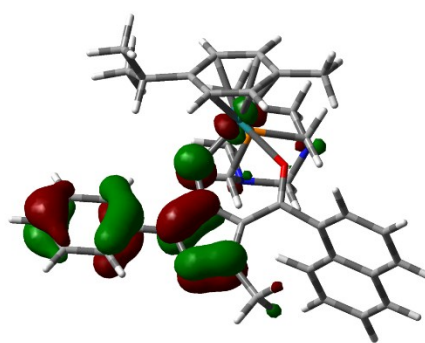
3c



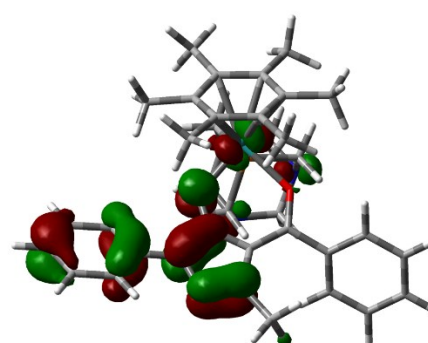
4c



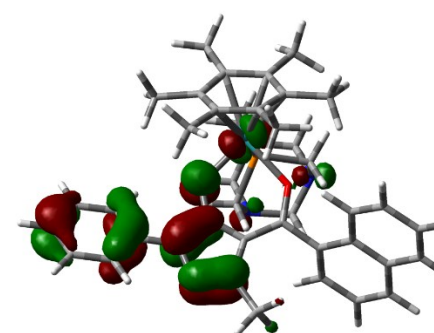
5c



6c

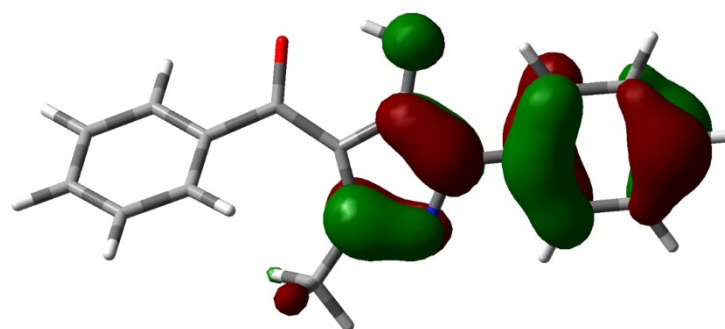


7c

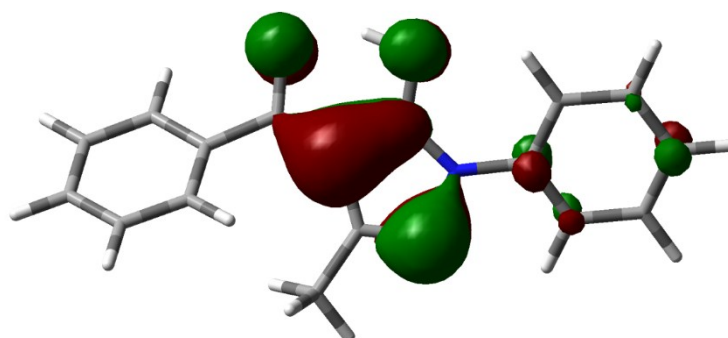


8c

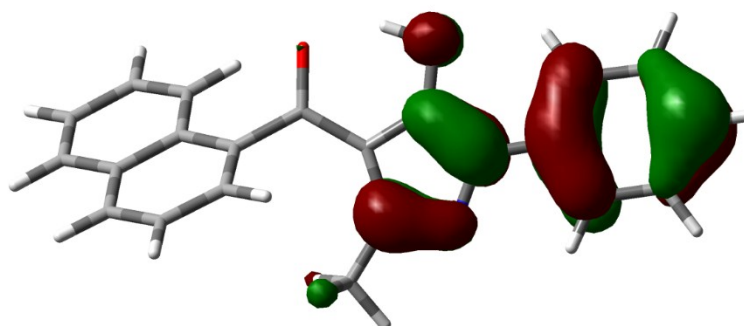
Figure S3. Selected MOs of compounds HQ^{Ph} and HQ^{naph} (Isovalue = 0.04).



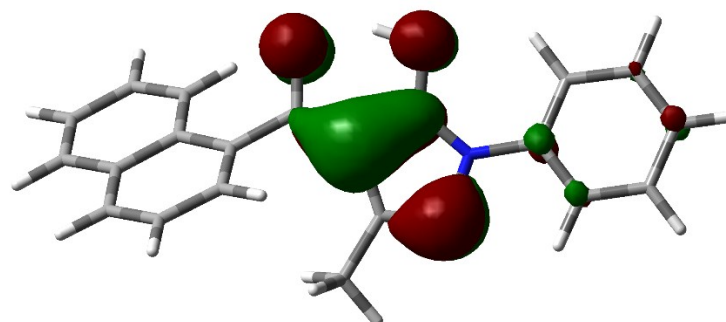
HOMO HQ^{Ph}



HOMO-1 HQ^{Ph}



HOMO-1 HQ^{naph}



HOMO-2 HQ^{naph}

Figure S4. Naphthyl rotation barrier that interconverts the conformers of proligand HQ^{naph}.

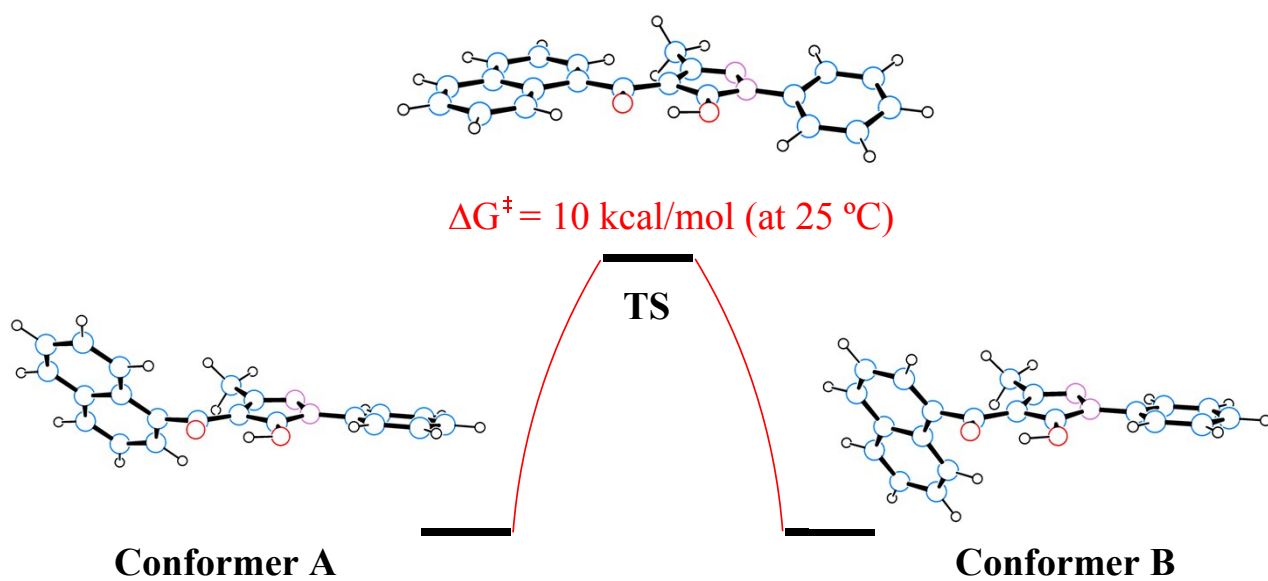
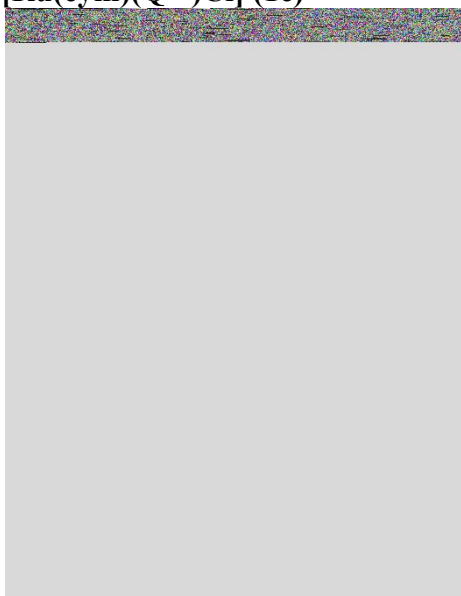


Table S5. Fractional coordinates of the computed compounds

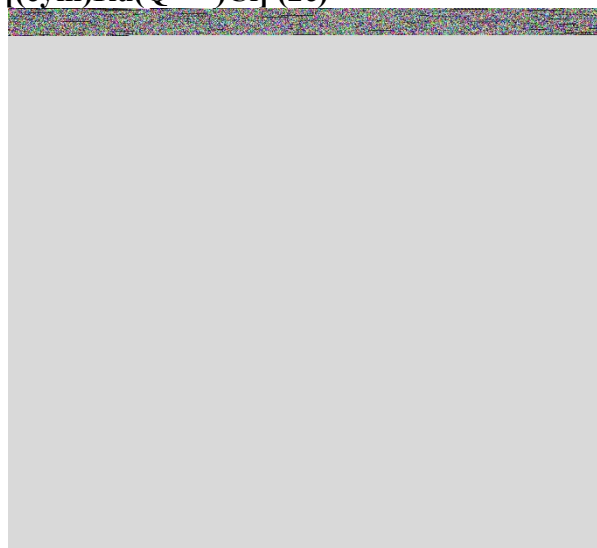
[Ru(cym)(Q^{Ph})Cl] (1c)



Ru	0.49471800	-1.45258200	-0.43195500
Cl	-0.23707400	-0.75468400	-2.64641100
O	-1.20241900	-0.45972700	0.30977500
O	1.50901800	0.38798700	-0.34950800
C	0.75665700	-2.78650300	1.37495500
H	0.41817000	-2.55696400	2.37809500
C	-4.01873100	-0.36833400	1.02385200
H	-3.15702200	-0.98526900	1.23612000
C	1.47909600	-3.22930000	-1.32164900
H	1.72979200	-3.29609300	-2.37457600
C	-5.30976900	-0.84203200	1.25884100
H	-5.43825200	-1.84333800	1.66227200
C	2.05288100	3.58520000	0.84662500
H	1.28252300	3.55290900	1.61167200
N	-2.54612100	1.44768600	0.25372100
C	2.04317500	-2.39139100	0.94957300
C	1.00876100	1.55722500	-0.23623600
C	-1.34218800	0.79855300	0.14526500
C	3.05158000	-1.69733500	1.84820800
H	3.54266100	-0.93898400	1.22476700
C	-4.95737900	1.72593200	0.23260000
H	-4.80384700	2.72170200	-0.16265100
C	-3.84003600	0.92152100	0.50222900
N	-2.41707500	2.80844200	-0.00965800
C	2.38896900	-2.62677300	-0.43084200
H	3.33244300	-2.24897500	-0.81099000
C	4.05243600	3.63168800	-1.10292200
H	4.82662000	3.65238300	-1.86515100
C	4.06275900	4.57156200	-0.06824900
H	4.84721400	5.32230100	-0.02304400
C	3.05353100	2.66112900	-1.15658600
H	3.04314400	1.91747800	-1.94735400
C	2.03515100	2.64331200	-0.19137100
C	0.17098300	-3.65037000	-0.88704700
C	-6.42549400	-0.04870300	0.99046300
H	-7.42698300	-0.42582700	1.17817000
C	-0.16829300	-3.39376100	0.45838000
H	-1.18043500	-3.59457700	0.79465800
C	-0.37088400	1.81971400	-0.12405000

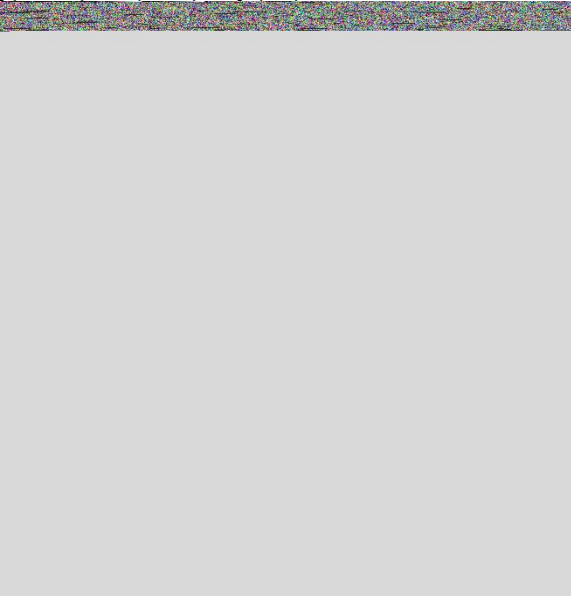
C	-6.23807500	1.23719200	0.47873900
H	-7.09572900	1.86937300	0.26401700
C	-1.14481800	3.03675500	-0.22408700
C	4.12326200	-2.71115200	2.30291300
H	3.68056600	-3.49376300	2.93075000
H	4.89797900	-2.20475100	2.88939800
H	4.60942100	-3.19827300	1.45033200
C	-0.72830200	4.42397400	-0.61440500
H	-1.62667800	5.01232800	-0.81837100
H	-0.10129000	4.40921500	-1.51234400
H	-0.15517500	4.92741600	0.17029600
C	3.06748400	4.54103800	0.91096300
H	3.08103000	5.26015600	1.72551400
C	-0.80532100	-4.23925800	-1.86705000
H	-0.48422100	-5.24403500	-2.16984500
H	-0.86833100	-3.60800500	-2.75947700
H	-1.80504900	-4.31502100	-1.43042300
C	2.42906700	-0.97276300	3.04845600
H	1.65555500	-0.26698200	2.72939800
H	3.20286600	-0.40963400	3.58080500
H	1.98626800	-1.67324400	3.76696300

[(cym)Ru(Q^{naph})Cl] (2c)



Ru	0.59459800	1.60802200	-0.36113300
Cl	0.35527600	0.66787100	-2.60165000
O	1.77544400	-0.07268600	0.07136000
O	-1.10142600	0.47027900	0.11772000
C	-2.57498500	-1.27089100	0.58506800
N	2.02755100	-2.38572900	0.16810600
C	3.43800200	-2.53481900	0.14750500
C	3.99373400	-3.73478500	0.61384800
H	3.33394800	-4.51491600	0.97251100
C	-0.01264900	-3.11961500	0.28787400
C	-4.93531300	-1.56990100	-0.04899200
C	-3.60597400	-1.16232300	-0.40420000
N	1.23169000	-3.52652900	0.25451900
C	-4.18317600	-2.12749100	2.19704200
H	-4.38919500	-2.48870300	3.20079100
C	-2.86653500	-1.74516100	1.84980200
H	-2.07283200	-1.81839400	2.58863400
C	1.27176800	-1.24280100	0.12845500
C	-1.18542100	-0.79321100	0.28179300
C	-0.09418100	-1.67614900	0.22646300
C	4.27224800	-1.51983400	-0.34292800

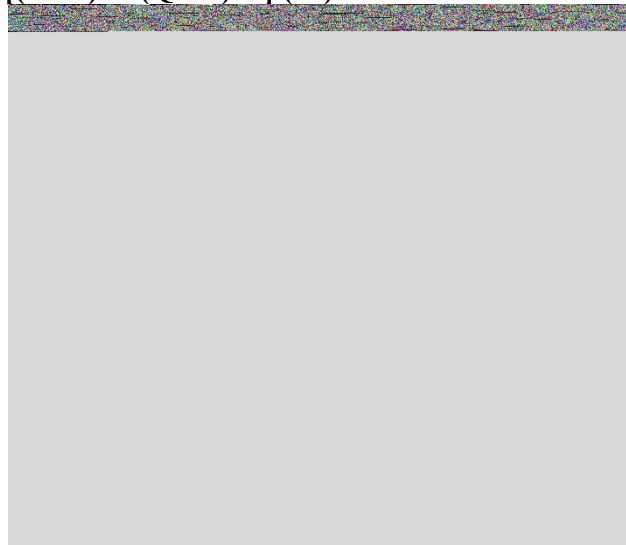
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H	-0.65342200	-5.13670600	0.18652500
H	-1.82825900	-3.97935700	-0.48647100
H	-1.65823100	-4.13580600	1.25928100
C	-3.36155300	-0.69696000	-1.72723800
H	-2.36192900	-0.38218300	-2.01144700
C	-5.96549400	-1.49037600	-1.02503000
H	-6.97023300	-1.80117500	-0.74796900
C	5.65393500	-1.71186200	-0.34830000
H	6.29433700	-0.92255400	-0.73373600
C	5.37557600	-3.91032100	0.59540100
H	5.79627400	-4.84450800	0.95822700
C	6.21521600	-2.90092500	0.11952900
H	7.29249900	-3.04171600	0.10873900
C	-5.19263500	-2.04347900	1.26593300
H	-6.20628400	-2.34153700	1.52371300
C	-4.38588700	-0.63749600	-2.64664700
H	-4.18199800	-0.28248600	-3.65307200
C	-5.69892300	-1.03491400	-2.29588200
H	-6.49432800	-0.98124100	-3.03447300
C	0.27907200	3.65831800	-1.15259800
H	-0.21028600	3.85633000	-2.09983300
C	-0.49895400	3.50765700	0.01152900
H	-1.57829300	3.59601100	-0.05756100
C	-0.22173300	2.02401000	3.56556200
H	0.07297600	1.05012700	3.16130400
H	-0.97146500	1.85378900	4.34549200
H	0.65205200	2.47673800	4.05002900
C	1.48367700	2.87387500	1.28043700
H	1.96080600	2.48769100	2.17293800
C	1.70359000	3.43478900	-1.13348200
C	2.27389400	3.02453900	0.08917500
H	3.32161000	2.74350800	0.11759700
C	2.50751900	3.54607100	-2.39884400
H	2.02872200	2.97379300	-3.19992600
H	3.51996700	3.15755700	-2.25833500
H	2.58123000	4.59505200	-2.71272900
C	0.09350900	3.11618200	1.26777700
C	-1.19106200	4.31233400	3.05195300
H	-1.65546500	4.95344400	2.29450000
H	-0.30771200	4.83386500	3.43951200
H	-1.90331000	4.19410300	3.87603600
C	-0.80778800	2.93189600	2.47667800
H	-1.72243800	2.45329400	2.10258400

[(hmb)Ru(Q^{Ph})Cl] (3c)

Ru	0.32840600	-1.36470300	-0.14042800
Cl	0.48288700	-0.82626700	-2.52225800
N	-1.60522500	3.50555700	-0.03990500
N	-2.08055800	2.19842200	-0.09646400
O	-1.25936400	0.02481000	-0.08351900
O	1.66916900	0.24278300	0.14444100
C	3.52432700	2.36725800	1.11991000
H	3.24822900	1.82029800	2.01728000
C	4.70731700	3.10529900	1.08261800
H	5.35107700	3.13883200	1.95759800
C	5.06730600	3.79360400	-0.07880100
H	5.99302000	4.36194000	-0.10961100
C	4.23896800	3.74359100	-1.20183700
H	4.52240200	4.26415700	-2.11254100
C	3.04455900	3.02259200	-1.16071800
H	2.40284600	2.97048600	-2.03555600
C	2.67787400	2.33559300	0.00394500
C	1.43967600	1.48926800	0.01558300
C	0.15396900	2.05530500	-0.09300300
C	-1.05796700	1.28275500	-0.10642000
C	-3.47861200	1.97071800	-0.05861000
C	-4.03489500	0.79400700	-0.58088000
H	-3.39189700	0.04895500	-1.03024700
C	-5.41625600	0.60598000	-0.52600800
H	-5.84189600	-0.30595800	-0.93694100
C	-6.24992300	1.57746600	0.03070900
H	-7.32495400	1.42386800	0.06570800
C	-5.68817000	2.75343200	0.53304000
H	-6.32511700	3.52244000	0.96230500
C	-4.31006500	2.95500100	0.49368400
H	-3.86447500	3.86646200	0.87302400
C	-0.29707200	3.43093300	-0.04538400
C	0.48299800	4.70918000	0.02539500
H	1.04774800	4.89602000	-0.89373100
H	1.20626300	4.69660300	0.84786100
H	-0.21691000	5.53490300	0.17842300
C	0.82477900	-2.31376900	1.83201000
C	-0.56465000	-2.50370100	1.60218800
C	-1.01797700	-3.07590300	0.34651700
C	-0.07306400	-3.54925700	-0.60359000
C	1.34680500	-3.34686100	-0.37624300
C	1.79095600	-2.75969500	0.84143200

C	1.32479200	-1.60008900	3.06863000
H	0.56449400	-0.94405700	3.49278300
H	2.18839600	-0.97593200	2.83287900
H	1.62815800	-2.31598700	3.84483000
C	-1.60605600	-2.05534100	2.60453900
H	-1.18948600	-1.93546600	3.60486500
H	-2.40914700	-2.79497700	2.67439900
H	-2.05774900	-1.10371100	2.30103100
C	-2.50237500	-3.12562100	0.06118900
H	-2.70149000	-3.15043500	-1.01008800
H	-3.00323300	-2.23996100	0.45647100
H	-2.96573200	-4.01194400	0.51630300
C	-0.51994100	-4.20149800	-1.89258300
H	0.17315900	-4.99732200	-2.17774200
H	-0.54409800	-3.46762100	-2.70720100
H	-1.50923900	-4.65098400	-1.79508100
C	2.31139000	-3.73052400	-1.47490400
H	1.90934400	-3.44338800	-2.44839600
H	2.49362500	-4.81409000	-1.47597700
H	3.27053700	-3.22446700	-1.37271600
C	3.26179200	-2.52353300	1.11111300
H	3.49488900	-2.71089400	2.16301100
H	3.53583900	-1.48671100	0.88156500
H	3.89560500	-3.18331500	0.51878300

[(hmb)Ru(Q^{naph})Cl] (4c)



Ru	-0.58560800	-1.42704300	-0.01596100
Cl	-0.21469000	-0.88574700	-2.37747100
O	-1.63614100	0.39845200	0.10555300
O	1.19650200	-0.35408300	0.34414100
C	2.78664100	1.32155600	0.64351900
N	-1.69159200	2.71039000	-0.14580000
C	-3.08272100	2.94929500	-0.27162100
C	-3.59614600	4.18625400	0.14009600
H	-2.91768700	4.93018300	0.54025900
C	0.39277800	3.29711200	-0.02202100
C	5.19057200	1.31835100	0.10785300
C	3.84683500	0.96738000	-0.25370000
N	-0.81192800	3.78988200	-0.17548400
C	4.39361000	2.30191800	2.18581900
H	4.58681900	2.80748000	3.12790700
C	3.06456300	1.97489600	1.82922300
H	2.24883700	2.23379500	2.49908600
C	-1.03407000	1.51918200	0.01986600

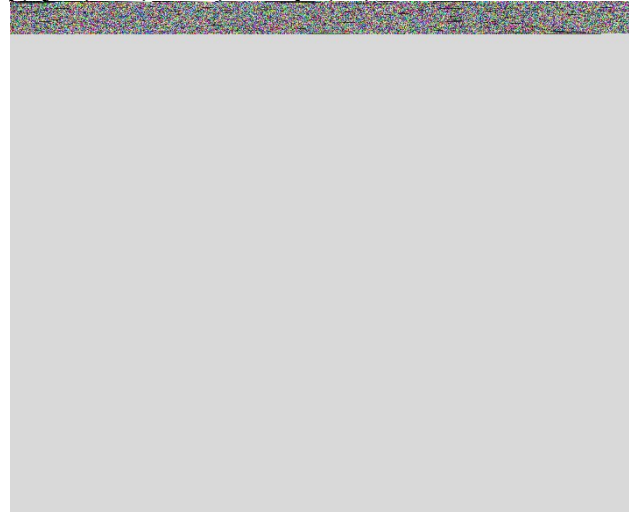
C	1.37524400	0.90912900	0.34412900
C	0.35831300	1.85686700	0.12389200
C	-3.93510800	1.98130000	-0.82115400
H	-3.52673500	1.04078100	-1.16714000
C	1.55985700	4.23603000	-0.08722700
H	1.19629400	5.22377300	-0.38257000
H	2.30181700	3.89720000	-0.81839600
H	2.07525900	4.32462200	0.87457600
C	3.62058800	0.31142700	-1.49692800
H	2.60999200	0.03872700	-1.78521700
C	6.25192400	0.99252500	-0.77974200
H	7.26734700	1.26155200	-0.49788500
C	-5.29872900	2.25374200	-0.93303500
H	-5.95472000	1.50229600	-1.36500500
C	-4.95955600	4.44489500	0.01330100
H	-5.35019200	5.40726500	0.33346500
C	-5.81961500	3.48024600	-0.51642300
H	-6.88237800	3.68544300	-0.61105300
C	5.43146700	1.98194100	1.34116100
H	6.45552200	2.23511800	1.60575400
C	4.67536800	0.01496800	-2.33228000
H	4.48498600	-0.48308600	-3.27901400
C	6.00233300	0.35457300	-1.97313800
H	6.82186800	0.11292500	-2.64475200
C	-0.48079100	-3.64876500	-0.44543900
C	0.34433100	-3.33683100	0.66930600
C	-1.57989900	-2.25483300	1.81631700
C	-1.86737500	-3.21272400	-0.46597300
C	-2.41646200	-2.54457300	0.66306500
C	-2.66886500	-3.44246900	-1.72667200
H	-2.05992000	-3.22809200	-2.60706600
H	-3.53985600	-2.79098800	-1.78406800
H	-3.01575500	-4.48322000	-1.78597000
C	-0.22513600	-2.68327900	1.83419100
C	0.67656500	-2.40989500	3.01907300
H	1.34613500	-3.25710600	3.19155500
H	1.30065900	-1.52634800	2.84328400
H	0.10904400	-2.25351300	3.93695100
C	1.82814200	-3.62839300	0.65693000
H	2.38492800	-2.79897400	1.09821000
H	2.06010100	-4.53959800	1.22504700
H	2.20578000	-3.75447000	-0.35712500
C	0.06932100	-4.37403400	-1.65340400
H	0.33790000	-3.65942300	-2.44084900
H	0.94933600	-4.96791800	-1.40334200
H	-0.67962200	-5.05845100	-2.06098300
C	-3.85217100	-2.06586900	0.68895600
H	-3.90809100	-0.98379000	0.52272400
H	-4.46469800	-2.56013100	-0.06439400
H	-4.30419000	-2.27680200	1.66300200
C	-2.16852600	-1.44896200	2.95266400
H	-2.81550200	-0.65763800	2.56899600
H	-2.76771000	-2.08358000	3.61978900
H	-1.39699500	-0.96505100	3.55129900

[(cym)Ru(Q^{Ph})PTA]⁺ (5c), cation of 5

Ru	0.06128800	-0.80716400	1.14585700
P	-1.03786200	-1.76632500	-0.69691400
O	1.19215800	0.27065300	-0.26102900
O	-1.43467900	0.66695800	0.98091500
N	1.51623900	3.70817100	-0.85004600
N	1.95745300	2.38870600	-0.86017300
N	-3.44718900	-2.37933900	-1.91463600
N	-1.61827000	-1.64817300	-3.40053300
N	-1.55991800	-3.89722300	-2.38759600
C	-2.60117000	2.62521800	0.49497800
C	3.29865900	2.11625700	-1.25558300
C	0.28280300	3.70045800	-0.41155300
C	1.00723300	1.53893100	-0.37834200
C	-3.08351700	3.24208300	-0.67005700
H	-2.50538000	3.18485600	-1.58763100
C	-3.37194200	2.67028700	1.66799400
C	-1.33415300	1.84285600	0.46778300
C	-0.14366600	2.34934500	-0.09091500
C	-3.05739000	-1.58662700	-3.09350500
H	-3.60501500	-1.97461700	-3.95811700
H	-3.35137100	-0.54335200	-2.94064000
C	-4.58549500	3.35355600	1.68423700
C	-0.74933800	-3.55343400	-1.21701900
H	0.31291300	-3.69907100	-1.44628600
H	-1.00368500	-4.22463700	-0.38751800
C	3.67232700	0.85127600	-1.72816900
H	2.93707600	0.06166000	-1.80654000
C	-0.41962200	5.01369200	-0.23783700
H	0.31109600	5.81676000	-0.35979100
H	-0.87609900	5.09502100	0.75417900
H	-1.21687300	5.15950000	-0.97273300
C	4.99662800	0.62554800	-2.10740400
H	5.28154000	-0.35411500	-2.48139500
C	4.24173800	3.14948100	-1.18141000
H	3.93115700	4.12674500	-0.83335100
C	-0.29210800	-2.55023800	2.56070300
H	-1.04487800	-3.32394800	2.44836500
C	0.99591700	-2.72680400	1.95369800
H	1.18838600	-3.62815600	1.38474500
C	5.94408400	1.64703500	-2.03011400
H	6.97093100	1.46559800	-2.33312700

C	5.55769400	2.90809500	-1.57037100
H	6.28394100	3.71362600	-1.51272500
C	-4.31149800	3.90322000	-0.65714800
H	-4.68386300	4.36754200	-1.56553700
C	-2.91876600	-1.80839300	-0.67432400
H	-3.25789300	-2.40331300	0.18188400
H	-3.29302900	-0.78947300	-0.53326300
C	-5.05862700	3.96820400	0.52107100
H	-6.00938200	4.49308000	0.53300300
C	1.98666800	-1.72635300	2.04210500
C	-0.81203800	-0.96687300	-2.38545200
H	-1.10067200	0.08802000	-2.32508800
H	0.24696600	-0.99957800	-2.66057700
C	1.67618500	-0.55190100	2.82190100
H	2.41057600	0.24508400	2.88419400
C	-3.00226000	-3.76842400	-2.11312800
H	-3.54556100	-4.17988500	-2.96942600
H	-3.25756900	-4.36123100	-1.22856000
C	-1.22683500	-3.05835500	-3.55347200
H	-0.15086700	-3.11735200	-3.74651500
H	-1.75401300	-3.46573800	-4.42169300
C	-0.61091200	-1.37455200	3.27263000
C	-1.96648000	-1.15304000	3.88606700
H	-2.68317600	-1.90854400	3.55348200
H	-2.35761700	-0.16753200	3.61523600
H	-1.90129200	-1.20379900	4.97977200
C	0.42474300	-0.38174900	3.41668100
H	0.19952500	0.54466800	3.93625100
C	3.36351400	-1.84134000	1.40999800
H	3.60023200	-0.84880200	1.00602000
C	3.44630000	-2.84398000	0.25245600
H	2.70729500	-2.62428200	-0.52569100
H	3.30551200	-3.87778300	0.59034500
H	4.43844300	-2.78944000	-0.20592700
C	4.40201900	-2.17563500	2.50458900
H	5.40759900	-2.18314600	2.07210700
H	4.21203700	-3.16412800	2.93868100
H	4.39302600	-1.44134200	3.31730800
H	-5.16560300	3.40411900	2.60100400
H	-3.00536600	2.18412500	2.56684700

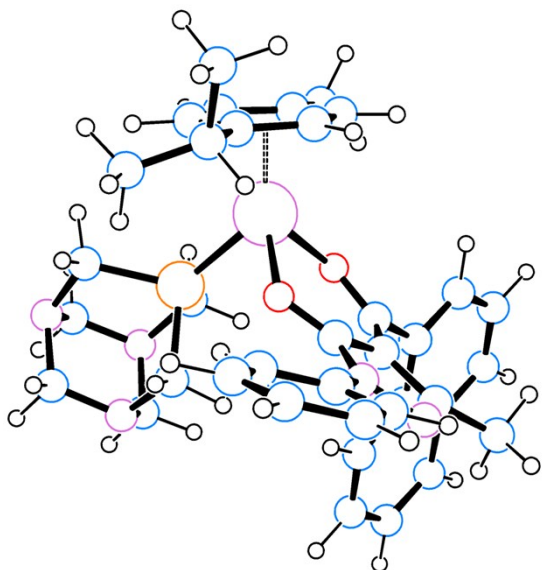
[(cym)Ru(Q^{naph})PTA]⁺ (6c), cation of 6



Ru	-0.51009200	0.65030300	1.18024900
P	-0.41976300	2.19574200	-0.58721400
O	-1.41743800	-0.68018700	-0.17685800
O	1.36409800	0.04594600	0.44296500
N	-0.37678400	-3.66052200	-1.69742500
N	-1.32790700	-2.75116500	-1.23885000
N	1.15290400	3.88899000	-2.11665900
N	-0.65520300	2.69689600	-3.29976300
N	-1.19548800	4.56716100	-1.78661400
C	3.08480700	-1.06637700	-0.68075900
C	-2.70592900	-3.10428300	-1.31162000
C	0.79975100	-3.13490900	-1.47163300
C	-0.74543800	-1.65148800	-0.68413800
C	3.44131300	-0.91910600	-2.01097600
H	2.66486600	-0.80639500	-2.76298500
C	4.09521100	-1.22290700	0.32401300
C	1.63780400	-0.95098600	-0.32273800
C	0.67309300	-1.83972000	-0.82622600
C	3.80330900	-1.43501200	1.69957700
H	2.76707400	-1.47574600	2.01899800
C	0.73656600	3.17793700	-3.33761900
H	0.83331100	3.86794000	-4.18165600
H	1.40774400	2.33015700	-3.50765200
C	5.46972300	-1.21116800	-0.08642100
C	-1.45771400	3.76943900	-0.58837500
H	-2.52059500	3.50372800	-0.54913500
H	-1.23020100	4.36431400	0.30454300
C	-3.70477900	-2.12241800	-1.34319900
H	-3.43688900	-1.07437700	-1.32112100
C	2.02251000	-3.92011700	-1.83664400
H	1.71541200	-4.92345600	-2.14120600
H	2.71385900	-4.00023700	-0.99109900
H	2.57463700	-3.45963600	-2.66183300
C	-5.04387500	-2.50995200	-1.41403700
H	-5.81644800	-1.74651500	-1.44656600
C	-3.04685800	-4.46170900	-1.36882900
H	-2.26077000	-5.20662100	-1.36415400
C	6.48697400	-1.38204600	0.89184600
H	7.52502200	-1.36821900	0.57008000
C	-0.58764900	2.21963200	2.81598900

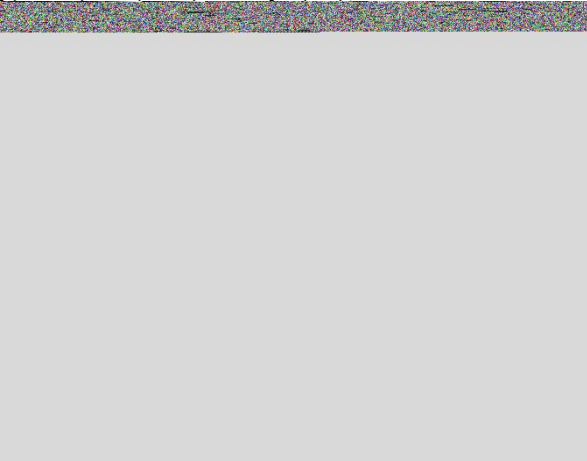
H	-0.30296200	3.26176800	2.71215000
C	-1.93590900	1.82538400	2.52277800
H	-2.64343600	2.57644800	2.19342100
C	-5.39288300	-3.86011400	-1.46363400
H	-6.43653000	-4.15389100	-1.52428900
C	-4.38829000	-4.83039800	-1.44566600
H	-4.64709600	-5.88423500	-1.49139000
C	4.79814300	-0.89733400	-2.40472300
H	5.05041000	-0.76885300	-3.45290900
C	1.24651300	2.98620300	-0.96704500
H	1.59364700	3.53934000	-0.08637100
H	1.97690100	2.19465800	-1.16242500
C	5.78876000	-1.03741100	-1.46009000
H	6.83487200	-1.02290000	-1.75461800
C	-2.32995000	0.47291500	2.59833800
C	6.17018700	-1.57152700	2.21711800
H	6.95618200	-1.70575800	2.95422000
C	-0.83657400	1.61548400	-2.32876700
H	-0.19331500	0.76758000	-2.58755700
H	-1.87132500	1.25865100	-2.35261800
C	4.81380800	-1.60547100	2.62082800
H	4.57123300	-1.77714500	3.66600100
C	-1.34785400	-0.48151600	3.05537200
H	-1.61816800	-1.53178800	3.10069900
C	0.21223300	4.99341800	-1.86992000
H	0.29941100	5.70550000	-2.69645200
H	0.49062600	5.50778500	-0.94422100
C	-1.54130800	3.83780900	-3.01904700
H	-2.57614700	3.48639900	-2.95420700
H	-1.46959600	4.53894400	-3.85639200
C	0.38692600	1.27450300	3.20409000
C	1.81255400	1.66426700	3.48618800
H	2.02332500	2.67861800	3.13668900
H	2.51167100	0.97962300	2.99577100
H	2.00602000	1.63172600	4.56565100
C	-0.03976500	-0.09457100	3.35095200
H	0.69206300	-0.84773200	3.62625900
C	-3.72904900	-0.01894300	2.26840100
H	-3.60025100	-0.95031000	1.70233200
C	-4.54525100	0.94330000	1.39668300
H	-4.01318300	1.20121000	0.47434700
H	-4.79728400	1.86865300	1.92863700
H	-5.48964400	0.46786300	1.11497400
C	-4.47926700	-0.34956600	3.57832800
H	-5.46006500	-0.77723100	3.34707700
H	-4.63592900	0.55307600	4.18017500
H	-3.93497400	-1.07543300	4.19203400

[(cym)Ru(Q^{naph})PTA]⁺ (i6c), Isomer cation of 6



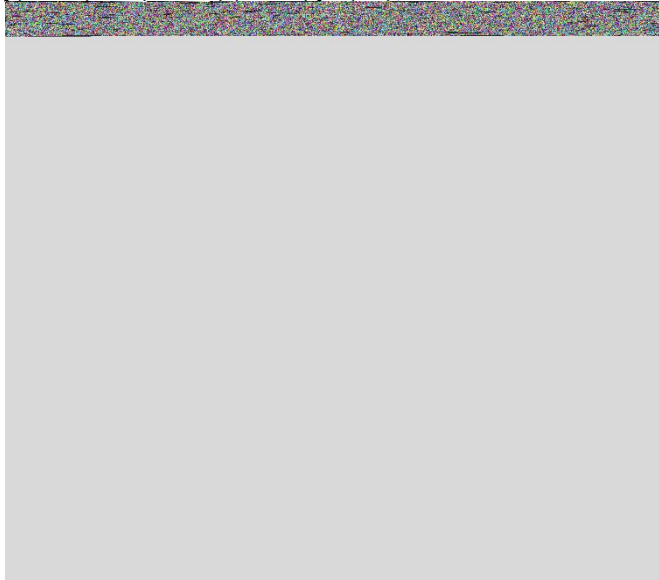
Ru	0.97353400	-0.89743700	1.10735100
P	0.13688500	-2.04541100	-0.77202600
O	1.34386300	0.72007400	-0.18803100
O	-1.00698400	-0.21599400	1.29905100
N	-0.03234600	3.93060600	-0.48411700
N	0.96986600	2.97496700	-0.64549100
N	-1.97846300	-3.44776400	-1.88129300
N	-0.75790000	-1.92524000	-3.39060900
N	0.27557800	-4.04949000	-2.68049000
C	-2.95058900	1.06382800	1.29631100
C	2.22062100	3.38128600	-1.19298300
C	-1.05268800	3.32959100	0.07138400
C	0.58887100	1.76056200	-0.15831400
C	-3.30154600	1.01753700	2.63493500
H	-2.52154000	0.94332300	3.38753100
C	-3.96648600	1.13885100	0.28609100
C	-1.50097600	0.91903300	0.94833100
C	-0.75632900	1.93038900	0.32048700
C	-3.69269700	1.15185600	-1.11103600
H	-2.66217800	1.14914200	-1.45142100
C	-2.06508200	-2.46272400	-2.97277500
H	-2.51877900	-2.95586600	-3.83818700
H	-2.71576400	-1.63857900	-2.66386800
C	-5.33888800	1.17839100	0.70704700
C	1.02670500	-3.52133000	-1.54079700
H	2.02615500	-3.21221900	-1.86870000
H	1.15246000	-4.30966200	-0.78882200
C	3.08538500	2.45744100	-1.79499400
H	2.80712700	1.41398200	-1.85760400
C	-2.28215000	4.12430900	0.38569500
H	-2.07836700	5.17956500	0.18945200
H	-2.57792200	4.00723100	1.43357100
H	-3.13191800	3.81259700	-0.23005700
C	4.30047500	2.89896300	-2.32134900
H	4.96549700	2.18128900	-2.79407500
C	2.56623000	4.73775400	-1.13522800
H	1.87794400	5.44145600	-0.68400500
C	-6.36570900	1.22834700	-0.27534400

H	-7.40002100	1.25867500	0.05723800
C	1.57050400	-2.75937200	2.25642000
H	1.20027500	-3.76432800	2.08136900
C	2.72393300	-2.29761600	1.53729200
H	3.19680000	-2.95877800	0.82141700
C	4.65530100	4.24711800	-2.26246700
H	5.59977200	4.58372500	-2.67938100
C	3.78025500	5.16143100	-1.67159300
H	4.04131700	6.21470700	-1.62553600
C	-4.65206200	1.08781900	3.03954600
H	-4.89728700	1.07635100	4.09717500
C	-1.56962400	-2.82789000	-0.62000800
H	-1.55403200	-3.58242100	0.17546800
H	-2.28737900	-2.05622100	-0.32541200
C	-5.64821200	1.16251500	2.09286900
H	-6.69141800	1.20621200	2.39469800
C	3.20764000	-0.98303900	1.70438500
C	-6.06468000	1.23788300	-1.61752700
H	-6.85860200	1.27745700	-2.35721000
C	-0.15724000	-1.07701700	-2.35911400
H	-0.81495600	-0.22887100	-2.14427500
H	0.79444400	-0.66857300	-2.71442400
C	-4.71311700	1.20172000	-2.03632700
H	-4.47868800	1.22200900	-3.09699600
C	2.53848600	-0.14704200	2.67250700
H	2.87172500	0.87840100	2.79796500
C	-1.06233400	-4.52498500	-2.28599500
H	-1.50237500	-5.04130600	-3.14478000
H	-0.96396300	-5.24491400	-1.46682700
C	0.12159800	-3.04823000	-3.75136900
H	1.10722900	-2.66220100	-4.03082900
H	-0.30922800	-3.55184800	-4.62224800
C	0.88554400	-1.91892200	3.16055200
C	-0.35180600	-2.36527600	3.89056800
H	-0.70736900	-3.33031400	3.51976400
H	-1.15716300	-1.63398600	3.76832700
H	-0.14419500	-2.46861600	4.96252000
C	1.42185600	-0.59817300	3.37840900
H	0.90025100	0.07931000	4.04762700
C	4.40633200	-0.42108700	0.95838900
H	4.13333500	0.60049600	0.66357400
C	4.77150300	-1.19028800	-0.31699600
H	3.91811600	-1.26799300	-0.99970800
H	5.14010500	-2.19976800	-0.09832100
H	5.57314300	-0.66374600	-0.84377000
C	5.61513100	-0.33766700	1.91776100
H	6.46174200	0.13329600	1.40803800
H	5.92843000	-1.33617300	2.24395900
H	5.39140500	0.25558600	2.81096200

[(hmb)Ru(Q^{Ph})PTA]⁺ (7c), cation of 7

Ru	-0.24878300	-0.87463100	0.93185600
P	-1.65422300	-1.03121200	-0.97043600
O	1.29314000	-0.37588700	-0.43008300
O	-0.85799400	1.15248500	0.84978000
N	3.22951600	2.52021600	-0.79732000
N	2.98938800	1.15383500	-0.89794000
N	-4.07060400	-0.34032300	-2.15100300
N	-2.07304500	-0.21026500	-3.59168500
N	-3.00444800	-2.40711800	-2.97386900
C	-0.95200100	3.45158100	0.46362400
C	4.04650000	0.30111300	-1.32730100
C	2.12901000	3.07478900	-0.35509500
C	1.73536200	0.83072800	-0.46528300
C	-1.02834100	4.28293500	-0.66520800
H	-0.49800100	4.00816300	-1.57221500
C	-1.67349600	3.79395500	1.61866700
C	-0.20243200	2.16508100	0.40534300
C	1.10303600	2.07438900	-0.12079600
C	-3.35292100	0.40332400	-3.20025400
H	-3.99465300	0.44341900	-4.08617600
H	-3.17413800	1.42769700	-2.85818000
C	-2.42506400	4.96600100	1.65678100
C	-2.14685700	-2.64962000	-1.81113800
H	-1.24318600	-3.18223500	-2.13076300
H	-2.67629700	-3.29320800	-1.09956400
C	3.78417300	-0.96919900	-1.85903000
H	2.76446500	-1.31647100	-1.95743400
C	2.13195800	4.55127000	-0.09223000
H	3.16269900	4.91052100	-0.14059500
H	1.71894500	4.78360600	0.89482900
H	1.54140600	5.10587400	-0.82762800
C	4.84873500	-1.77295700	-2.27068100
H	4.64105200	-2.75422200	-2.68857700
C	5.36503700	0.76505500	-1.22706500
H	5.54934700	1.75730600	-0.83462500
C	-1.41715500	-2.24105600	2.34648300
C	-0.40556000	-3.06026700	1.70855500
C	6.16484200	-1.32109100	-2.16810400
H	6.98707200	-1.94990800	-2.49618700
C	6.41440900	-0.04842000	-1.64952600
H	7.43374600	0.31848700	-1.57179700
C	-1.80227700	5.44290500	-0.63267900

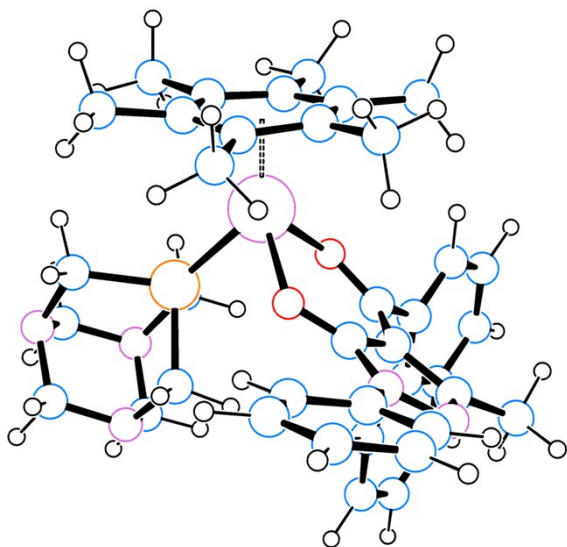
H	-1.86573800	6.07393800	-1.51429900
C	-3.37528000	-0.27197000	-0.86411900
H	-3.96074800	-0.79754700	-0.10101300
H	-3.27573700	0.77014600	-0.54302700
C	-2.49319000	5.79082900	0.53004400
H	-3.08698200	6.69980500	0.55775300
C	0.95082200	-2.64132900	1.72597100
C	-1.07715200	-0.12939900	-2.52128800
H	-0.88104500	0.91939500	-2.27475000
H	-0.13124100	-0.56789400	-2.85466800
C	1.36234700	-1.50862600	2.53458800
C	-4.25724100	-1.72900600	-2.60035900
H	-4.90838800	-1.71692700	-3.48008300
H	-4.75760900	-2.30139400	-1.81209100
C	-2.32171400	-1.60078100	-4.00079800
H	-1.37154700	-2.07762900	-4.26243900
H	-2.95529200	-1.58642400	-4.89324600
C	-1.02342100	-1.07816700	3.06809100
C	-2.03659100	-0.21088900	3.78442100
H	-3.00194300	-0.70218200	3.89541100
H	-2.19435500	0.73236000	3.24878400
H	-1.68418900	0.03096100	4.79130500
C	0.38361000	-0.71845900	3.17372400
H	-2.96181700	5.23537000	2.56173700
H	-1.62767300	3.14624300	2.48867700
C	-2.87456000	-2.64756300	2.27218400
H	-3.13592300	-3.31149500	3.10683400
H	-3.53973900	-1.78511000	2.31281900
H	-3.10044200	-3.18054900	1.34747600
C	-0.75398200	-4.39661200	1.07972900
H	-0.08071800	-5.16821400	1.46746600
H	-1.76917600	-4.71163000	1.31835400
H	-0.64965900	-4.39622300	-0.00864500
C	2.00430000	-3.42285600	0.97614600
H	2.54695900	-4.09370700	1.65560800
H	1.56905400	-4.03425300	0.18568400
H	2.73195200	-2.75499800	0.51048600
C	2.83826600	-1.19617300	2.61617300
H	3.40255500	-2.10959100	2.82868900
H	3.21449300	-0.79932300	1.66627000
H	3.07149200	-0.48080300	3.40333100
C	0.75912900	0.53053400	3.93907800
H	0.87066900	0.31101400	5.00916800
H	1.69590200	0.96087300	3.58604500
H	-0.00639500	1.30117300	3.83941100

[(hmb)Ru(Q^{naph})(PTA)]⁺ (8c), cation of 8

Ru	-0.62950600	0.74843800	1.03555400
P	-0.35297900	2.10714700	-0.87997500
O	-1.60663300	-0.64108000	-0.22511600
O	1.22164900	-0.04567200	0.36095300
N	-0.74414800	-3.78423300	-1.51184800
N	-1.64092500	-2.79261900	-1.12021000
N	1.45009900	3.52716300	-2.44809800
N	-0.22278200	2.17191700	-3.65537700
N	-0.90105700	4.26258200	-2.54416000
C	2.85303600	-1.29730200	-0.77242200
C	-3.03642400	-3.07375600	-1.16169700
C	0.46079700	-3.30593000	-1.33462400
C	-0.99431500	-1.68542900	-0.65283300
C	3.14004500	-1.25272700	-2.12755500
H	2.32756000	-1.16021100	-2.84338300
C	3.91442500	-1.43858600	0.18047500
C	1.42938000	-1.09272100	-0.35598800
C	0.41023100	-1.96240000	-0.78539300
C	3.69355400	-1.55831900	1.57925600
H	2.67728300	-1.52876200	1.95432300
C	1.17570700	2.62860700	-3.58259400
H	1.40314000	3.16994900	-4.50640000
H	1.83757800	1.75900800	-3.52003900
C	5.26226800	-1.51580300	-0.30493600
C	-1.33697700	3.67166000	-1.27822000
H	-2.40432000	3.42805600	-1.33604500
H	-1.20351100	4.40578000	-0.47573200
C	-3.98303900	-2.04274200	-1.23704400
H	-3.65982700	-1.01097300	-1.27394900
C	1.63690400	-4.18064500	-1.64672900
H	1.27548900	-5.18885600	-1.86287500
H	2.33727600	-4.22518600	-0.80596000
H	2.19815500	-3.81894700	-2.51401500
C	-5.34171500	-2.36141400	-1.27424600
H	-6.07271400	-1.56006100	-1.33881800
C	-3.45074800	-4.41205500	-1.14214100
H	-2.70556100	-5.19694000	-1.10501400
C	6.32560900	-1.67877400	0.62446300
H	7.34298400	-1.73278200	0.24582600
C	-0.58398100	2.39867300	2.61858100
C	-1.98081100	2.13743900	2.33826300
C	-5.76286600	-3.69138800	-1.24795600

H	-6.82135300	-3.93135500	-1.28265100
C	-4.81076400	-4.71157200	-1.18702800
H	-5.12559600	-5.75101300	-1.17362400
C	4.47142400	-1.31545600	-2.59676900
H	4.66650800	-1.26603800	-3.66375900
C	1.36688900	2.82216100	-1.16704900
H	1.61381800	3.51146400	-0.35096600
H	2.09295200	2.00415100	-1.13624400
C	5.50905200	-1.44028500	-1.70191500
H	6.53599000	-1.49195100	-2.05409400
C	-2.46480000	0.80285300	2.37700100
C	6.07736300	-1.77933200	1.97395100
H	6.89771600	-1.91010800	2.67331000
C	-0.56428800	1.26774400	-2.55518700
H	0.07173300	0.37779100	-2.59414500
H	-1.60082600	0.93007200	-2.65735300
C	4.74624700	-1.72609900	2.45231500
H	4.55676800	-1.82780700	3.51757200
C	-1.63837700	-0.25168400	2.93816300
C	0.51644800	4.66155500	-2.50863700
H	0.72823000	5.22972400	-3.41991100
H	0.68699100	5.31780500	-1.64871600
C	-1.10347000	3.34823600	-3.68159700
H	-2.14774800	3.02007700	-3.70163800
H	-0.90150500	3.90635900	-4.60126300
C	0.26597900	1.33347300	3.03677700
C	1.72745100	1.56556700	3.34943900
H	2.05508200	2.57207400	3.09643800
H	2.36533800	0.86568600	2.80197300
H	1.91236200	1.42647700	4.42157500
C	-0.29718300	0.01261400	3.27469700
C	-3.87286800	0.46265800	1.94523300
H	-3.90771800	-0.51689700	1.46635000
H	-4.55226400	0.44291800	2.80778200
H	-4.26323600	1.18250100	1.22557600
C	-2.24412700	-1.62433700	3.11166100
H	-3.20480900	-1.55371400	3.63223600
H	-2.43718000	-2.09461300	2.14078700
H	-1.60461700	-2.29117000	3.68797600
C	0.55843100	-1.08952400	3.86320400
H	0.18032500	-1.36553700	4.85530200
H	0.54198400	-1.99151100	3.24518400
H	1.59670900	-0.78864700	3.98517700
C	-0.06977400	3.82178400	2.54265400
H	-0.04578100	4.26850800	3.54543500
H	0.94145000	3.87719300	2.13787600
H	-0.70533200	4.45370200	1.92198900
C	-2.92028600	3.29929400	2.08107700
H	-2.79005900	4.04879400	2.86934300
H	-2.74756300	3.80133700	1.12583300
H	-3.96397400	2.98929700	2.10722400

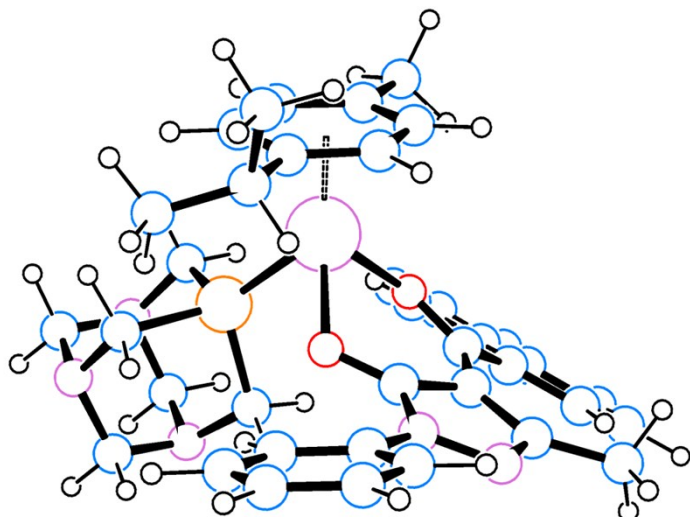
[(hmb)Ru(Q^{naph})(PTA)]⁺ (i8c), Isomer cation of 8



Ru	1.13966800	-0.84118200	0.81914100
P	0.18946400	-1.95033000	-1.05209700
O	1.33484800	0.85116300	-0.43984900
O	-0.86863400	-0.26031500	1.14977200
N	-0.18643400	4.00987300	-0.46622800
N	0.83681100	3.10801400	-0.75110200
N	-2.03741800	-3.25240500	-2.08691000
N	-0.88889800	-1.67844200	-3.60028900
N	0.13823200	-3.85620700	-3.07625300
C	-2.86501600	0.92609600	1.33254200
C	2.03341700	3.59727900	-1.34886900
C	-1.14193100	3.33557800	0.12053300
C	0.53953300	1.85141800	-0.30783600
C	-3.12709200	0.77089700	2.68349000
H	-2.29695300	0.67429800	3.37728600
C	-3.94816000	1.03555100	0.39764900
C	-1.43502700	0.86336400	0.88884600
C	-0.77570000	1.93881100	0.26778300
C	-3.76918600	1.16077700	-1.00935400
H	-2.76422400	1.21830200	-1.41424900
C	-2.17573400	-2.20913800	-3.11682600
H	-2.70397300	-2.64462600	-3.97100600
H	-2.78157300	-1.38900700	-2.71895200
C	-5.29037500	0.99309500	0.90743500
C	0.97867100	-3.40283900	-1.96623400
H	1.95973200	-3.10216100	-2.35213000
H	1.13311600	-4.23562700	-1.27074300
C	2.88250000	2.75037400	-2.07420600
H	2.63213800	1.70494400	-2.19615300
C	-2.37496500	4.06093800	0.56384600
H	-2.21746700	5.13416800	0.43312400
H	-2.60284300	3.85904100	1.61573500
H	-3.25045600	3.76372900	-0.02231100
C	4.04484300	3.27161500	-2.64511400
H	4.69806300	2.61397400	-3.21208500
C	2.34062900	4.95772200	-1.21378000
H	1.66263400	5.60217200	-0.66813500
C	-6.38169000	1.07822000	-0.00021000
H	-7.39185900	1.04588900	0.39962900
C	1.93366300	-2.67657900	1.94592500
C	3.03046600	-2.14437000	1.16174300
C	4.36127500	4.62394100	-2.51000900
H	5.26438700	5.02273400	-2.96225100

C	3.50119800	5.46209300	-1.79678800
H	3.73226600	6.51806800	-1.69073500
C	-4.44891600	0.75991500	3.17793400
H	-4.62292200	0.66319000	4.24532300
C	-1.52234400	-2.71115200	-0.82751000
H	-1.46941000	-3.51054100	-0.07884800
H	-2.20021000	-1.94581000	-0.43875900
C	-5.50742700	0.86483300	2.30470500
H	-6.52950500	0.84766200	2.67391900
C	3.36112600	-0.76514700	1.26831600
C	-6.17149700	1.19944500	-1.35405000
H	-7.01384800	1.26569900	-2.03603100
C	-0.19654600	-0.90061400	-2.57049200
H	-0.81585200	-0.05044800	-2.26802100
H	0.73776000	-0.49436000	-2.97192400
C	-4.85037700	1.24330400	-1.86029900
H	-4.68810100	1.35054600	-2.92918500
C	2.75040500	0.05074700	2.30370200
C	-1.17976000	-4.32421900	-2.61262700
H	-1.69115600	-4.78433100	-3.46410400
H	-1.04142500	-5.09028300	-1.84232300
C	-0.06559600	-2.79797700	-4.08046600
H	0.90738500	-2.41822200	-4.40907500
H	-0.56785500	-3.24631000	-4.94351900
C	1.23785300	-1.83439400	2.85912000
C	0.07832800	-2.35277200	3.68058500
H	-0.12294800	-3.40680800	3.49923400
H	-0.83698800	-1.79553100	3.45568100
H	0.28892500	-2.24238500	4.75025700
C	1.68695900	-0.46748900	3.06980000
C	4.40031700	-0.12690700	0.37444800
H	4.13415400	0.90586200	0.14512000
H	5.38692500	-0.12697900	0.85635900
H	4.49045700	-0.64747900	-0.57912900
C	3.24416900	1.46550600	2.50005900
H	4.33699800	1.49449600	2.46612500
H	2.87838000	2.13281800	1.71094400
H	2.93537500	1.87577600	3.46124800
C	0.98855000	0.40998400	4.08572800
H	1.59978300	0.50243100	4.99300100
H	0.81835900	1.41655500	3.69731000
H	0.02287900	0.00501200	4.38391100
C	1.57415300	-4.14538100	1.83912300
H	1.93093500	-4.68469300	2.72605400
H	0.49556300	-4.30196400	1.77461200
H	2.02801300	-4.61951300	0.96982600
C	3.85168400	-3.08400700	0.30267300
H	4.27687900	-3.87025100	0.93786700
H	3.26478900	-3.57753900	-0.47497400
H	4.68616000	-2.57925100	-0.18047800

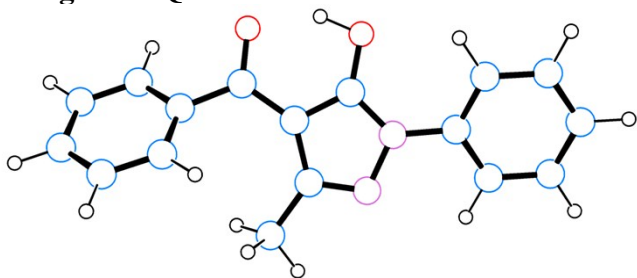
Transition state of the naphthyl rotation in [(cym)Ru(Q^{naph})PTA]⁺ (6c)



Ru	0.41973100	-0.56476600	1.21164400
P	-0.34857000	-2.03324000	-0.48629600
O	1.30647600	0.35578200	-0.43622800
O	-1.18767100	0.67128500	0.69181000
N	1.67755500	3.74214200	-1.12187000
N	2.08162800	2.43109900	-1.07634600
N	-1.98289300	-4.07940900	-1.39844600
N	-1.49198200	-2.26844600	-3.00055000
N	0.24890400	-3.91790300	-2.43370200
C	-2.67154900	2.31737500	-0.01318600
C	3.42253700	2.10912000	-1.43734000
C	0.43118100	3.79009100	-0.70950100
C	1.10365600	1.62605300	-0.57551500
C	-2.87734700	3.66676500	-0.25757300
H	-2.02950700	4.31786000	-0.31343600
C	-3.84441700	1.45520800	0.09367000
C	-1.26580600	1.82240000	0.13239700
C	-0.05015400	2.45795600	-0.33596900
C	-3.84267600	0.05435800	0.35837600
H	-2.90561100	-0.43982100	0.54924100
C	-2.49912200	-3.19422600	-2.45968700
H	-2.85727500	-3.82577900	-3.27871000
H	-3.34577000	-2.61973600	-2.07107900
C	-5.14003300	2.05814800	-0.10325700
C	0.89096000	-3.14915600	-1.36666900
H	1.69237200	-2.52946800	-1.78448700
H	1.34511100	-3.83615600	-0.64304800
C	3.75881900	0.84399000	-1.93531100
H	2.99291800	0.09017200	-2.05823500
C	-0.11859200	5.19205300	-0.64194600
H	0.71721200	5.87226500	-0.82115000
H	-0.54558600	5.43291800	0.33775200
H	-0.87200600	5.39284700	-1.41153700
C	5.08375500	0.57392000	-2.28261500
H	5.34014300	-0.40575700	-2.67651300
C	4.40365100	3.10096300	-1.30864100
H	4.12114900	4.08146700	-0.94515900
C	-6.32047200	1.26858500	-0.04702900
H	-7.27504300	1.76333900	-0.20549900
C	0.31216300	-2.04816500	2.93832000
H	-0.27680400	-2.95924100	2.96290700
C	1.64061600	-2.08646700	2.39866900
H	2.02839300	-3.02449600	2.02024500

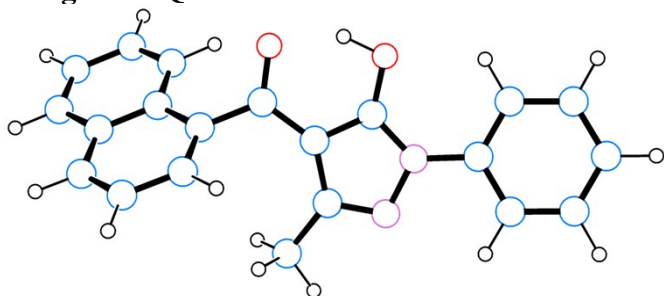
C	6.06844300	1.55391100	-2.15008500
H	7.09542700	1.33914100	-2.43016400
C	5.71989100	2.81761800	-1.66739100
H	6.47562600	3.59146600	-1.56891800
C	-4.14838500	4.24654100	-0.41380200
H	-4.23241200	5.31406500	-0.59180300
C	-1.67076900	-3.34119500	-0.17321600
H	-1.32307400	-4.04058600	0.59682800
H	-2.57597300	-2.85498200	0.20690200
C	-5.26311100	3.44989400	-0.34943400
H	-6.25644300	3.87037700	-0.48216400
C	2.42523900	-0.91570800	2.31004400
C	-6.26772000	-0.08189600	0.20081700
H	-7.17608700	-0.67507500	0.24278300
C	-1.10924700	-1.24994000	-2.02059500
H	-1.98717200	-0.66560200	-1.72996900
H	-0.37697100	-0.56285900	-2.45619100
C	-5.00987300	-0.68353100	0.40763200
H	-4.95712900	-1.74863000	0.62116700
C	1.85399800	0.30621600	2.82010500
H	2.42127300	1.22775900	2.73684900
C	-0.80809300	-4.80124000	-1.91480200
H	-1.14032600	-5.44769700	-2.73303100
H	-0.39524800	-5.43546900	-1.12322400
C	-0.33388600	-3.04446100	-3.46777700
H	0.43528300	-2.36035400	-3.83991100
H	-0.66044500	-3.67845400	-4.29811100
C	-0.25938100	-0.84472700	3.40185600
C	-1.65902900	-0.77533000	3.94973400
H	-2.21168700	-1.69753500	3.75123800
H	-2.21065400	0.05933100	3.50592300
H	-1.63344500	-0.62334000	5.03584200
C	0.55846900	0.33932500	3.34519300
H	0.13119100	1.28824300	3.65547900
C	3.83957500	-0.88343000	1.75547300
H	3.90668700	0.01711600	1.13199800
C	4.20333800	-2.08443500	0.87506800
H	3.49336700	-2.21120400	0.05147500
H	4.24778800	-3.01764800	1.44957100
H	5.19345800	-1.92711100	0.43701000
C	4.84040600	-0.73309400	2.92385300
H	5.85684800	-0.63396500	2.52983000
H	4.81507300	-1.61093600	3.57994100
H	4.63061300	0.15199400	3.53401200

Proligand HQ^{Ph}



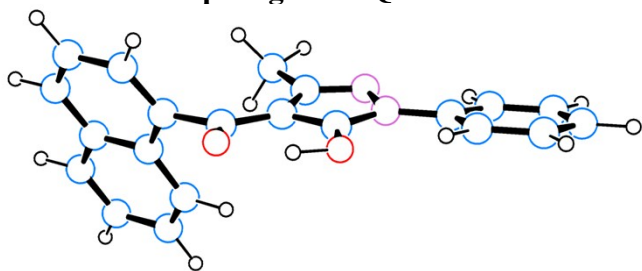
O	-1.00768600	-2.02808400	0.06452000
O	1.55059300	-2.18463700	-0.18937500
C	3.07569900	-0.39989700	0.00582900
N	-1.70447800	0.23120200	-0.00711900
C	-3.12328200	0.12207800	0.02321300
C	-3.88826700	1.21997000	-0.38985900
H	-3.38423100	2.11941800	-0.72000200
C	0.18565300	1.29225600	-0.16712900
C	5.39832100	-0.56091600	-0.66994200
C	4.08185400	-1.00368700	-0.76400200
N	-1.11859800	1.48422600	-0.14031500
C	4.74028200	1.04767500	1.01288900
H	4.99871500	1.82916600	1.72212500
C	3.41651100	0.62174600	0.90224500
H	2.65209200	1.05578600	1.53852600
C	-0.75530000	-0.73017000	0.01632400
C	1.68859500	-0.94186300	-0.08403900
C	0.50750500	-0.10607700	-0.05063600
C	-3.74915400	-1.04932400	0.46800700
H	-3.15969000	-1.89553200	0.79503100
C	1.07036200	2.48821900	-0.35755000
H	0.46184100	3.32170800	-0.71750200
H	1.86615100	2.28719600	-1.08116700
H	1.55072500	2.80010300	0.57618300
C	-5.14234400	-1.11480600	0.48245700
H	-5.62326800	-2.02631800	0.82658800
C	-5.27824700	1.13799500	-0.36102800
H	-5.86628100	1.99325800	-0.68268300
C	-5.91368000	-0.02783900	0.07093700
H	-6.99821200	-0.08734500	0.08837300
C	5.73001200	0.46589000	0.21890800
H	6.75954100	0.80445700	0.29878800
H	-0.08971500	-2.43612600	-0.04151400
H	6.16905600	-1.02151200	-1.28183400
H	3.81443200	-1.81799800	-1.42978100

Proligand HQ^{naph}



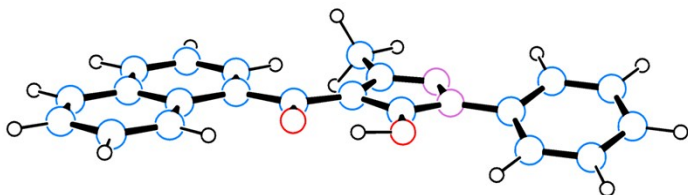
O	1.72322900	-1.72961300	-0.96997900
O	-0.85836300	-1.66746100	-1.04571600
C	-2.19360400	0.23508900	-0.55438100
N	2.56008900	0.19808800	0.12420000
C	3.96830200	-0.01404200	0.12764200
C	4.80148100	1.05205300	0.49041700
H	4.35576900	2.00088900	0.76008300
C	0.73881500	1.31028000	0.54532600
C	-4.60385400	0.37643400	-0.06250900
C	-3.37694700	-0.36642200	-0.00736200
N	2.04593200	1.35107500	0.70945600
C	-3.47877800	2.19733400	-1.21801700
H	-3.50344900	3.16981300	-1.70130700
C	-2.26077500	1.48631100	-1.14158400
H	-1.36398500	1.91567800	-1.57826900
C	1.55865200	-0.55540800	-0.38192300
C	-0.89013100	-0.49682400	-0.59472100
C	0.34226800	0.12239400	-0.16274300
C	4.51946100	-1.25527200	-0.21674200
H	3.87972500	-2.08230400	-0.49268500
C	-0.08842900	2.41080900	1.13799500
H	0.54774700	3.02132900	1.78377100
H	-0.91774900	2.01012100	1.72990400
H	-0.52470000	3.05816300	0.37043600
C	-3.39046800	-1.64640500	0.61238300
H	-2.47667100	-2.22714700	0.64226300
C	-5.78189800	-0.18471400	0.49995300
H	-6.70453300	0.38882300	0.45200800
C	5.90522800	-1.41398100	-0.20116500
H	6.32691100	-2.37858600	-0.47016900
C	6.18228700	0.87188400	0.50455600
H	6.82179600	1.70364500	0.78728200
C	6.74343300	-0.35848500	0.15748000
H	7.82132400	-0.49291100	0.16752000
C	-4.62271000	1.65493900	-0.68159400
H	-5.56411500	2.19737900	-0.72712200
C	-4.55089700	-2.15862500	1.14896800
H	-4.53950500	-3.13960900	1.61615000
C	-5.75935600	-1.42472800	1.09426500
H	-6.66638700	-1.84400100	1.52097200
H	0.77426300	-2.02456000	-1.14834600

Rotamer of the proligand HQ^{naph}



O	-1.85336300	1.81522200	-1.13448100
O	0.67665400	2.35656300	-1.02198100
C	2.32505600	1.06409100	0.08107500
N	-2.35344000	-0.05291700	0.23916500
C	-3.76431400	-0.19120800	0.10550200
C	-4.37369100	-1.34091500	0.62454500
H	-3.76076500	-2.08704200	1.11357800
C	-0.38611000	-0.60375600	0.98740900
C	4.39326900	-0.27323200	0.08696700
C	3.03383100	-0.10567300	-0.34249400
N	-1.65832000	-0.93893100	1.05975400
C	4.29695300	1.84655900	1.27357900
H	4.76711600	2.60721700	1.89024900
C	2.96327300	2.02457600	0.84437800
H	2.42200300	2.92360500	1.12381500
C	-1.49927100	0.82964900	-0.32506100
C	0.90631300	1.34150800	-0.32385900
C	-0.19544000	0.51699200	0.10772700
C	-4.53670800	0.79399800	-0.52389700
H	-4.07141000	1.68555300	-0.92144000
C	0.61507300	-1.36422400	1.80020000
H	0.08745800	-2.04821100	2.46955000
H	1.23521800	-0.68762700	2.39791400
H	1.29020900	-1.94504300	1.16316400
C	2.47119200	-1.09118100	-1.20129500
H	1.45279300	-0.96751500	-1.55587000
C	5.11485900	-1.42379200	-0.33211400
H	6.14284800	-1.54171300	0.00233900
C	-5.91543100	0.61301000	-0.63389300
H	-6.50870900	1.38017900	-1.12391400
C	-5.75224100	-1.50059300	0.50855800
H	-6.21726500	-2.39512500	0.91391700
C	-6.53147900	-0.52873600	-0.12183400
H	-7.60612200	-0.65952800	-0.21158300
C	4.99333100	0.71789600	0.90782500
H	6.02090300	0.57372900	1.23298300
C	3.20134000	-2.19164500	-1.59216900
H	2.75227000	-2.93073600	-2.24992000
C	4.53496700	-2.36506900	-1.15037000
H	5.09895000	-3.23839000	-1.46595000
H	-0.97812000	2.28978500	-1.30424400

Transition state of the naphthyl rotation in the proligand HQ^{naph}



O	-1.57729900	-1.78867400	-0.08717800
O	0.86794300	-1.53208500	-0.16015200
C	2.26177400	0.35766700	-0.00846900
N	-2.66683600	0.27104000	0.04165100
C	-4.03434800	-0.12701000	0.02666900
C	-4.99603900	0.81576000	-0.35773400
H	-4.67649200	1.81320200	-0.63238500
C	-1.03890800	1.70770800	0.04935300
C	4.74226700	0.31048900	0.02598400
C	3.49683500	-0.41468900	-0.02479400
N	-2.35395800	1.61149300	0.07480300
C	3.57519700	2.43297000	0.10878400
H	3.57397600	3.51789400	0.15978400
C	2.35331100	1.73706100	0.05970700
H	1.45138500	2.31545200	0.07440000
C	-1.54170600	-0.47228800	-0.01953300
C	0.90561500	-0.27690700	-0.06360700
C	-0.41032100	0.39430800	-0.00898000
C	-4.42214300	-1.41912200	0.40194700
H	-3.68112300	-2.14536800	0.70694300
C	-0.54432600	3.12920200	0.08058400
H	-1.42423700	3.77676700	0.09633900
H	0.04905900	3.38968700	-0.80301200
H	0.04959100	3.35155600	0.97427500
C	3.59179500	-1.83543800	-0.08269600
H	2.68609200	-2.41665100	-0.12092200
C	5.98035200	-0.38613500	0.01303300
H	6.89766600	0.19656600	0.05175600
C	-5.77447100	-1.76022400	0.37510100
H	-6.07006300	-2.76465600	0.66559500
C	-6.34221300	0.45928500	-0.37063600
H	-7.08304900	1.19569600	-0.67001400
C	-6.73974500	-0.82937300	-0.00889800
H	-7.79071600	-1.10386600	-0.02431800
C	4.75117000	1.72762600	0.09118400
H	5.70904500	2.24118000	0.12777300
C	4.81266900	-2.47879600	-0.09222300
H	4.83551700	-3.56458300	-0.13675800
C	6.02397100	-1.75800100	-0.04564200
H	6.97580800	-2.28182500	-0.05513000
H	-0.58647200	-2.01727100	-0.14567400