

## TABLE CAPTIONS

**Table S1.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $[\text{Rh}(\text{ppy})_2\text{phi}]\text{Cl}\cdot\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$ .

**Table S2.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for  $[\text{Rh}(\text{ppy})_2\text{phi}]\text{Cl}\cdot\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$ .

**Table S3.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for  $[\text{Rh}(\text{ppy})_2\text{phi}]\text{Cl}\cdot\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$ .

**Table S4.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $[\text{Rh}(\text{ppy})_2\text{phi}]\text{Cl}\cdot\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$ .

**Table S5.** Torsion angles [ $^\circ$ ] for  $[\text{Rh}(\text{ppy})_2\text{phi}]\text{Cl}\cdot\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$ .

**Table S6.** Hydrogen bonds for  $[\text{Rh}(\text{ppy})_2\text{phi}]\text{Cl}\cdot\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$  [ $\text{\AA}$  and  $^\circ$ ].

## FIGURE CAPTIONS

**Figure S1.** Crystal packing of  $[\text{Rh}(\text{ppy})_2\text{phi}]\text{Cl}\cdot\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$  showing boundaries of the unit cell viewed down the  $b$ -axis. All fragments within the range [0.1, 0.9] along the cell edge are included. Rh, N, and Cl atoms are shaded. Hydrogen atoms are at arbitrary scale. The partial overlapping, or  $\pi$ -stacking, of the phi ligands can be seen.

Table S1

Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for JLK1 -  $[\text{Rh}(\text{ppy})_2\text{phi}]^+\text{Cl}^- \cdot \text{H}_2\text{O} \cdot \text{CH}_2\text{Cl}_2$ .  
 $U(\text{eq})$  is defined as the trace of the orthogonalized  $U^{\text{ij}}$  tensor.

	x	y	z	$U_{\text{eq}}$
Rh	2079(1)	7256(1)	2977(1)	20(1)
N1	2717(1)	6467(2)	3957(1)	26(1)
N2	2994(1)	6285(2)	2559(1)	21(1)
N3	2581(1)	9102(2)	2930(1)	26(1)
N4	1441(1)	5547(2)	2990(1)	20(1)
C1	3269(1)	5696(2)	3835(1)	24(1)
C2	3708(1)	4889(3)	4401(1)	25(1)
C3	3522(2)	4796(3)	5147(2)	37(1)
C4	3918(2)	3989(3)	5674(2)	43(1)
C5	4498(2)	3245(3)	5456(2)	41(1)
C6	4702(2)	3321(3)	4720(2)	34(1)
C7	4313(1)	4152(3)	4181(2)	27(1)
C8	4543(1)	4258(2)	3402(2)	26(1)
C9	5184(2)	3647(3)	3199(2)	35(1)
C10	5394(2)	3747(3)	2473(2)	37(1)
C11	4978(2)	4454(3)	1919(2)	32(1)
C12	4341(1)	5067(3)	2097(2)	26(1)
C13	4119(1)	4983(2)	2835(2)	23(1)
C14	3449(1)	5670(2)	3029(1)	21(1)
C15	3055(2)	9613(3)	3482(2)	34(1)
C16	3368(2)	10909(3)	3408(2)	45(1)
C17	3194(2)	11654(3)	2771(2)	45(1)
C18	2713(2)	11143(3)	2216(2)	37(1)
C19	2404(1)	9854(3)	2298(2)	27(1)
C20	1893(1)	9172(2)	1743(2)	25(1)
C21	1682(2)	9720(3)	1027(2)	32(1)
C22	1244(2)	8967(3)	508(2)	34(1)
C23	1015(2)	7679(3)	710(2)	32(1)
C24	1207(1)	7157(3)	1426(2)	24(1)
C25	1650(1)	7884(2)	1961(1)	22(1)
C26	1623(1)	4302(3)	2755(1)	24(1)
C27	1164(1)	3184(3)	2757(2)	28(1)
C28	485(2)	3366(3)	3014(2)	28(1)
C29	288(1)	4632(3)	3264(1)	26(1)
C30	773(1)	5729(2)	3256(1)	21(1)
C31	645(1)	7124(2)	3518(1)	22(1)
C32	5(1)	7525(3)	3838(1)	27(1)
C33	-71(2)	8869(3)	4064(2)	30(1)
C34	475(2)	9804(3)	3974(2)	30(1)
C35	1110(1)	9415(3)	3659(1)	26(1)
C36	1215(1)	8065(2)	3429(1)	22(1)
Cl1 <sup>a</sup>	3222(1)	8018(1)	5676(1)	37(1)
O1A <sup>b</sup>	3035(4)	7823(7)	6073(5)	51(2)
O1 <sup>a</sup>	4271(4)	9793(7)	4881(4)	104(2)
Cl1A <sup>b</sup>	4060(1)	9372(3)	5083(2)	30(1)

Cl2	2023(1)	2504(1)	4539(1)	60(1)
Cl3	2146(1)	1056(1)	5974(1)	66(1)
C37	2481(2)	1215(4)	5095(2)	68(1)

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<sup>a</sup> Population: 0.658(4)

<sup>b</sup> Population: 0.342(4)

Table S2

Bond lengths [Å] and angles [°] for JLK1 –  
[Rh(ppy)<sub>2</sub>phi]<sup>+</sup>Cl<sup>-</sup>·H<sub>2</sub>O·CH<sub>2</sub>Cl<sub>2</sub>.

Rh-C25	1.996(3)	C21-H21	1.07(3)
Rh-C36	2.003(2)	C22-C23	1.383(4)
Rh-N3	2.033(2)	C22-H22	0.96(3)
Rh-N4	2.0439(19)	C23-C24	1.382(4)
Rh-N2	2.122(2)	C23-H23	1.01(3)
Rh-N1	2.153(2)	C24-C25	1.391(4)
N1-C1	1.300(3)	C24-H24	0.84(3)
N1-H1	0.82(3)	C26-C27	1.382(3)
N2-C14	1.281(3)	C26-H26	0.86(3)
N2-H2	0.82(2)	C27-C28	1.379(4)
N3-C15	1.350(3)	C27-H27	0.94(3)
N3-C19	1.353(3)	C28-C29	1.372(4)
N4-C26	1.338(3)	C28-H28	0.87(3)
N4-C30	1.367(3)	C29-C30	1.396(3)
C1-C2	1.464(3)	C29-H29	0.90(3)
C1-C14	1.487(3)	C30-C31	1.465(3)
C2-C3	1.391(4)	C31-C32	1.407(3)
C2-C7	1.411(4)	C31-C36	1.416(3)
C3-C4	1.381(4)	C32-C33	1.383(4)
C3-H3	0.87(3)	C32-H32	0.99(3)
C4-C5	1.375(5)	C33-C34	1.378(4)
C4-H4	0.94(3)	C33-H33	0.90(3)
C5-C6	1.384(4)	C34-C35	1.392(4)
C5-H5	1.01(3)	C34-H34	0.92(3)
C6-C7	1.402(4)	C35-C36	1.399(3)
C6-H6	1.02(3)	C35-H35	0.98(3)
C7-C8	1.475(4)		
C8-C9	1.399(4)	C11...O1A	0.829(8)
C8-C13	1.410(3)	C11...C11A	2.347(3)
C9-C10	1.374(4)	O1...C11A	0.687(7)
C9-H9	0.81(3)		
C10-C11	1.378(4)	C12-C37	1.768(4)
C10-H10	0.93(3)	C13-C37	1.725(4)
C11-C12	1.380(4)	C37-H37A	0.9900
C11-H11	0.97(3)	C37-H37B	0.9900
C12-C13	1.399(4)		
C12-H12	0.93(3)	C25-Rh-C36	88.17(9)
C13-C14	1.473(3)	C25-Rh-N3	80.66(9)
C15-C16	1.402(4)	C36-Rh-N3	92.65(9)
C15-H15	0.92(3)	C25-Rh-N4	94.38(9)
C16-C17	1.356(5)	C36-Rh-N4	80.79(9)
C16-H16	0.86(3)	N3-Rh-N4	171.94(8)
C17-C18	1.360(4)	C25-Rh-N2	95.25(9)
C17-H17	0.91(3)	C36-Rh-N2	175.86(9)
C18-C19	1.395(4)	N3-Rh-N2	90.21(8)
C18-H18	0.96(3)	N4-Rh-N2	96.60(7)
C19-C20	1.462(4)	C25-Rh-N1	169.05(9)
C20-C21	1.399(4)	C36-Rh-N1	102.72(9)
C20-C25	1.401(3)	N3-Rh-N1	97.49(8)
C21-C22	1.381(4)		

N4-Rh-N1	88.57(8)	N2-C14-C1	115.2(2)
N2-Rh-N1	73.92(8)	C13-C14-C1	119.4(2)
C1-N1-Rh	117.17(17)	N3-C15-C16	120.9(3)
C1-N1-H1	115(2)	N3-C15-H15	116.2(19)
Rh-N1-H1	127.5(19)	C16-C15-H15	122.5(19)
C14-N2-Rh	118.74(17)	C17-C16-C15	119.5(3)
C14-N2-H2	116.7(18)	C17-C16-H16	132(2)
Rh-N2-H2	124.5(18)	C15-C16-H16	108(2)
C15-N3-C19	119.4(2)	C16-C17-C18	119.7(3)
C15-N3-Rh	124.7(2)	C16-C17-H17	122(2)
C19-N3-Rh	115.87(16)	C18-C17-H17	118(2)
C26-N4-C30	118.9(2)	C17-C18-C19	120.3(3)
C26-N4-Rh	125.39(17)	C17-C18-H18	116.6(19)
C30-N4-Rh	115.75(15)	C19-C18-H18	123.1(19)
N1-C1-C2	126.4(2)	N3-C19-C18	120.2(3)
N1-C1-C14	114.2(2)	N3-C19-C20	113.8(2)
C2-C1-C14	119.3(2)	C18-C19-C20	126.0(3)
C3-C2-C7	119.5(2)	C21-C20-C25	121.4(2)
C3-C2-C1	121.1(2)	C21-C20-C19	123.1(2)
C7-C2-C1	119.4(2)	C25-C20-C19	115.4(2)
C4-C3-C2	121.1(3)	C22-C21-C20	119.9(3)
C4-C3-H3	120(2)	C22-C21-H21	124.9(15)
C2-C3-H3	119(2)	C20-C21-H21	115.1(15)
C5-C4-C3	119.6(3)	C21-C22-C23	119.2(3)
C5-C4-H4	120.9(19)	C21-C22-H22	118.1(17)
C3-C4-H4	119.3(19)	C23-C22-H22	122.6(17)
C4-C5-C6	120.9(3)	C24-C23-C22	120.7(3)
C4-C5-H5	120.9(18)	C24-C23-H23	115.2(16)
C6-C5-H5	118.3(18)	C22-C23-H23	124.0(16)
C5-C6-C7	120.4(3)	C23-C24-C25	121.6(3)
C5-C6-H6	115.6(16)	C23-C24-H24	115.8(18)
C7-C6-H6	124.0(16)	C25-C24-H24	122.6(18)
C6-C7-C2	118.6(3)	C24-C25-C20	117.1(2)
C6-C7-C8	120.2(2)	C24-C25-Rh	128.27(19)
C2-C7-C8	121.2(2)	C20-C25-Rh	114.31(18)
C9-C8-C13	117.5(2)	N4-C26-C27	123.2(2)
C9-C8-C7	121.6(2)	N4-C26-H26	114.7(17)
C13-C8-C7	120.9(2)	C27-C26-H26	121.9(17)
C10-C9-C8	121.3(3)	C28-C27-C26	118.1(3)
C10-C9-H9	121(2)	C28-C27-H27	121.4(17)
C8-C9-H9	118(2)	C26-C27-H27	120.5(17)
C9-C10-C11	121.0(3)	C29-C28-C27	119.7(3)
C9-C10-H10	123.9(18)	C29-C28-H28	119.9(19)
C11-C10-H10	114.9(18)	C27-C28-H28	120.4(19)
C10-C11-C12	119.3(3)	C28-C29-C30	120.1(2)
C10-C11-H11	117.0(17)	C28-C29-H29	122.1(17)
C12-C11-H11	123.4(17)	C30-C29-H29	117.8(17)
C11-C12-C13	120.6(3)	N4-C30-C29	120.0(2)
C11-C12-H12	118.8(16)	N4-C30-C31	113.8(2)
C13-C12-H12	120.6(16)	C29-C30-C31	126.2(2)
C12-C13-C8	120.3(2)	C32-C31-C36	121.4(2)
C12-C13-C14	120.5(2)	C32-C31-C30	123.3(2)
C8-C13-C14	119.2(2)	C36-C31-C30	115.4(2)
N2-C14-C13	125.4(2)	C33-C32-C31	119.2(2)

C33-C32-H32	118.3(16)	C35-C36-C31	117.2(2)
C31-C32-H32	122.4(16)	C35-C36-Rh	128.49(19)
C34-C33-C32	120.3(2)	C31-C36-Rh	114.28(17)
C34-C33-H33	120.6(18)		
C32-C33-H33	119.0(18)	Cl3-C37-Cl2	112.0(2)
C33-C34-C35	120.9(3)	Cl3-C37-H37A	109.2
C33-C34-H34	119.7(17)	Cl2-C37-H37A	109.2
C35-C34-H34	119.3(18)	Cl3-C37-H37B	109.2
C34-C35-C36	121.0(3)	Cl2-C37-H37B	109.2
C34-C35-H35	119.2(16)	H37A-C37-H37B	107.9
C36-C35-H35	119.8(16)		

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Table S3

Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for JLK1 -  
 $[\text{Rh}(\text{ppy})_2\text{phi}]^+\text{Cl}^-\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$ . The anisotropic displacement factor exponent  
 takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Rh	127(1)	189(1)	274(1)	-48(1)	21(1)	-3(1)
N1	195(11)	303(13)	279(12)	-67(10)	20(9)	-21(9)
N2	172(11)	184(11)	267(11)	-38(9)	35(9)	-37(8)
N3	126(10)	224(12)	425(14)	-103(10)	57(9)	-18(8)
N4	151(10)	233(11)	222(11)	-6(8)	-2(8)	5(8)
C1	161(12)	227(14)	318(14)	-45(11)	2(11)	-48(10)
C2	208(13)	246(14)	293(14)	-20(11)	-13(11)	-59(11)
C3	251(16)	475(19)	374(17)	1(14)	8(13)	-33(13)
C4	355(18)	580(20)	336(17)	95(15)	4(14)	-119(15)
C5	409(18)	338(17)	457(19)	101(14)	-103(15)	-89(14)
C6	353(17)	247(15)	410(17)	4(13)	-64(13)	-8(13)
C7	263(14)	198(14)	347(15)	-11(11)	-31(12)	-64(11)
C8	245(14)	176(13)	346(15)	-66(11)	-14(11)	-11(10)
C9	304(16)	289(16)	434(19)	-46(13)	-26(13)	112(12)
C10	277(16)	329(17)	495(19)	-108(14)	52(14)	128(13)
C11	253(15)	331(16)	379(16)	-74(13)	59(13)	14(12)
C12	190(13)	241(14)	347(15)	-45(11)	26(11)	-9(11)
C13	157(12)	169(13)	362(15)	-54(11)	-9(11)	-17(10)
C14	128(12)	184(13)	313(14)	-45(10)	18(10)	-54(10)
C15	225(15)	287(17)	520(19)	-131(13)	24(13)	-9(12)
C16	238(16)	382(19)	730(30)	-273(18)	12(16)	-59(13)
C17	337(17)	220(16)	820(30)	-69(17)	121(17)	-72(13)
C18	284(16)	242(16)	610(20)	-34(14)	152(15)	-23(12)
C19	178(13)	213(14)	440(17)	-50(12)	121(12)	12(10)
C20	189(13)	206(14)	378(15)	-9(11)	121(11)	12(10)
C21	277(15)	266(15)	432(17)	61(13)	154(13)	72(12)
C22	362(17)	347(17)	315(16)	63(13)	94(13)	97(13)
C23	298(15)	376(17)	301(15)	-42(12)	56(12)	34(13)
C24	185(12)	222(14)	322(14)	-2(12)	35(11)	13(11)
C25	163(12)	206(13)	298(13)	-25(10)	70(10)	30(10)
C26	178(13)	248(14)	301(15)	-22(11)	29(11)	4(11)
C27	270(14)	212(14)	351(15)	-16(11)	27(12)	-19(11)
C28	252(14)	271(15)	320(15)	32(12)	12(11)	-94(12)
C29	178(13)	342(16)	263(14)	22(11)	34(11)	-32(11)
C30	163(12)	273(14)	189(12)	15(10)	-1(10)	5(10)
C31	184(12)	266(14)	194(12)	-2(10)	-4(10)	28(10)
C32	185(13)	387(18)	231(13)	30(11)	30(10)	48(11)
C33	229(14)	410(17)	257(14)	10(12)	62(11)	142(12)
C34	337(16)	308(16)	264(15)	-44(12)	14(12)	152(13)
C35	227(14)	272(15)	276(14)	-36(11)	-1(11)	25(11)
C36	181(12)	238(14)	230(13)	-19(10)	1(10)	36(10)
C11	322(7)	434(8)	358(9)	-58(6)	-28(5)	25(5)
O1A	660(50)	550(40)	380(40)	0(30)	360(40)	-140(40)
O1	890(50)	1150(50)	1050(50)	250(40)	-130(40)	-130(40)
Cl1A	212(12)	375(15)	316(13)	49(10)	36(9)	33(9)

Cl2	672(6)	578(6)	531(5)	-117(4)	-100(4)	36(4)
Cl3	763(7)	533(6)	698(6)	16(4)	234(5)	-57(5)
C37	670(30)	860(30)	490(20)	-80(20)	12(19)	270(20)

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Table S4

Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for JLK1 -  $[\text{Rh}(\text{ppy})_2\text{phi}]^+\text{Cl}^-\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$ .

	x	y	z	$U_{\text{iso}}$
H1	2621(14)	6500(30)	4401(15)	31
H2	3090(14)	6300(30)	2114(14)	25
H3	3149(16)	5260(30)	5283(16)	44
H4	3811(16)	4010(30)	6187(18)	51
H5	4787(18)	2620(30)	5829(18)	49
H6	5155(16)	2780(30)	4617(16)	41
H9	5436(16)	3250(30)	3526(17)	42
H10	5796(16)	3300(30)	2306(16)	44
H11	5178(15)	4570(30)	1435(16)	38
H12	4062(15)	5540(30)	1721(15)	31
H15	3118(16)	9110(30)	3921(17)	41
H16	3615(18)	11110(30)	3831(19)	54
H17	3361(19)	12520(30)	2716(18)	55
H18	2593(15)	11720(30)	1786(17)	45
H21	1914(15)	10700(30)	914(15)	38
H22	1101(15)	9370(30)	25(16)	41
H23	685(16)	7070(30)	366(16)	39
H24	1041(14)	6380(30)	1515(15)	29
H26	2037(15)	4260(30)	2569(15)	29
H27	1312(15)	2330(30)	2583(16)	33
H28	186(16)	2680(30)	3026(16)	34
H29	-145(15)	4780(30)	3444(14)	31
H32	-403(15)	6890(30)	3893(14)	32
H33	-470(15)	9110(30)	4290(16)	36
H34	432(15)	10690(30)	4152(15)	36
H35	1493(14)	10090(30)	3613(14)	31
H37A	2427	330	4823	81
H37B	3006	1437	5164	81

Table S5

Torsion angles [°] for JLK1 - [Rh(ppy)<sub>2</sub>phi]<sup>+</sup>Cl<sup>-</sup>·H<sub>2</sub>O·CH<sub>2</sub>Cl<sub>2</sub>.

C25-Rh-N1-C1	-15.8(6)	C13-C8-C9-C10	-0.2(4)
C36-Rh-N1-C1	170.26(18)	C7-C8-C9-C10	179.8(3)
N3-Rh-N1-C1	-95.30(19)	C8-C9-C10-C11	0.0(5)
N4-Rh-N1-C1	90.03(19)	C9-C10-C11-C12	-0.1(4)
N2-Rh-N1-C1	-7.25(18)	C10-C11-C12-C13	0.4(4)
C25-Rh-N2-C14	-178.47(18)	C11-C12-C13-C8	-0.6(4)
C36-Rh-N2-C14	-32.8(13)	C11-C12-C13-C14	178.4(2)
N3-Rh-N2-C14	100.88(18)	C9-C8-C13-C12	0.5(4)
N4-Rh-N2-C14	-83.44(18)	C7-C8-C13-C12	-179.5(2)
N1-Rh-N2-C14	3.15(17)	C9-C8-C13-C14	-178.5(2)
C25-Rh-N3-C15	179.7(2)	C7-C8-C13-C14	1.5(3)
C36-Rh-N3-C15	92.0(2)	Rh-N2-C14-C13	-178.19(17)
N4-Rh-N3-C15	127.3(6)	Rh-N2-C14-C1	0.8(3)
N2-Rh-N3-C15	-85.0(2)	C12-C13-C14-N2	5.7(4)
N1-Rh-N3-C15	-11.2(2)	C8-C13-C14-N2	-175.3(2)
C25-Rh-N3-C19	0.94(17)	C12-C13-C14-C1	-173.2(2)
C36-Rh-N3-C19	-86.77(18)	C8-C13-C14-C1	5.8(3)
N4-Rh-N3-C19	-51.5(7)	N1-C1-C14-N2	-7.0(3)
N2-Rh-N3-C19	96.23(17)	C2-C1-C14-N2	172.9(2)
N1-Rh-N3-C19	170.03(17)	N1-C1-C14-C13	172.0(2)
C25-Rh-N4-C26	93.3(2)	C2-C1-C14-C13	-8.1(3)
C36-Rh-N4-C26	-179.2(2)	C19-N3-C15-C16	-0.2(4)
N3-Rh-N4-C26	145.0(5)	Rh-N3-C15-C16	-178.9(2)
N2-Rh-N4-C26	-2.5(2)	N3-C15-C16-C17	-0.4(4)
N1-Rh-N4-C26	-76.1(2)	C15-C16-C17-C18	0.7(5)
C25-Rh-N4-C30	-85.87(17)	C16-C17-C18-C19	-0.5(5)
C36-Rh-N4-C30	1.57(16)	C15-N3-C19-C18	0.5(4)
N3-Rh-N4-C30	-34.2(7)	Rh-N3-C19-C18	179.30(19)
N2-Rh-N4-C30	178.32(16)	C15-N3-C19-C20	179.3(2)
N1-Rh-N4-C30	104.69(16)	Rh-N3-C19-C20	-1.9(3)
Rh-N1-C1-C2	-170.11(18)	C17-C18-C19-N3	-0.1(4)
Rh-N1-C1-C14	9.8(3)	C17-C18-C19-C20	-178.8(3)
N1-C1-C2-C3	5.3(4)	N3-C19-C20-C21	-174.8(2)
C14-C1-C2-C3	-174.7(2)	C18-C19-C20-C21	4.0(4)
N1-C1-C2-C7	-177.1(2)	N3-C19-C20-C25	2.1(3)
C14-C1-C2-C7	3.0(3)	C18-C19-C20-C25	-179.2(2)
C7-C2-C3-C4	-0.4(4)	C25-C20-C21-C22	-2.0(4)
C1-C2-C3-C4	177.3(3)	C19-C20-C21-C22	174.6(2)
C2-C3-C4-C5	-1.1(5)	C20-C21-C22-C23	0.4(4)
C3-C4-C5-C6	1.6(5)	C21-C22-C23-C24	1.4(4)
C4-C5-C6-C7	-0.6(4)	C22-C23-C24-C25	-1.7(4)
C5-C6-C7-C2	-0.9(4)	C23-C24-C25-C20	0.1(4)
C5-C6-C7-C8	178.4(2)	C23-C24-C25-Rh	-172.78(19)
C3-C2-C7-C6	1.4(4)	C21-C20-C25-C24	1.8(4)
C1-C2-C7-C6	-176.3(2)	C19-C20-C25-C24	-175.2(2)
C3-C2-C7-C8	-178.0(2)	C21-C20-C25-Rh	175.62(18)
C1-C2-C7-C8	4.3(3)	C19-C20-C25-Rh	-1.3(3)
C6-C7-C8-C9	-6.1(4)	C36-Rh-C25-C24	-93.7(2)
C2-C7-C8-C9	173.2(2)	N3-Rh-C25-C24	173.3(2)
C6-C7-C8-C13	173.9(2)	N4-Rh-C25-C24	-13.1(2)
C2-C7-C8-C13	-6.7(4)	N2-Rh-C25-C24	83.9(2)

N1-Rh-C25-C24	92.2(5)	C36-C31-C32-C33	0.5(4)
C36-Rh-C25-C20	93.23(18)	C30-C31-C32-C33	-179.5(2)
N3-Rh-C25-C20	0.25(17)	C31-C32-C33-C34	0.2(4)
N4-Rh-C25-C20	173.85(17)	C32-C33-C34-C35	-0.2(4)
N2-Rh-C25-C20	-89.10(18)	C33-C34-C35-C36	-0.4(4)
N1-Rh-C25-C20	-80.9(5)	C34-C35-C36-C31	1.1(4)
C30-N4-C26-C27	0.9(4)	C34-C35-C36-Rh	-179.12(19)
Rh-N4-C26-C27	-178.26(19)	C32-C31-C36-C35	-1.2(3)
N4-C26-C27-C28	0.0(4)	C30-C31-C36-C35	178.9(2)
C26-C27-C28-C29	-0.5(4)	C32-C31-C36-Rh	179.04(18)
C27-C28-C29-C30	0.0(4)	C30-C31-C36-Rh	-0.9(3)
C26-N4-C30-C29	-1.4(3)	C25-Rh-C36-C35	-85.3(2)
Rh-N4-C30-C29	177.88(18)	N3-Rh-C36-C35	-4.8(2)
C26-N4-C30-C31	178.3(2)	N4-Rh-C36-C35	179.9(2)
Rh-N4-C30-C31	-2.5(2)	N2-Rh-C36-C35	128.9(11)
C28-C29-C30-N4	0.9(4)	N1-Rh-C36-C35	93.5(2)
C28-C29-C30-C31	-178.7(2)	C25-Rh-C36-C31	94.44(18)
N4-C30-C31-C32	-177.8(2)	N3-Rh-C36-C31	175.01(17)
C29-C30-C31-C32	1.9(4)	N4-Rh-C36-C31	-0.29(17)
N4-C30-C31-C36	2.2(3)	N2-Rh-C36-C31	-51.4(13)
C29-C30-C31-C36	-178.1(2)	N1-Rh-C36-C31	-86.70(18)

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Table S6

Hydrogen bonds for JLK1 -  $[\text{Rh}(\text{ppy})_2\text{phi}]^+\text{Cl}^-\text{H}_2\text{O}\cdot\text{CH}_2\text{Cl}_2$   
 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1...Cl1	0.82(3)	2.84(3)	3.450(3)	132(2)
N2-H2...Cl1 <sup>①</sup>	0.82(2)	2.66(3)	3.454(3)	165(2)
N2-H2...O1A <sup>①</sup>	0.82(2)	2.02(3)	2.772(9)	152(3)

Symmetry transformations used to generate equivalent atoms:

<sup>①</sup>  $x, -y+3/2, z-1/2$

