THE DEVELOPMENT OF LAUE TECHNIQUES FOR SINGLE PULSE DIFFRACTION OF CHEMICAL COMPLEXES: TIME-RESOLVED LAUE DIFFRACTION ON A BINUCLEAR-RHODIUM ORGANOMETALLIC COMPLEX.

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Supplementary Material

Table S1. Number of reflections before and after averaging, cut-off and R_{merge} values for individual data sets.

Data set	# reflections recorded	# reflections after averaging over 10 frame-sequence	# reflections after merging over equivalents	sin θ/λ max [Å^{-1}]	R_{merge}
19	30069	3380	1196	0.40	0.0196
20	15489	1844	588	0.40	0.0204
24	14464	1719	540	0.38	0.0274
27	27675	3439	760	0.51	0.0237
28	42288	5386	1281	0.41	0.0214
29	37112	4778	1150	0.42	0.0175

Table S2. Details on the filtering of the measurements.

Data set	% I/σ(I) > 3.0 for both ON and OFF frames	% I/σ(I) >10.0 for both ON and OFF frames	% Reflections measured on all 10 repeated frames	σ(R) <0.5
19	94.9	62.8	79.4	89.0
20	93.3	52.9	71.4	92.7
24	93.4	57.4	70.0	91.7
27	91.0	48.2	64.5	86.9
28	93.7	58.1	63.1	87.1
29	94.4	59.8	63.5	87.2

Table S3. Final refined values of excited-state occupancies and k_B parameters for each of six datasets.

Data set	Laser power (mJ/mm^2)	occupancy	k_B
19	0.60	0.059(3)	1.141(3)
20	0.60	0.103(6)	1.252(3)

24	0.55	0.081(7)	1.299(7)
27	0.45	0.058(6)	1.142(6)
28	0.45	0.052(4)	1.112(4)
29	0.45	0.058(3)	1.091(3)

Table S4. Final coordinates of the excited-state rhodium atoms.

atom	x	y	z
Rh1E	0.6437(4)	0.2804(3)	0.1953(2)
Rh2E	0.8056(4)	0.2525(3)	0.1270(2)

Table S5. List of non-hydrogen atoms belonging to each of the rigid PNP ligands.

#1	P1, P2, N1, O1, O2, O3, O4, C1, C2, C3, C4, C5
#2	P3, P4, N2, O5, O6, O7, O8, C6, C7, C8, C9, C10
#3	P7, P8, N4, O13, O14, O15, O16, C16, C17, C18, C19, C20
#4	P5, P6, N3, O9, O10, O11, O12, C11, C12, C13, C14, C15

Table S6. Final coordinates of the anchor points of the four rigid PNP ligands.

	initial			final		
anchor	x	y	z	x	y	z
#1	0.7300	0.2690	0.1610	0.7312(15)	0.2664(10)	0.1581(11)
#2	0.7300	0.2690	0.1610	0.7181(15)	0.2665(14)	0.1629(5)
#3	0.6462	0.2870	0.1959	0.6436(19)	0.2848(9)	0.1950(4)
#4	0.8146	0.2519	0.1254	0.8084(13)	0.2524(10)	0.1273(8)

Table S7. Eulerian rotation angles φ, χ, ψ (°), of the four PNP rigid bodies.

	angle		
	φ	χ	ψ
#1	0.3(4)	2.5(3)	1.0(7)
#2	0.8(6)	-1.3(3)	0.3(5)
#3	-2.6(4)	1.8(7)	0.7(3)
#4	0.9(5)	-0.1(5)	0.9(4)

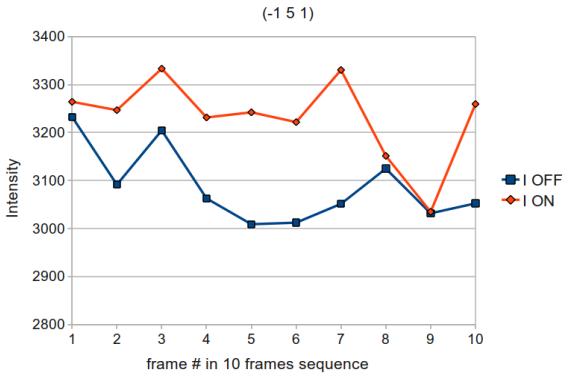
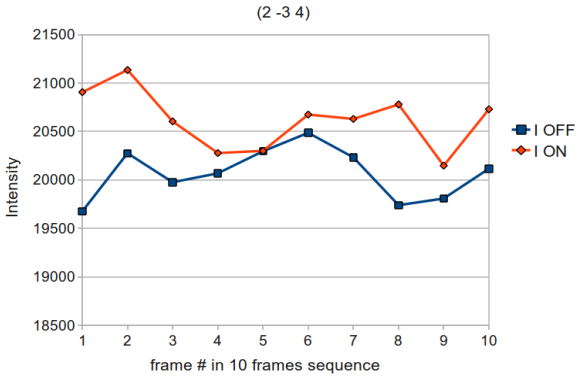


Fig. S1.



Intensities of 10 repeated measurements for two reflections with $I_{ON}>I_{OFF}$ from data set 29.