Supplementary Material (ESI) for Dalton Transactions

[Supporting information]

Photocrystallographic Analysis for Elucidation of the Effect of the Crystal Packing for the Molecular Structure and the Photophysical Property of [$AuCl(PPh_3)_2$]

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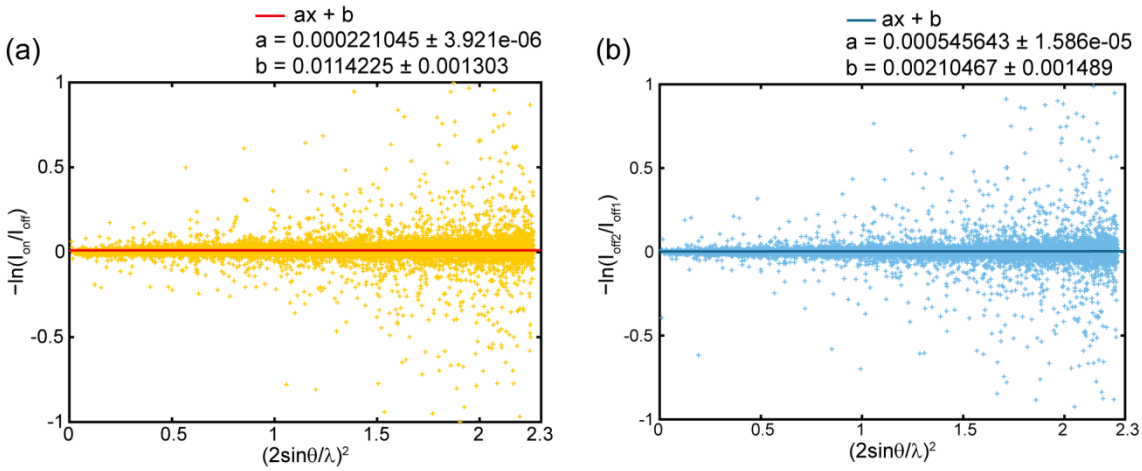

Fig. S1. Wilson-type plot: (a) $(2\sin\theta/\lambda)^2$ vs. $-\ln(I_{on}/I_{off})$; (b) $(2\sin\theta/\lambda)^2$ vs. $-\ln(I_{off2}/I_{off1})$.

The inclement from the linear-fit to the Wilson type plot means change of the averaged temperature factor ($\Delta B/2$). The value of $\Delta B/2$ from $(2\sin\theta/\lambda)^2$ vs. $-\ln(I_{on}/I_{off})$ (Fig. 1(a)) is approximately same as one from $(2\sin\theta/\lambda)^2$ vs. $-\ln(I_{off2}/I_{off1})$ (Fig. 1(b)), which I_{off2} is measured after the data collection of the light-on stage and I_{off1} is corresponding to the light-off stage. It indicates that the difference of temperature between the light-on and light-off stage can be regarded as almost zero and had little effect on the examining structural change by photoexcitation.

Data collected at 118 K were used to plot above. At this temperature, because the cell volume was hardly changed by photoexcitation, the ratios of diffraction intensity (I_{on}/I_{off}) to every $(2\sin\theta/\lambda)^2$ were obtainable.

Table S1. Geometric parameters of [$AuCl(PPh_3)_2$] at every temperature (Å, °)

	177Koff	177Kon	156Koff	156Kon	137Koff	137Kon
Au1—Cl1	2.5432 (3)	2.5380 (5)	2.5438 (4)	2.5420 (4)	2.5443 (3)	2.5439 (4)
Au1—P1	2.3244 (3)	2.3179 (5)	2.3254 (4)	2.3211 (4)	2.3238 (3)	2.3230 (4)
Au1—P2	2.3127 (3)	2.3051 (5)	2.3134 (4)	2.3089 (4)	2.3122 (3)	2.3100 (4)
C111—C112	1.3955 (19)	1.384 (3)	1.397 (2)	1.396 (2)	1.3944 (19)	1.394 (2)
C111—C116	1.3933 (18)	1.389 (2)	1.396 (2)	1.391 (2)	1.3955 (18)	1.3958 (19)
C112—C113	1.388 (2)	1.383 (3)	1.390 (2)	1.385 (2)	1.390 (2)	1.389 (2)
C112—H112	0.97 (2)	0.97 (3)	0.97 (2)	0.97 (2)	0.97 (2)	0.98 (2)
C113—C114	1.386 (2)	1.381 (3)	1.387 (2)	1.383 (2)	1.388 (2)	1.388 (2)
C113—H113	0.91 (2)	0.94 (3)	0.93 (3)	0.92 (3)	0.93 (2)	0.93 (2)
C114—C115	1.382 (2)	1.379 (3)	1.386 (2)	1.384 (3)	1.390 (2)	1.386 (2)
C114—H114	0.95 (2)	0.96 (3)	0.97 (2)	0.95 (3)	0.96 (2)	0.94 (2)
C115—C116	1.390 (2)	1.391 (3)	1.391 (2)	1.388 (2)	1.3898 (19)	1.390 (2)
C115—H115	0.95 (2)	0.93 (3)	0.96 (2)	0.97 (2)	0.97 (2)	0.97 (2)
C116—H116	0.93 (2)	0.93 (3)	0.94 (2)	0.92 (2)	0.93 (2)	0.95 (2)
C121—C122	1.385 (2)	1.382 (3)	1.386 (2)	1.385 (3)	1.388 (2)	1.386 (2)
C121—C126	1.388 (2)	1.383 (3)	1.389 (2)	1.385 (2)	1.391 (2)	1.389 (2)
C122—C123	1.394 (2)	1.390 (3)	1.392 (3)	1.392 (3)	1.394 (2)	1.394 (3)
C122—H122	0.96 (3)	0.95 (4)	0.93 (3)	0.94 (3)	0.96 (3)	0.96 (3)
C123—C124	1.370 (3)	1.371 (4)	1.376 (3)	1.373 (3)	1.379 (3)	1.378 (3)
C123—H123	0.94 (3)	0.99 (4)	0.99 (3)	0.99 (3)	0.96 (3)	0.96 (3)
C124—C125	1.372 (3)	1.364 (5)	1.375 (3)	1.378 (4)	1.377 (3)	1.378 (3)
C124—H124	0.95 (3)	0.90 (4)	0.90 (3)	0.94 (3)	0.93 (3)	0.93 (3)
C125—C126	1.390 (3)	1.387 (4)	1.388 (3)	1.390 (3)	1.390 (2)	1.389 (3)
C125—H125	0.92 (3)	0.92 (4)	0.91 (3)	0.93 (3)	0.96 (3)	0.96 (3)
C126—H126	0.94 (3)	0.91 (3)	0.96 (3)	0.96 (3)	0.93 (3)	0.94 (3)
C131—C132	1.3935 (19)	1.392 (3)	1.396 (2)	1.393 (2)	1.3950 (19)	1.396 (2)
C131—C136	1.3967 (19)	1.387 (3)	1.396 (2)	1.394 (2)	1.3984 (19)	1.398 (2)
C132—C133	1.390 (2)	1.382 (3)	1.392 (2)	1.388 (2)	1.394 (2)	1.394 (2)
C132—H132	0.95 (2)	0.94 (3)	1.00 (2)	0.94 (3)	0.96 (2)	0.95 (2)
C133—C134	1.382 (3)	1.379 (3)	1.385 (3)	1.381 (3)	1.386 (2)	1.386 (2)
C133—H133	0.96 (2)	0.95 (3)	0.99 (3)	0.96 (3)	0.96 (2)	0.98 (2)
C134—C135	1.387 (3)	1.384 (3)	1.389 (3)	1.390 (3)	1.392 (2)	1.390 (3)
C134—H134	0.94 (2)	0.95 (3)	0.95 (3)	0.97 (3)	0.97 (2)	0.96 (2)
C135—C136	1.387 (2)	1.381 (3)	1.389 (2)	1.386 (2)	1.389 (2)	1.386 (2)

C135—H135	0.92 (2)	0.93 (3)	0.94 (3)	0.92 (3)	0.95 (2)	0.94 (2)
C136—H136	0.98 (2)	0.96 (3)	0.93 (2)	0.95 (3)	0.95 (2)	0.96 (2)
C211—C212	1.391 (2)	1.377 (3)	1.394 (2)	1.393 (2)	1.395 (2)	1.392 (2)
C211—C216	1.389 (2)	1.387 (3)	1.391 (2)	1.389 (2)	1.393 (2)	1.394 (2)
C212—C213	1.389 (2)	1.386 (3)	1.391 (3)	1.389 (3)	1.388 (2)	1.389 (2)
C212—H212	0.89 (2)	0.86 (3)	0.95 (3)	0.92 (3)	0.94 (2)	0.93 (3)
C213—C214	1.378 (3)	1.373 (4)	1.378 (3)	1.380 (3)	1.378 (3)	1.380 (3)
C213—H213	0.95 (3)	0.96 (4)	0.91 (3)	0.97 (3)	0.96 (3)	0.96 (3)
C214—C215	1.373 (3)	1.367 (4)	1.375 (3)	1.369 (3)	1.382 (3)	1.379 (3)
C214—H214	0.92 (2)	0.93 (3)	0.92 (3)	0.92 (3)	0.91 (2)	0.92 (3)
C215—C216	1.394 (2)	1.384 (3)	1.395 (2)	1.392 (3)	1.395 (2)	1.393 (2)
C215—H215	0.96 (3)	0.96 (3)	0.96 (3)	0.95 (3)	0.93 (3)	0.93 (3)
C216—H216	0.97 (2)	0.94 (3)	0.98 (3)	0.95 (3)	0.96 (2)	0.96 (2)
C221—C222	1.3948 (19)	1.388 (3)	1.397 (2)	1.396 (2)	1.3966 (19)	1.394 (2)
C221—C226	1.392 (2)	1.390 (3)	1.391 (2)	1.392 (2)	1.3928 (19)	1.393 (2)
C222—C223	1.386 (2)	1.384 (3)	1.390 (3)	1.386 (3)	1.392 (2)	1.392 (2)
C222—H222	0.96 (2)	0.93 (3)	0.98 (3)	0.98 (3)	0.97 (2)	0.95 (2)
C223—C224	1.387 (3)	1.384 (4)	1.387 (3)	1.386 (3)	1.389 (2)	1.388 (3)
C223—H223	0.94 (2)	0.94 (3)	0.93 (3)	0.93 (3)	0.94 (2)	0.94 (3)
C224—C225	1.381 (2)	1.377 (3)	1.386 (3)	1.384 (3)	1.386 (2)	1.386 (2)
C224—H224	0.95 (2)	0.96 (3)	0.94 (3)	0.93 (3)	0.94 (2)	0.93 (2)
C225—C226	1.393 (2)	1.386 (3)	1.391 (2)	1.389 (2)	1.390 (2)	1.390 (2)
C225—H225	0.99 (2)	0.97 (3)	0.96 (3)	0.96 (3)	0.98 (2)	0.98 (2)
C226—H226	0.92 (2)	0.93 (3)	0.92 (2)	0.93 (3)	0.94 (2)	0.94 (2)
C231—C232	1.380 (2)	1.377 (3)	1.382 (3)	1.382 (3)	1.384 (2)	1.382 (2)
C231—C236	1.387 (2)	1.376 (3)	1.392 (2)	1.389 (3)	1.391 (2)	1.389 (2)
C232—C233	1.389 (3)	1.383 (4)	1.390 (3)	1.391 (3)	1.392 (3)	1.389 (3)
C232—H232	0.86 (3)	0.80 (4)	0.87 (3)	0.88 (3)	0.92 (3)	0.91 (3)
C233—C234	1.369 (3)	1.368 (5)	1.373 (4)	1.371 (4)	1.380 (3)	1.378 (3)
C233—H233	0.91 (3)	0.90 (5)	0.92 (4)	0.94 (4)	0.91 (3)	0.93 (3)
C234—C235	1.377 (3)	1.372 (4)	1.380 (3)	1.376 (3)	1.381 (3)	1.381 (3)
C234—H234	0.96 (3)	0.96 (4)	0.90 (3)	0.97 (3)	0.98 (3)	0.96 (3)
C235—C236	1.389 (3)	1.383 (4)	1.387 (3)	1.388 (3)	1.389 (2)	1.391 (3)
C235—H235	0.95 (3)	0.94 (4)	0.93 (3)	0.96 (3)	0.95 (3)	0.96 (3)
C236—H236	0.99 (2)	0.96 (3)	0.95 (3)	0.96 (3)	0.96 (2)	0.96 (3)
P1—C111	1.8137 (13)	1.8098 (18)	1.8135 (14)	1.8109 (15)	1.8135 (13)	1.8112 (14)

P1—C121	1.8206 (14)	1.8156 (19)	1.8226 (15)	1.8214 (16)	1.8218 (14)	1.8206 (15)
P1—C131	1.8145 (13)	1.8048 (18)	1.8171 (15)	1.8132 (15)	1.8142 (13)	1.8124 (14)
P2—C211	1.8211 (14)	1.813 (2)	1.8217 (16)	1.8182 (16)	1.8218 (14)	1.8212 (15)
P2—C221	1.8143 (14)	1.809 (2)	1.8168 (16)	1.8123 (16)	1.8154 (14)	1.8170 (15)
P2—C231	1.8201 (14)	1.816 (2)	1.8201 (16)	1.8164 (17)	1.8221 (14)	1.8220 (15)
C111—C112—H112	119.2 (13)	118.0 (17)	118.5 (14)	119.3 (15)	118.8 (13)	118.9 (14)
C111—C116—H116	121.9 (13)	123.5 (17)	120.5 (14)	122.0 (15)	121.5 (13)	122.1 (13)
C111—P1—Au1	119.55 (4)	119.52 (6)	119.56 (5)	119.46 (5)	119.56 (4)	119.50 (5)
C111—P1—C121	106.09 (6)	106.02 (9)	106.10 (7)	106.12 (7)	106.07 (6)	106.10 (7)
C111—P1—C131	104.01 (6)	104.11 (8)	103.92 (7)	103.99 (7)	103.86 (6)	104.00 (6)
C112—C111—P1	121.34 (10)	121.34 (14)	121.38 (11)	121.30 (11)	121.37 (10)	121.27 (11)
C112—C113—H113	120.8 (14)	121.7 (18)	120.7 (16)	121.7 (16)	120.5 (14)	120.7 (15)
C113—C112—C111	120.38 (13)	120.47 (18)	120.39 (15)	120.30 (15)	120.50 (13)	120.38 (14)
C113—C112—H112	120.4 (13)	121.5 (17)	121.1 (14)	120.4 (15)	120.7 (13)	120.7 (14)
C113—C114—H114	119.8 (13)	121.7 (18)	120.9 (15)	122.0 (15)	120.5 (13)	120.4 (14)
C114—C113—C112	119.99 (14)	120.21 (19)	120.06 (15)	120.17 (16)	119.93 (14)	119.97 (14)
C114—C113—H113	119.2 (14)	118.1 (18)	119.2 (15)	118.1 (16)	119.6 (14)	119.3 (15)
C114—C115—C116	120.48 (13)	120.43 (18)	120.54 (15)	120.28 (15)	120.38 (13)	120.34 (14)
C114—C115—H115	119.9 (14)	120.7 (19)	120.0 (15)	119.6 (15)	119.9 (13)	119.4 (14)
C115—C114—C113	119.93 (13)	119.69 (18)	119.82 (15)	119.91 (15)	119.87 (13)	119.95 (14)
C115—C114—H114	120.2 (13)	118.6 (18)	119.3 (15)	118.1 (15)	119.6 (13)	119.6 (14)
C115—C116—C111	119.94 (13)	119.78 (18)	119.89 (14)	120.12 (15)	119.99 (13)	119.98 (14)
C115—C116—H116	118.1 (13)	116.6 (17)	119.6 (14)	117.8 (15)	118.5 (13)	117.8 (13)
C116—C111—C112	119.28 (12)	119.40 (17)	119.29 (14)	119.21 (14)	119.33 (12)	119.37 (13)
C116—C111—P1	119.38 (10)	119.25 (14)	119.33 (11)	119.49 (12)	119.29 (10)	119.36 (11)
C116—C115—H115	119.6 (14)	118.8 (19)	119.5 (15)	120.1 (15)	119.7 (13)	120.2 (14)
C121—C122—C123	120.14 (17)	120.6 (2)	120.40 (19)	120.56 (19)	120.25 (16)	120.58 (17)
C121—C122—H122	119.5 (16)	120 (2)	120.9 (18)	119.3 (18)	118.4 (15)	119.5 (16)
C121—C126—C125	120.33 (18)	120.3 (2)	120.40 (19)	120.5 (2)	120.40 (16)	120.45 (17)
C121—C126—H126	120.4 (16)	118 (2)	120.7 (17)	118.5 (17)	119.8 (16)	119.9 (16)
C121—P1—Au1	113.09 (5)	113.27 (7)	113.07 (5)	113.13 (6)	113.20 (5)	113.19 (5)
C122—C121—C126	118.70 (14)	118.5 (2)	118.69 (16)	118.72 (16)	118.80 (14)	118.66 (15)
C122—C121—P1	123.17 (12)	123.38 (16)	123.17 (13)	123.13 (13)	123.14 (11)	123.19 (12)
C122—C123—H123	119.0 (18)	118 (2)	118.8 (19)	119.3 (19)	117.6 (17)	117.9 (18)
C123—C122—H122	120.4 (16)	119 (2)	118.7 (18)	120.1 (18)	121.3 (15)	120.0 (16)

C123—C124—C125	119.30 (17)	119.3 (2)	119.38 (19)	119.58 (19)	119.31 (16)	119.42 (17)
C123—C124—H124	120.1 (17)	120 (2)	121 (2)	120.3 (19)	119.6 (17)	120.3 (18)
C124—C123—C122	120.82 (19)	120.4 (3)	120.5 (2)	120.3 (2)	120.61 (18)	120.29 (19)
C124—C123—H123	120.2 (18)	121 (2)	120.7 (19)	120.3 (19)	121.7 (17)	121.7 (18)
C124—C125—C126	120.71 (19)	120.9 (3)	120.6 (2)	120.4 (2)	120.63 (17)	120.60 (18)
C124—C125—H125	120.8 (18)	122 (2)	124 (2)	123 (2)	122.0 (16)	121.6 (17)
C125—C124—H124	120.6 (17)	121 (2)	120 (2)	120.1 (19)	121.1 (17)	120.3 (18)
C125—C126—H126	119.2 (16)	122 (2)	118.9 (17)	121.0 (17)	119.8 (16)	119.6 (16)
C126—C121—P1	118.10 (12)	118.11 (17)	118.10 (13)	118.10 (14)	118.03 (11)	118.12 (12)
C126—C125—H125	118.4 (18)	117 (2)	116 (2)	116 (2)	117.4 (16)	117.8 (17)
C131—C132—H132	120.1 (13)	120.6 (18)	119.9 (14)	120.6 (15)	120.0 (13)	119.1 (14)
C131—C136—H136	119.3 (13)	119.2 (18)	119.5 (15)	119.4 (15)	119.7 (13)	119.7 (14)
C131—P1—Au1	108.41 (4)	108.29 (6)	108.44 (5)	108.41 (5)	108.53 (4)	108.47 (5)
C131—P1—C121	104.32 (6)	104.25 (9)	104.38 (7)	104.35 (7)	104.20 (6)	104.18 (7)
C132—C131—P1	123.20 (11)	123.03 (15)	123.07 (12)	123.10 (12)	123.28 (10)	123.17 (11)
C132—C133—H133	120.5 (14)	120.5 (19)	119.3 (15)	121.6 (16)	121.0 (14)	120.6 (14)
C133—C132—C131	120.05 (14)	119.9 (2)	119.95 (16)	120.05 (16)	120.16 (14)	119.97 (15)
C133—C132—H132	119.9 (13)	119.5 (18)	120.1 (14)	119.4 (15)	119.8 (13)	120.9 (14)
C133—C134—C135	120.18 (14)	120.3 (2)	120.08 (16)	120.26 (16)	120.02 (14)	119.98 (15)
C133—C134—H134	119.1 (14)	120.7 (19)	118.8 (15)	120.2 (16)	119.8 (14)	120.0 (14)
C134—C133—C132	120.18 (15)	120.1 (2)	120.25 (16)	120.08 (17)	120.15 (14)	120.22 (15)
C134—C133—H133	119.4 (14)	119.4 (19)	120.5 (15)	118.3 (16)	118.8 (14)	119.2 (15)
C134—C135—H135	122.7 (14)	123.5 (19)	122.4 (16)	123.4 (16)	122.2 (14)	122.5 (15)
C135—C134—H134	120.7 (14)	118.9 (19)	121.1 (16)	119.5 (16)	120.2 (14)	120.0 (15)
C135—C136—C131	120.18 (14)	120.3 (2)	120.20 (16)	120.15 (16)	120.26 (14)	120.24 (15)
C135—C136—H136	120.5 (13)	120.4 (18)	120.3 (15)	120.4 (15)	120.0 (13)	120.0 (14)
C132—C131—C136	119.41 (13)	119.61 (18)	119.47 (14)	119.58 (15)	119.36 (13)	119.41 (13)
C136—C131—P1	117.38 (10)	117.34 (15)	117.45 (12)	117.31 (12)	117.35 (10)	117.42 (11)
C136—C135—C134	120.00 (15)	119.8 (2)	120.05 (16)	119.88 (17)	120.05 (14)	120.18 (15)
C136—C135—H135	117.1 (14)	116.4 (19)	117.4 (16)	116.6 (16)	117.5 (14)	117.2 (15)
C211—C212—H212	121.2 (15)	119 (2)	118.5 (16)	119.4 (17)	119.2 (14)	119.1 (15)
C211—C216—C215	120.41 (16)	120.7 (2)	120.24 (17)	120.31 (18)	120.28 (15)	120.19 (16)
C211—C216—H216	120.0 (13)	120.5 (18)	119.1 (15)	120.1 (16)	120.7 (14)	120.4 (14)
C211—P2—Au1	109.36 (5)	109.45 (7)	109.42 (5)	109.54 (5)	109.47 (5)	109.50 (5)
C212—C211—P2	118.31 (12)	118.32 (16)	118.18 (13)	118.08 (13)	118.23 (11)	118.14 (12)
C212—C213—H213	120.0 (16)	119 (2)	118.6 (18)	120.2 (17)	120.7 (15)	121.3 (16)

C213—C212—C211	120.60 (17)	120.6 (2)	120.45 (18)	120.37 (19)	120.61 (16)	120.49 (17)
C213—C212—H212	118.2 (15)	121 (2)	121.0 (16)	120.3 (17)	120.2 (14)	120.4 (15)
C213—C214—H214	119.1 (16)	121 (2)	119.4 (18)	118.9 (18)	120.2 (16)	119.9 (17)
C214—C213—C212	120.16 (17)	120.1 (2)	120.30 (18)	120.16 (19)	120.23 (16)	120.19 (17)
C214—C213—H213	119.9 (15)	120 (2)	121.1 (18)	119.6 (17)	119.1 (15)	118.5 (16)
C214—C215—C216	120.31 (17)	120.0 (2)	120.47 (19)	120.40 (19)	120.16 (16)	120.29 (17)
C214—C215—H215	121.3 (15)	120 (2)	121.5 (17)	120.5 (17)	119.5 (15)	119.8 (16)
C215—C214—C213	119.91 (16)	120.0 (2)	119.80 (17)	119.99 (18)	119.97 (15)	119.93 (16)
C215—C214—H214	120.9 (16)	119 (2)	120.8 (18)	121.1 (18)	119.8 (16)	120.2 (17)
C215—C216—H216	119.5 (13)	118.8 (18)	120.6 (15)	119.6 (16)	119.0 (14)	119.4 (14)
C216—C211—C212	118.61 (14)	118.55 (19)	118.72 (15)	118.76 (16)	118.74 (13)	118.89 (14)
C216—C211—P2	123.01 (11)	123.07 (16)	123.04 (12)	123.10 (13)	122.97 (11)	122.92 (11)
C216—C215—H215	118.4 (15)	120 (2)	118.1 (17)	119.1 (17)	120.3 (15)	119.8 (16)
C221—C222—H222	118.0 (14)	118.2 (19)	118.7 (15)	117.7 (16)	118.5 (14)	119.0 (15)
C221—C226—H226	119.3 (13)	118.8 (18)	118.1 (15)	119.5 (15)	118.8 (13)	118.6 (14)
C221—P2—Au1	119.58 (5)	119.49 (6)	119.53 (5)	119.50 (5)	119.50 (5)	119.52 (5)
C221—P2—C211	105.83 (6)	105.80 (9)	105.87 (7)	105.74 (7)	105.86 (6)	105.86 (7)
C221—P2—C231	104.33 (7)	104.47 (9)	104.29 (7)	104.44 (8)	104.43 (6)	104.36 (7)
C222—C221—P2	122.00 (11)	121.89 (16)	121.86 (12)	121.96 (13)	121.80 (11)	121.80 (12)
C222—C223—C224	120.07 (15)	120.2 (2)	120.03 (16)	119.96 (17)	120.06 (14)	120.05 (15)
C222—C223—H223	119.8 (15)	119 (2)	117.7 (16)	118.9 (17)	118.1 (15)	118.3 (15)
C223—C222—C221	120.24 (15)	120.1 (2)	120.10 (16)	120.21 (17)	120.03 (14)	119.99 (15)
C223—C222—H222	121.7 (14)	121.7 (19)	121.2 (15)	122.1 (16)	121.5 (14)	121.0 (15)
C223—C224—H224	117.9 (14)	117.6 (19)	118.2 (16)	119.7 (17)	119.5 (14)	119.6 (15)
C224—C223—H223	120.1 (15)	120.7 (19)	122.3 (16)	121.1 (17)	121.8 (14)	121.7 (15)
C224—C225—C226	120.10 (16)	120.1 (2)	120.00 (17)	119.88 (18)	120.11 (15)	120.02 (16)
C224—C225—H225	121.0 (14)	120.6 (19)	119.1 (16)	118.9 (16)	118.3 (14)	118.9 (15)
C225—C224—C223	120.12 (15)	120.0 (2)	120.14 (16)	120.30 (17)	120.06 (14)	120.14 (15)
C225—C224—H224	122.0 (14)	122.4 (19)	121.6 (16)	120.0 (17)	120.5 (14)	120.2 (16)
C225—C226—H226	120.6 (13)	121.0 (18)	121.6 (15)	120.30 (16)	120.24 (13)	120.19 (14)
C221—C226—C225	120.09 (14)	120.2 (2)	120.26 (15)	120.2 (15)	121.0 (13)	121.2 (14)
C226—C221—C222	119.38 (13)	119.40 (19)	119.46 (15)	119.35 (15)	119.50 (13)	119.61 (14)
C226—C221—P2	118.60 (10)	118.69 (15)	118.66 (12)	118.68 (12)	118.69 (10)	118.57 (11)
C226—C225—H225	118.9 (14)	119.3 (19)	120.9 (16)	121.2 (16)	121.6 (14)	121.1 (15)
C231—C232—C233	120.51 (19)	120.7 (3)	120.4 (2)	120.4 (2)	120.36 (17)	120.52 (18)
C231—C232—H232	121.7 (19)	122 (3)	122 (2)	122 (2)	121.5 (17)	121.3 (18)

C231—C236—H236	119.2 (14)	120 (2)	119.8 (16)	118.3 (17)	119.7 (15)	119.5 (15)
C231—P2—Au1	111.20 (5)	111.09 (7)	111.19 (5)	111.13 (6)	111.05 (5)	111.09 (5)
C231—P2—C211	105.54 (6)	105.55 (9)	105.55 (7)	105.48 (7)	105.55 (6)	105.51 (7)
C232—C231—C236	118.63 (15)	118.7 (2)	118.71 (17)	118.64 (17)	118.96 (14)	118.91 (15)
C232—C231—P2	123.47 (13)	123.50 (17)	123.36 (14)	123.46 (14)	123.26 (12)	123.38 (13)
C232—C233—H233	119 (2)	121 (3)	118 (2)	121 (2)	121 (2)	121 (2)
C233—C232—H232	117.8 (19)	117 (3)	117 (2)	118 (2)	118.1 (17)	118.1 (18)
C233—C234—C235	119.30 (19)	119.0 (3)	119.4 (2)	119.4 (2)	119.26 (17)	119.29 (18)
C233—C234—H234	120.9 (17)	120 (2)	119 (2)	120.1 (19)	119.7 (16)	119.6 (17)
C234—C233—C232	120.7 (2)	120.5 (3)	120.7 (2)	120.7 (2)	120.54 (18)	120.5 (2)
C234—C233—H233	120 (2)	118 (3)	121 (2)	118 (2)	118 (2)	118 (2)
C234—C235—C236	120.41 (18)	120.8 (3)	120.4 (2)	120.4 (2)	120.52 (17)	120.44 (18)
C234—C235—H235	120.0 (16)	120 (2)	122.3 (18)	120.3 (18)	120.6 (16)	121.4 (17)
C235—C234—H234	119.7 (17)	121 (2)	122 (2)	120.5 (19)	121.1 (16)	121.1 (17)
C231—C236—C235	120.41 (17)	120.3 (2)	120.48 (18)	120.49 (19)	120.35 (16)	120.31 (17)
C235—C236—H236	120.2 (14)	120 (2)	119.7 (16)	121.1 (17)	119.9 (15)	120.2 (15)
C236—C231—P2	117.84 (12)	117.75 (17)	117.84 (13)	117.79 (13)	117.67 (11)	117.58 (12)
C236—C235—H235	119.6 (16)	119 (2)	117.2 (18)	119.3 (18)	118.8 (16)	118.1 (17)
P1—Au1—Cl1	108.733 (12)	108.802 (16)	108.686 (13)	108.738 (14)	108.649 (12)	108.688 (12)
P2—Au1—Cl1	114.206 (12)	114.189 (17)	114.205 (14)	114.193 (14)	114.185 (12)	114.168 (13)
P2—Au1—P1	136.695 (12)	136.642 (16)	136.754 (13)	136.711 (14)	136.814 (12)	136.790 (13)
Au1—P1—C111—C112	−154.15 (10)	−154.18 (14)	−154.11 (11)	−154.07 (12)	−154.00 (10)	−154.03 (11)
Au1—P1—C111—C116	25.52 (13)	25.47 (17)	25.66 (14)	25.61 (15)	25.64 (12)	25.62 (13)
Au1—P1—C121—C122	−149.87 (14)	−150.0 (2)	−149.73 (15)	−149.83 (16)	−149.33 (13)	−149.33 (14)
Au1—P1—C121—C126	32.22 (15)	32.4 (2)	32.68 (16)	32.85 (17)	32.84 (14)	32.86 (15)
Au1—P1—C131—C132	−131.57 (12)	−131.50 (16)	−131.69 (13)	−131.63 (13)	−131.70 (11)	−131.86 (12)
Au1—P1—C131—C136	47.40 (12)	47.15 (16)	47.19 (13)	47.05 (14)	47.04 (11)	47.17 (12)
Au1—P2—C211—C212	31.16 (14)	31.53 (19)	30.75 (15)	30.83 (15)	30.37 (13)	30.47 (14)
Au1—P2—C211—C216	−145.75 (12)	−145.61 (17)	−146.43 (13)	−146.26 (14)	−146.95 (11)	−146.91 (12)
Au1—P2—C221—C222	−161.87 (11)	−161.83 (15)	−161.80 (12)	−161.75 (12)	−161.87 (10)	−161.73 (11)
Au1—P2—C221—C226	19.97 (13)	20.13 (19)	19.80 (15)	19.84 (15)	19.76 (13)	19.82 (14)
Au1—P2—C231—C232	−119.34 (18)	−119.4 (3)	−119.01 (19)	−119.1 (2)	−119.13 (16)	−119.08 (17)
Au1—P2—C231—C236	57.60 (15)	57.2 (2)	57.30 (16)	57.03 (17)	57.01 (14)	56.89 (15)
C111—C112—C113—C114	−0.3 (2)	−0.9 (3)	−0.4 (3)	−0.8 (3)	−0.4 (2)	−0.6 (3)
C111—P1—C121—C122	−16.95 (17)	−17.0 (2)	−16.81 (18)	−16.96 (19)	−16.32 (15)	−16.38 (17)

C111—P1—C121—C126	165.14 (14)	165.31 (19)	165.60 (15)	165.72 (15)	165.84 (13)	165.81 (14)
C111—P1—C131—C132	100.20 (13)	100.33 (18)	100.11 (14)	100.25 (15)	100.08 (13)	99.94 (13)
C111—P1—C131—C136	−80.83 (12)	−81.03 (17)	−81.01 (13)	−81.07 (14)	−81.19 (12)	−81.03 (13)
C112—C111—C116—C115	−0.7 (2)	−0.9 (3)	−0.7 (2)	−0.8 (2)	−0.9 (2)	−0.9 (2)
C112—C113—C114—C115	0.1 (3)	1.1 (3)	0.2 (3)	0.7 (3)	0.1 (2)	0.5 (3)
C113—C114—C115—C116	−0.2 (2)	−1.2 (3)	−0.3 (3)	−0.7 (3)	−0.2 (2)	−0.6 (2)
C114—C115—C116—C111	0.5 (2)	1.1 (3)	0.5 (2)	0.7 (3)	0.6 (2)	0.8 (2)
C116—C111—C112—C113	0.6 (2)	0.8 (3)	0.6 (2)	0.9 (3)	0.8 (2)	0.8 (2)
C121—C122—C123—C124	−0.3 (4)	−0.6 (5)	−0.5 (4)	−0.5 (4)	−0.6 (3)	−0.7 (4)
C121—P1—C111—C112	76.60 (13)	76.40 (18)	76.65 (14)	76.66 (15)	76.60 (13)	76.60 (13)
C121—P1—C111—C116	−103.73 (12)	−103.95 (16)	−103.58 (13)	−103.67 (13)	−103.76 (11)	−103.75 (12)
C121—P1—C131—C132	−10.81 (14)	−10.62 (19)	−10.90 (15)	−10.80 (16)	−10.81 (14)	−11.02 (15)
C121—P1—C131—C136	168.16 (11)	168.03 (15)	167.98 (13)	167.88 (13)	167.93 (11)	168.00 (12)
C122—C121—C126—C125	−1.2 (3)	−0.8 (4)	−0.8 (3)	−0.4 (3)	−1.1 (3)	−1.1 (3)
C122—C123—C124—C125	−0.1 (4)	0.4 (6)	0.2 (4)	0.0 (4)	0.2 (4)	0.3 (4)
C123—C124—C125—C126	−0.1 (4)	−0.5 (6)	−0.2 (4)	0.2 (4)	−0.3 (4)	−0.4 (4)
C124—C125—C126—C121	0.8 (4)	0.6 (5)	0.5 (4)	0.0 (4)	0.7 (3)	0.8 (4)
C126—C121—C122—C123	0.9 (3)	0.8 (4)	0.8 (3)	0.7 (3)	1.0 (3)	1.0 (3)
C131—C132—C133—C134	−0.3 (3)	−0.3 (4)	−0.2 (3)	−0.4 (3)	−0.7 (2)	−0.6 (3)
C131—P1—C111—C112	−33.11 (13)	−33.25 (18)	−33.09 (15)	−33.09 (15)	−32.92 (13)	−32.96 (14)
C131—P1—C111—C116	146.56 (11)	146.41 (15)	146.68 (12)	146.58 (13)	146.73 (11)	146.70 (12)
C131—P1—C121—C122	92.54 (16)	92.5 (2)	92.61 (17)	92.54 (18)	92.95 (15)	93.05 (16)
C131—P1—C121—C126	−85.37 (15)	−85.1 (2)	−84.98 (16)	−84.78 (17)	−84.88 (14)	−84.77 (15)
C132—C131—C136—C135	0.6 (2)	0.2 (3)	0.3 (2)	0.2 (3)	0.2 (2)	0.6 (2)
C132—C133—C134—C135	0.8 (3)	0.5 (4)	0.5 (3)	0.8 (3)	0.9 (2)	0.8 (3)
C133—C134—C135—C136	−0.6 (3)	−0.4 (3)	−0.4 (3)	−0.6 (3)	−0.6 (2)	−0.3 (3)
C134—C135—C136—C131	−0.1 (2)	0.0 (3)	0.0 (3)	0.2 (3)	0.0 (2)	−0.4 (2)
C136—C131—C132—C133	−0.4 (2)	−0.1 (3)	−0.2 (3)	0.0 (3)	0.2 (2)	−0.1 (2)
C211—C212—C213—C214	−0.9 (3)	−1.1 (4)	−0.8 (3)	−0.8 (3)	−0.7 (3)	−0.9 (3)
C211—P2—C221—C222	74.27 (14)	74.27 (19)	74.26 (15)	74.28 (16)	74.15 (13)	74.24 (14)
C211—P2—C221—C226	−103.89 (12)	−103.77 (17)	−104.14 (13)	−104.13 (14)	−104.22 (12)	−104.21 (13)
C211—P2—C231—C232	−0.8 (2)	−0.8 (3)	−0.5 (2)	−0.4 (2)	−0.59 (18)	−0.50 (19)
C211—P2—C231—C236	176.09 (14)	175.7 (2)	175.86 (15)	175.67 (16)	175.55 (13)	175.47 (14)
C212—C211—C216—C215	0.2 (2)	0.3 (3)	0.1 (3)	0.2 (3)	0.0 (2)	−0.1 (3)
C212—C213—C214—C215	0.1 (3)	0.0 (4)	−0.2 (3)	−0.1 (3)	−0.2 (3)	0.0 (3)
C213—C214—C215—C216	0.8 (3)	1.3 (4)	1.1 (3)	1.0 (3)	1.1 (3)	0.9 (3)

C214—C215—C216—C211	−0.9 (3)	−1.4 (4)	−1.0 (3)	−1.1 (3)	−0.9 (3)	−0.9 (3)
C216—C211—C212—C213	0.7 (3)	0.9 (4)	0.8 (3)	0.7 (3)	0.9 (2)	1.0 (3)
C221—C222—C223—C224	−0.4 (3)	−0.7 (4)	−0.8 (3)	−0.6 (3)	−0.6 (2)	−1.0 (3)
C221—P2—C211—C212	161.21 (13)	161.52 (18)	160.80 (14)	160.84 (14)	160.42 (12)	160.57 (13)
C221—P2—C211—C216	−15.69 (14)	−15.6 (2)	−16.38 (16)	−16.25 (17)	−16.91 (14)	−16.81 (15)
C221—P2—C231—C232	110.45 (19)	110.5 (3)	110.9 (2)	110.8 (2)	110.79 (17)	110.83 (18)
C221—P2—C231—C236	−72.61 (15)	−72.9 (2)	−72.81 (16)	−73.12 (17)	−73.07 (14)	−73.19 (15)
C222—C221—C226—C225	−0.5 (2)	−0.4 (3)	−0.8 (3)	−0.8 (3)	−0.6 (2)	−0.7 (2)
C222—C223—C224—C225	0.2 (3)	0.3 (4)	0.4 (3)	0.3 (3)	0.4 (3)	0.6 (3)
C223—C224—C225—C226	−0.2 (3)	0.0 (4)	−0.3 (3)	−0.3 (3)	−0.2 (3)	−0.3 (3)
C224—C225—C226—C221	0.3 (3)	0.0 (4)	0.5 (3)	0.6 (3)	0.3 (2)	0.3 (3)
C226—C221—C222—C223	0.6 (2)	0.7 (3)	0.9 (3)	0.8 (3)	0.8 (2)	1.0 (2)
C231—C232—C233—C234	−1.0 (5)	−0.6 (7)	−1.0 (5)	−1.0 (5)	−0.9 (4)	−0.6 (5)
C231—P2—C211—C212	−88.55 (14)	−88.10 (19)	−88.99 (15)	−88.86 (15)	−89.22 (13)	−89.16 (14)
C231—P2—C211—C216	94.54 (14)	94.76 (19)	93.84 (15)	94.05 (16)	93.46 (13)	93.46 (14)
C231—P2—C221—C222	−36.83 (14)	−36.9 (2)	−36.84 (16)	−36.75 (16)	−37.00 (14)	−36.84 (15)
C231—P2—C221—C226	145.01 (12)	145.08 (16)	144.76 (13)	144.83 (14)	144.63 (11)	144.71 (12)
C232—C231—C236—C235	1.2 (3)	0.8 (4)	0.9 (3)	0.4 (3)	0.6 (3)	0.5 (3)
C232—C233—C234—C235	1.6 (5)	0.8 (7)	1.5 (5)	1.6 (5)	1.4 (4)	1.2 (5)
C233—C234—C235—C236	−0.8 (4)	−0.2 (6)	−0.8 (4)	−1.2 (5)	−1.0 (4)	−0.9 (4)
C234—C235—C236—C231	−0.6 (4)	−0.6 (5)	−0.4 (4)	0.2 (4)	0.0 (3)	0.0 (3)
C236—C231—C232—C233	−0.4 (4)	−0.2 (5)	−0.2 (4)	0.0 (4)	−0.1 (3)	−0.2 (4)
Cl1—Au1—P1—C111	7.16 (5)	7.14 (7)	7.13 (6)	7.14 (6)	7.16 (5)	7.18 (6)
Cl1—Au1—P1—C121	133.18 (5)	133.21 (7)	133.14 (5)	133.17 (6)	133.27 (5)	133.28 (5)
Cl1—Au1—P1—C131	−111.65 (5)	−111.68 (6)	−111.60 (5)	−111.60 (5)	−111.57 (5)	−111.63 (5)
Cl1—Au1—P2—C211	104.39 (5)	104.33 (7)	104.25 (5)	104.19 (6)	104.11 (5)	104.12 (5)
Cl1—Au1—P2—C221	−17.74 (5)	−17.77 (8)	−17.94 (6)	−17.92 (6)	−18.10 (5)	−18.14 (6)
Cl1—Au1—P2—C231	−139.44 (5)	−139.50 (7)	−139.54 (6)	−139.65 (6)	−139.74 (5)	−139.73 (5)
P1—Au1—P2—C211	−67.64 (5)	−67.69 (7)	−67.89 (6)	−67.93 (6)	−68.07 (5)	−68.02 (5)
P1—Au1—P2—C221	170.22 (5)	170.20 (7)	169.91 (6)	169.96 (6)	169.72 (5)	169.72 (5)
P1—Au1—P2—C231	48.52 (6)	48.48 (8)	48.32 (6)	48.23 (6)	48.09 (5)	48.12 (6)
P1—C111—C112—C113	−179.69 (12)	−179.52 (17)	−179.66 (13)	−179.44 (14)	−179.56 (12)	−179.50 (13)
P1—C111—C116—C115	179.59 (11)	179.43 (16)	179.57 (12)	179.49 (13)	179.45 (11)	179.40 (12)
P1—C121—C122—C123	−176.95 (18)	−176.9 (3)	−176.77 (19)	−176.6 (2)	−176.86 (16)	−176.79 (17)
P1—C121—C126—C125	176.86 (19)	177.0 (3)	176.9 (2)	177.0 (2)	176.88 (16)	176.85 (18)
P1—C131—C132—C133	178.57 (13)	178.53 (18)	178.66 (14)	178.62 (14)	178.88 (12)	178.95 (13)

P1—C131—C136—C135	−178.45 (12)	−178.46 (17)	−178.63 (13)	−178.55 (14)	−178.61 (12)	−178.50 (13)
P2—Au1—P1—C111	179.49 (5)	179.46 (7)	179.56 (5)	179.55 (6)	179.62 (5)	179.62 (5)
P2—Au1—P1—C121	−54.49 (5)	−54.47 (7)	−54.42 (6)	−54.42 (6)	−54.26 (5)	−54.28 (5)
P2—Au1—P1—C131	60.68 (5)	60.63 (7)	60.83 (5)	60.81 (6)	60.89 (5)	60.80 (5)
P2—C211—C212—C213	−176.32 (15)	−176.4 (2)	−176.48 (16)	−176.50 (16)	−176.58 (13)	−176.51 (14)
P2—C211—C216—C215	177.07 (14)	177.46 (19)	177.22 (15)	177.30 (15)	177.28 (13)	177.29 (14)
P2—C221—C222—C223	−177.59 (13)	−177.32 (18)	−177.46 (14)	−177.56 (15)	−177.59 (12)	−177.41 (13)
P2—C221—C226—C225	177.71 (13)	177.73 (18)	177.66 (14)	177.61 (14)	177.79 (12)	177.78 (13)
P2—C231—C232—C233	176.5 (2)	176.3 (3)	176.1 (3)	176.1 (3)	175.9 (2)	175.7 (2)
P2—C231—C236—C235	−175.88 (17)	−175.9 (2)	−175.63 (18)	−175.89 (19)	−175.70 (15)	−175.64 (16)

	118Koff	118Kon	215Koff	215Kon
Au1—Cl1	2.5439 (3)	2.5431 (3)	2.5428 (4)	2.5415 (4)
Au1—P1	2.3230 (4)	2.3221 (3)	2.3265 (4)	2.3242 (4)
Au1—P2	2.3121 (4)	2.3110 (3)	2.3138 (4)	2.3115 (4)
C111—C112	1.398 (2)	1.3979 (19)	1.395 (2)	1.391 (2)
C111—C116	1.3936 (18)	1.3937 (18)	1.391 (2)	1.390 (2)
C112—C113	1.392 (2)	1.391 (2)	1.390 (2)	1.388 (2)
C112—H112	0.97 (2)	0.98 (2)	0.98 (2)	0.97 (2)
C113—C114	1.389 (2)	1.388 (2)	1.382 (3)	1.383 (3)
C113—H113	0.95 (2)	0.93 (2)	0.93 (3)	0.93 (3)
C114—C115	1.393 (2)	1.389 (2)	1.381 (3)	1.378 (3)
C114—H114	0.95 (2)	0.95 (2)	0.94 (3)	0.94 (3)
C115—C116	1.389 (2)	1.3897 (19)	1.390 (2)	1.392 (2)
C115—H115	0.97 (2)	0.96 (2)	0.97 (2)	0.98 (2)
C116—H116	0.90 (2)	0.94 (2)	0.92 (2)	0.92 (2)
C121—C122	1.392 (2)	1.390 (2)	1.382 (3)	1.382 (3)
C121—C126	1.391 (2)	1.391 (2)	1.385 (3)	1.382 (3)
C122—C123	1.395 (2)	1.395 (2)	1.396 (3)	1.395 (3)
C122—H122	0.95 (3)	0.93 (3)	0.96 (3)	0.95 (3)
C123—C124	1.379 (3)	1.378 (3)	1.363 (4)	1.359 (4)
C123—H123	0.98 (3)	0.98 (3)	0.95 (4)	0.97 (4)
C124—C125	1.379 (3)	1.380 (3)	1.363 (4)	1.365 (4)
C124—H124	0.95 (3)	0.95 (3)	0.91 (3)	0.92 (3)
C125—C126	1.394 (2)	1.393 (2)	1.387 (3)	1.390 (3)
C125—H125	0.91 (3)	0.94 (3)	0.91 (4)	0.92 (4)

C126—H126	0.97 (3)	0.94 (3)	0.91 (3)	0.93 (3)
C131—C132	1.397 (2)	1.3952 (19)	1.393 (2)	1.391 (2)
C131—C136	1.398 (2)	1.3981 (19)	1.392 (2)	1.392 (2)
C132—C133	1.393 (2)	1.393 (2)	1.391 (3)	1.389 (3)
C132—H132	0.95 (2)	0.97 (2)	0.96 (2)	0.96 (3)
C133—C134	1.390 (2)	1.388 (2)	1.380 (3)	1.378 (3)
C133—H133	0.94 (2)	0.94 (2)	0.93 (3)	0.93 (3)
C134—C135	1.388 (2)	1.389 (2)	1.384 (3)	1.382 (3)
C134—H134	0.97 (2)	0.95 (2)	0.95 (3)	0.96 (3)
C135—C136	1.389 (2)	1.387 (2)	1.388 (3)	1.386 (3)
C135—H135	0.96 (2)	0.96 (2)	0.93 (3)	0.92 (3)
C136—H136	0.95 (2)	0.95 (2)	0.93 (2)	0.98 (2)
C211—C212	1.395 (2)	1.393 (2)	1.391 (2)	1.387 (3)
C211—C216	1.394 (2)	1.392 (2)	1.390 (2)	1.390 (3)
C212—C213	1.389 (2)	1.388 (2)	1.389 (3)	1.388 (3)
C212—H212	0.90 (3)	0.89 (2)	0.90 (3)	0.90 (3)
C213—C214	1.386 (3)	1.384 (3)	1.367 (4)	1.369 (4)
C213—H213	0.95 (3)	0.96 (3)	0.93 (3)	0.96 (3)
C214—C215	1.378 (3)	1.377 (3)	1.370 (3)	1.368 (4)
C214—H214	0.93 (3)	0.91 (2)	0.92 (3)	0.92 (3)
C215—C216	1.394 (2)	1.392 (2)	1.389 (3)	1.389 (3)
C215—H215	0.94 (3)	0.96 (3)	0.97 (3)	0.97 (3)
C216—H216	0.96 (3)	0.95 (2)	0.97 (3)	0.96 (3)
C221—C222	1.399 (2)	1.3954 (19)	1.395 (2)	1.388 (2)
C221—C226	1.395 (2)	1.3952 (19)	1.389 (2)	1.391 (2)
C222—C223	1.391 (2)	1.390 (2)	1.387 (3)	1.387 (3)
C222—H222	0.99 (2)	0.98 (2)	0.96 (3)	0.94 (3)
C223—C224	1.389 (2)	1.389 (2)	1.381 (3)	1.378 (3)
C223—H223	0.92 (3)	0.93 (2)	0.92 (3)	0.92 (3)
C224—C225	1.389 (2)	1.388 (2)	1.378 (3)	1.378 (3)
C224—H224	0.97 (3)	0.96 (2)	0.97 (3)	0.97 (3)
C225—C226	1.389 (2)	1.389 (2)	1.391 (2)	1.391 (3)
C225—H225	0.94 (2)	0.96 (2)	0.98 (3)	0.96 (3)
C226—H226	0.94 (2)	0.95 (2)	0.93 (2)	0.93 (3)
C231—C232	1.386 (2)	1.385 (2)	1.374 (3)	1.375 (3)
C231—C236	1.390 (2)	1.389 (2)	1.383 (3)	1.380 (3)

C232—C233	1.394 (3)	1.395 (3)	1.394 (3)	1.391 (4)
C232—H232	0.91 (3)	0.93 (3)	0.86 (3)	0.85 (4)
C233—C234	1.380 (3)	1.379 (3)	1.362 (4)	1.361 (4)
C233—H233	0.95 (3)	0.95 (3)	0.90 (4)	0.88 (4)
C234—C235	1.384 (3)	1.381 (3)	1.369 (4)	1.368 (4)
C234—H234	0.97 (3)	0.97 (3)	0.94 (3)	0.93 (4)
C235—C236	1.393 (2)	1.392 (2)	1.385 (3)	1.386 (3)
C235—H235	0.96 (3)	0.93 (3)	0.97 (3)	0.94 (3)
C236—H236	0.95 (3)	0.95 (2)	0.94 (3)	0.95 (3)
P1—C111	1.8137 (14)	1.8121 (13)	1.8133 (15)	1.8117 (15)
P1—C121	1.8211 (14)	1.8210 (14)	1.8201 (16)	1.8180 (17)
P1—C131	1.8131 (14)	1.8122 (13)	1.8154 (15)	1.8131 (16)
P2—C211	1.8206 (14)	1.8191 (14)	1.8200 (16)	1.8175 (17)
P2—C221	1.8147 (14)	1.8145 (14)	1.8155 (16)	1.8142 (17)
P2—C231	1.8216 (15)	1.8204 (14)	1.8214 (17)	1.8201 (18)
C111—C112—H112	119.0 (14)	119.3 (13)	119.3 (14)	119.6 (15)
C111—C116—H116	123.9 (14)	122.9 (13)	122.5 (14)	123.0 (14)
C111—P1—Au1	119.53 (5)	119.51 (4)	119.56 (5)	119.57 (5)
C111—P1—C121	106.04 (6)	106.04 (6)	105.98 (7)	105.98 (7)
C131—P1—C111	104.01 (6)	104.01 (6)	104.09 (7)	104.12 (7)
C112—C111—P1	121.11 (10)	121.16 (10)	121.44 (11)	121.44 (12)
C112—C113—H113	120.5 (15)	120.6 (14)	120.6 (15)	120.6 (16)
C113—C112—C111	120.30 (13)	120.33 (13)	120.39 (15)	120.45 (16)
C113—C112—H112	120.7 (14)	120.4 (13)	120.3 (14)	119.9 (15)
C113—C114—H114	120.0 (15)	119.6 (14)	119.4 (15)	119.7 (16)
C114—C113—C112	119.93 (14)	119.86 (13)	119.92 (16)	119.90 (17)
C114—C113—H113	119.5 (15)	119.5 (14)	119.5 (15)	119.5 (16)
C114—C115—H115	119.3 (14)	118.7 (14)	120.3 (15)	119.8 (15)
C113—C114—C115	119.93 (14)	120.04 (13)	120.11 (16)	120.15 (16)
C115—C114—H114	120.1 (15)	120.3 (14)	120.5 (15)	120.2 (16)
C115—C116—C111	120.13 (13)	120.05 (13)	120.20 (15)	120.14 (16)
C115—C116—H116	116.0 (14)	117.0 (13)	117.1 (14)	116.7 (14)
C116—C111—C112	119.46 (13)	119.40 (12)	119.11 (14)	119.17 (14)
C116—C111—P1	119.43 (10)	119.44 (10)	119.45 (12)	119.38 (12)
C116—C115—C114	120.24 (13)	120.30 (13)	120.26 (15)	120.18 (16)

C116—C115—H115	120.5 (14)	121.0 (14)	119.5 (15)	120.1 (15)
C121—C122—C123	120.09 (16)	120.20 (16)	120.2 (2)	120.4 (2)
C121—C122—H122	120.3 (16)	119.1 (16)	120.2 (18)	119.6 (19)
C121—C126—C125	120.18 (17)	120.23 (16)	120.6 (2)	120.6 (2)
C121—C126—H126	120.5 (16)	120.3 (16)	119.3 (19)	119.2 (19)
C121—P1—Au1	113.14 (5)	113.20 (5)	113.09 (6)	113.12 (6)
C122—C121—P1	122.89 (12)	123.04 (11)	123.47 (14)	123.49 (14)
C122—C123—H123	118.5 (18)	119.2 (17)	119 (2)	118 (2)
C123—C122—H122	119.6 (16)	120.7 (16)	119.6 (18)	120.0 (19)
C123—C124—C125	119.54 (16)	119.54 (16)	119.4 (2)	119.7 (2)
C123—C124—H124	118.7 (18)	118.3 (16)	120 (2)	121 (2)
C124—C123—C122	120.54 (18)	120.52 (17)	120.8 (2)	120.6 (2)
C124—C123—H123	120.9 (17)	120.2 (17)	120 (2)	121 (2)
C124—C125—C126	120.54 (17)	120.50 (17)	120.7 (2)	120.5 (2)
C124—C125—H125	121.5 (18)	120.3 (17)	123 (2)	122 (2)
C125—C124—H124	121.8 (18)	122.2 (16)	120 (2)	119 (2)
C125—C126—H126	119.2 (16)	119.5 (16)	120.0 (19)	120.0 (19)
C126—C121—C122	119.09 (14)	119.01 (14)	118.30 (17)	118.28 (18)
C126—C121—P1	117.98 (12)	117.90 (11)	118.20 (14)	118.20 (15)
C126—C125—H125	117.9 (18)	119.2 (17)	117 (2)	118 (2)
C131—C132—H132	119.2 (14)	119.7 (13)	119.4 (14)	119.1 (15)
C131—C136—H136	119.6 (14)	120.4 (14)	119.2 (15)	120.3 (15)
C131—P1—Au1	108.52 (5)	108.46 (4)	108.30 (5)	108.32 (5)
C131—P1—C121	104.22 (6)	104.22 (6)	104.49 (7)	104.39 (7)
C132—C131—C136	119.45 (13)	119.63 (13)	119.16 (15)	119.32 (15)
C132—C131—P1	123.14 (11)	122.99 (11)	123.23 (12)	123.25 (13)
C132—C133—H133	120.7 (15)	121.1 (14)	122.5 (16)	123.9 (17)
C133—C132—C131	120.00 (14)	119.84 (14)	120.20 (17)	120.09 (18)
C133—C132—H132	120.8 (14)	120.5 (13)	120.3 (14)	120.8 (15)
C135—C134—C133	120.09 (14)	120.12 (14)	120.26 (17)	120.20 (18)
C133—C134—H134	120.1 (14)	120.0 (14)	118.7 (16)	119.2 (16)
C134—C133—C132	120.14 (15)	120.19 (14)	120.04 (18)	120.12 (19)
C134—C133—H133	119.2 (15)	118.7 (14)	117.5 (16)	115.9 (17)
C134—C135—C136	120.05 (15)	120.03 (14)	119.88 (18)	120.01 (18)
C134—C135—H135	121.4 (15)	122.6 (14)	122.1 (16)	122.7 (17)
C135—C134—H134	119.7 (15)	119.9 (14)	121.0 (16)	120.6 (16)

C135—C136—C131	120.27 (14)	120.19 (14)	120.46 (17)	120.25 (17)
C135—C136—H136	120.1 (14)	119.4 (14)	120.3 (15)	119.5 (15)
C136—C131—P1	117.40 (11)	117.38 (10)	117.60 (12)	117.42 (12)
C136—C135—H135	118.3 (15)	117.1 (14)	117.9 (16)	117.2 (17)
C211—C212—H212	119.7 (16)	119.6 (16)	120.6 (17)	121.8 (18)
C211—C216—H216	121.5 (15)	121.2 (14)	120.3 (15)	121.6 (16)
C211—P2—Au1	109.53 (5)	109.52 (5)	109.27 (5)	109.33 (5)
C211—P2—C231	105.53 (7)	105.55 (6)	105.57 (7)	105.51 (8)
C212—C211—P2	118.13 (12)	118.19 (11)	118.54 (13)	118.50 (14)
C212—C213—H213	121.9 (16)	121.9 (15)	118.8 (19)	120.1 (18)
C213—C212—C211	120.61 (16)	120.69 (15)	120.6 (2)	120.7 (2)
C213—C212—H212	119.7 (16)	119.7 (15)	118.8 (17)	117.5 (18)
C213—C214—H214	117.2 (16)	119.0 (16)	118.4 (18)	118.4 (19)
C214—C213—C212	120.02 (16)	119.96 (16)	120.5 (2)	120.3 (2)
C214—C213—H213	118.1 (16)	118.1 (15)	120.7 (19)	119.6 (18)
C214—C215—C216	120.50 (16)	120.25 (16)	120.5 (2)	120.4 (2)
C214—C215—H215	121.6 (16)	120.2 (15)	121.6 (17)	120.5 (17)
C215—C214—C213	119.86 (15)	119.97 (15)	119.75 (19)	119.9 (2)
C215—C214—H214	122.9 (17)	121.0 (16)	121.9 (18)	121.7 (19)
C215—C216—C211	120.10 (15)	120.39 (15)	120.54 (19)	120.51 (19)
C215—C216—H216	118.4 (15)	118.4 (14)	119.1 (15)	117.9 (16)
C216—C211—C212	118.88 (14)	118.72 (13)	118.11 (16)	118.18 (17)
C216—C211—P2	122.93 (11)	123.03 (11)	123.26 (13)	123.22 (13)
C216—C215—H215	117.9 (16)	119.6 (15)	117.9 (17)	119.0 (17)
C221—C222—H222	118.8 (15)	118.0 (14)	117.6 (15)	117.7 (16)
C221—C226—H226	118.5 (14)	118.7 (13)	119.5 (15)	119.3 (15)
C221—P2—Au1	119.48 (5)	119.54 (5)	119.54 (5)	119.54 (5)
C221—P2—C211	105.95 (7)	105.87 (6)	105.78 (7)	105.74 (8)
C221—P2—C231	104.46 (7)	104.42 (7)	104.28 (8)	104.28 (8)
C222—C221—P2	121.83 (11)	121.90 (11)	121.94 (13)	122.00 (14)
C222—C223—H223	118.7 (16)	120.0 (15)	119.4 (17)	119.5 (17)
C223—C222—C221	120.05 (14)	120.13 (14)	120.20 (18)	120.20 (18)
C223—C222—H222	121.2 (15)	121.8 (14)	122.2 (15)	122.1 (16)
C223—C224—H224	119.8 (15)	119.2 (14)	118.0 (16)	118.6 (16)
C224—C223—C222	120.05 (15)	120.05 (14)	120.06 (17)	120.17 (18)
C224—C223—H223	121.2 (16)	120.0 (15)	120.6 (17)	120.3 (17)

C224—C225—C226	120.07 (15)	120.13 (15)	120.17 (19)	120.15 (19)
C224—C225—H225	119.6 (16)	119.9 (15)	122.0 (16)	121.9 (16)
C223—C224—C225	120.14 (15)	120.07 (14)	120.19 (18)	120.14 (18)
C225—C224—H224	120.1 (15)	120.7 (14)	121.8 (16)	121.3 (16)
C225—C226—C221	120.21 (14)	120.09 (13)	120.08 (16)	119.98 (17)
C225—C226—H226	121.2 (14)	121.2 (13)	120.4 (15)	120.7 (15)
C226—C221—C222	119.48 (13)	119.53 (13)	119.28 (16)	119.35 (16)
C226—C221—P2	118.67 (11)	118.55 (10)	118.75 (12)	118.62 (12)
C226—C225—H225	120.3 (16)	119.9 (15)	117.8 (16)	117.9 (16)
C231—C232—C233	120.31 (17)	120.38 (17)	120.3 (2)	120.2 (2)
C231—C232—H232	121.9 (18)	121.0 (17)	123 (2)	121 (2)
C231—C236—C235	120.48 (16)	120.44 (15)	120.7 (2)	120.5 (2)
C231—C236—H236	119.4 (16)	119.7 (15)	118.9 (18)	119.6 (18)
C231—P2—Au1	110.92 (5)	110.97 (5)	111.42 (6)	111.43 (6)
C232—C231—C236	119.00 (15)	118.93 (14)	118.51 (18)	118.68 (19)
C232—C231—P2	123.22 (12)	123.26 (12)	123.43 (15)	123.43 (16)
C232—C233—H233	120.1 (19)	119.8 (19)	120 (3)	120 (3)
C233—C232—H232	117.8 (18)	118.7 (17)	116 (2)	118 (2)
C233—C234—C235	119.48 (17)	119.39 (17)	119.4 (2)	119.2 (2)
C233—C234—H234	118.3 (17)	119.6 (16)	122 (2)	121 (2)
C234—C233—C232	120.50 (18)	120.46 (18)	120.7 (3)	120.8 (3)
C234—C233—H233	119.1 (19)	119.5 (19)	119 (3)	119 (3)
C234—C235—C236	120.22 (17)	120.39 (16)	120.4 (2)	120.5 (2)
C234—C235—H235	120.5 (16)	120.3 (16)	119.9 (19)	121 (2)
C235—C234—H234	122.2 (17)	121.0 (16)	119 (2)	119 (2)
C235—C236—H236	120.1 (16)	119.9 (15)	120.0 (18)	119.5 (18)
C236—C231—P2	117.67 (12)	117.69 (11)	118.01 (14)	117.83 (15)
C236—C235—H235	119.2 (16)	119.2 (16)	119.7 (19)	119 (2)
P1—Au1—Cl1	108.609 (12)	108.598 (12)	108.805 (14)	108.847 (14)
P2—Au1—Cl1	114.145 (12)	114.177 (12)	114.249 (14)	114.244 (15)
P2—Au1—P1	136.900 (13)	136.881 (12)	136.569 (13)	136.534 (14)
Au1—P1—C111—C112	−153.68 (10)	−153.76 (10)	−154.05 (12)	−153.99 (12)
Au1—P1—C111—C116	25.55 (13)	25.57 (13)	25.49 (15)	25.40 (15)
Au1—P1—C121—C122	−149.12 (13)	−149.11 (13)	−150.55 (18)	−150.58 (18)
Au1—P1—C121—C126	33.29 (14)	33.19 (14)	31.45 (18)	31.54 (19)

Au1—P1—C131—C132	−132.05 (12)	−131.99 (11)	−131.33 (13)	−131.23 (14)
Au1—P1—C131—C136	47.16 (12)	47.19 (12)	47.64 (14)	47.60 (14)
Au1—P2—C211—C212	29.95 (13)	30.00 (13)	32.04 (16)	31.97 (17)
Au1—P2—C211—C216	−147.33 (12)	−147.23 (12)	−144.50 (14)	−144.38 (15)
Au1—P2—C221—C222	−161.82 (11)	−161.82 (11)	−161.94 (13)	−161.87 (13)
Au1—P2—C221—C226	19.91 (14)	19.73 (13)	20.13 (16)	20.10 (16)
Au1—P2—C231—C232	−119.20 (16)	−119.14 (16)	−119.4 (2)	−119.4 (2)
Au1—P2—C231—C236	56.93 (14)	56.80 (14)	57.99 (18)	57.75 (19)
C111—C112—C113—C114	−0.8 (2)	−0.7 (2)	−0.7 (3)	−0.9 (3)
C111—P1—C121—C122	−16.23 (16)	−16.20 (15)	−17.7 (2)	−17.7 (2)
C111—P1—C121—C126	166.19 (13)	166.10 (13)	164.28 (17)	164.41 (17)
C111—P1—C131—C132	99.68 (13)	99.81 (13)	100.45 (15)	100.51 (15)
C111—P1—C131—C136	−81.11 (12)	−81.02 (12)	−80.58 (14)	−80.66 (14)
C112—C111—C116—C115	−1.2 (2)	−1.2 (2)	−0.6 (2)	−0.7 (3)
C112—C113—C114—C115	0.4 (2)	0.4 (2)	0.2 (3)	0.3 (3)
C113—C114—C115—C116	−0.4 (2)	−0.5 (2)	0.2 (3)	0.1 (3)
C114—C115—C116—C111	0.8 (2)	0.9 (2)	0.0 (3)	0.2 (3)
C116—C111—C112—C113	1.2 (2)	1.1 (2)	0.9 (3)	1.1 (3)
C121—C122—C123—C124	−0.1 (3)	−0.4 (3)	−0.9 (5)	−1.0 (5)
C121—P1—C111—C112	77.06 (13)	76.91 (13)	76.81 (15)	76.81 (15)
C121—P1—C111—C116	−103.72 (12)	−103.76 (11)	−103.66 (14)	−103.79 (14)
C121—P1—C131—C132	−11.23 (14)	−11.12 (14)	−10.53 (16)	−10.44 (17)
C121—P1—C131—C136	167.98 (11)	168.06 (11)	168.44 (13)	168.39 (13)
C122—C121—C126—C125	−0.8 (3)	−0.9 (3)	−1.4 (4)	−1.2 (4)
C122—C123—C124—C125	−0.5 (4)	0.0 (3)	0.9 (5)	1.1 (5)
C123—C124—C125—C126	0.4 (4)	0.0 (3)	−1.1 (5)	−1.2 (5)
C124—C125—C126—C121	0.2 (3)	0.5 (3)	1.4 (5)	1.3 (5)
C126—C121—C122—C123	0.7 (3)	0.9 (3)	1.1 (4)	1.1 (4)
C131—C132—C133—C134	−0.4 (2)	−0.6 (2)	−0.4 (3)	−0.3 (3)
C131—P1—C111—C112	−32.52 (13)	−32.68 (13)	−33.08 (15)	−32.98 (16)
C131—P1—C111—C116	146.71 (11)	146.65 (11)	146.45 (13)	146.42 (13)
C131—P1—C121—C122	93.20 (15)	93.24 (15)	91.89 (19)	91.9 (2)
C131—P1—C121—C126	−84.39 (14)	−84.46 (14)	−86.12 (18)	−85.99 (18)
C132—C131—C136—C135	0.6 (2)	0.6 (2)	0.8 (3)	0.7 (3)
C132—C133—C134—C135	0.7 (3)	0.8 (2)	0.8 (3)	0.7 (3)
C133—C134—C135—C136	−0.4 (2)	−0.4 (2)	−0.5 (3)	−0.3 (3)

C134—C135—C136—C131	−0.3 (2)	−0.3 (2)	−0.4 (3)	−0.4 (3)
C136—C131—C132—C133	−0.3 (2)	−0.1 (2)	−0.4 (3)	−0.4 (3)
C211—C212—C213—C214	−0.7 (3)	−0.8 (3)	−0.9 (4)	−0.5 (4)
C211—P2—C221—C222	74.05 (14)	74.11 (13)	74.40 (16)	74.41 (16)
C211—P2—C221—C226	−104.21 (12)	−104.34 (12)	−103.53 (14)	−103.62 (14)
C211—P2—C231—C232	−0.67 (18)	−0.58 (18)	−0.9 (2)	−0.8 (3)
C211—P2—C231—C236	175.46 (13)	175.35 (13)	176.49 (17)	176.30 (17)
C212—C211—C216—C215	0.2 (2)	0.2 (2)	0.5 (3)	0.6 (3)
C212—C213—C214—C215	−0.4 (3)	−0.2 (3)	0.2 (4)	0.0 (4)
C213—C214—C215—C216	1.3 (3)	1.2 (3)	0.8 (4)	0.9 (4)
C214—C215—C216—C211	−1.2 (3)	−1.2 (3)	−1.2 (3)	−1.2 (4)
C216—C211—C212—C213	0.8 (2)	0.8 (2)	0.5 (3)	0.2 (3)
C221—C222—C223—C224	−0.8 (3)	−0.7 (2)	−0.3 (3)	−0.6 (3)
C221—P2—C211—C212	160.08 (12)	160.13 (12)	161.95 (15)	161.89 (16)
C221—P2—C211—C216	−17.20 (15)	−17.11 (14)	−14.60 (17)	−14.46 (17)
C221—P2—C231—C232	110.81 (17)	110.80 (16)	110.3 (2)	110.3 (2)
C221—P2—C231—C236	−73.06 (14)	−73.27 (14)	−72.28 (18)	−72.53 (19)
C222—C221—C226—C225	−0.4 (2)	−0.6 (2)	−0.5 (3)	−0.6 (3)
C222—C223—C224—C225	0.4 (3)	0.4 (3)	0.4 (3)	0.6 (3)
C223—C224—C225—C226	−0.1 (3)	−0.1 (3)	−0.6 (3)	−0.6 (3)
C224—C225—C226—C221	0.1 (2)	0.2 (2)	0.7 (3)	0.7 (3)
C226—C221—C222—C223	0.7 (2)	0.8 (2)	0.3 (3)	0.6 (3)
C231—C232—C233—C234	−0.2 (4)	−0.6 (4)	−0.7 (7)	−0.8 (7)
C231—P2—C211—C212	−89.51 (13)	−89.52 (13)	−87.89 (16)	−87.98 (17)
C231—P2—C211—C216	93.22 (14)	93.24 (13)	95.57 (16)	95.67 (17)
C231—P2—C221—C222	−37.13 (14)	−37.04 (14)	−36.68 (16)	−36.59 (17)
C231—P2—C221—C226	144.61 (12)	144.52 (12)	145.39 (14)	145.38 (14)
C232—C231—C236—C235	1.0 (3)	0.8 (3)	1.5 (4)	1.2 (4)
C232—C233—C234—C235	0.6 (4)	0.8 (4)	1.2 (6)	1.2 (7)
C233—C234—C235—C236	−0.2 (4)	−0.3 (3)	−0.3 (5)	−0.4 (6)
C234—C235—C236—C231	−0.7 (3)	−0.5 (3)	−1.1 (4)	−0.8 (5)
C236—C231—C232—C233	−0.6 (3)	−0.2 (3)	−0.7 (5)	−0.4 (5)
Cl1—Au1—P1—C111	7.31 (5)	7.27 (5)	7.19 (6)	7.19 (6)
Cl1—Au1—P1—C121	133.28 (5)	133.29 (5)	133.05 (6)	133.08 (6)
Cl1—Au1—P1—C131	−111.58 (5)	−111.56 (5)	−111.65 (5)	−111.71 (5)
Cl1—Au1—P2—C211	104.05 (5)	104.02 (5)	104.60 (6)	104.64 (6)

Cl1—Au1—P2—C221	−18.33 (6)	−18.27 (5)	−17.35 (6)	−17.32 (7)
Cl1—Au1—P2—C231	−139.87 (5)	−139.85 (5)	−139.14 (6)	−139.13 (6)
P1—Au1—P2—C211	−68.19 (5)	−68.22 (5)	−67.31 (6)	−67.30 (6)
P1—Au1—P2—C221	169.42 (5)	169.49 (5)	170.74 (6)	170.74 (6)
P1—Au1—P2—C231	47.89 (6)	47.91 (5)	48.95 (6)	48.93 (7)
P1—C111—C112—C113	−179.58 (12)	−179.57 (12)	−179.53 (14)	−179.54 (15)
P1—C111—C116—C115	179.56 (11)	179.47 (11)	179.89 (13)	179.88 (14)
P1—C121—C122—C123	−176.85 (16)	−176.82 (16)	−176.9 (2)	−176.8 (2)
P1—C121—C126—C125	176.89 (16)	176.89 (16)	176.7 (2)	176.8 (2)
P1—C131—C132—C133	178.94 (12)	179.05 (12)	178.54 (15)	178.40 (16)
P1—C131—C136—C135	−178.62 (12)	−178.64 (12)	−178.21 (14)	−178.14 (15)
P2—Au1—P1—C111	179.84 (5)	179.81 (5)	179.40 (6)	179.42 (6)
P2—Au1—P1—C121	−54.19 (5)	−54.17 (5)	−54.74 (6)	−54.68 (6)
P2—Au1—P1—C131	60.95 (5)	60.98 (5)	60.57 (6)	60.52 (6)
P2—C211—C212—C213	−176.60 (14)	−176.54 (13)	−176.22 (18)	−176.29 (19)
P2—C211—C216—C215	177.42 (13)	177.41 (13)	177.06 (16)	176.96 (17)
P2—C221—C222—C223	−177.52 (13)	−177.62 (12)	−177.57 (16)	−177.45 (16)
P2—C221—C226—C225	177.91 (12)	177.92 (12)	177.46 (15)	177.47 (16)
P2—C231—C232—C233	175.5 (2)	175.7 (2)	176.7 (3)	176.7 (3)
P2—C231—C236—C235	−175.26 (15)	−175.32 (15)	−176.0 (2)	−176.1 (2)

Table S2. Difference of bond lengths (Å), bond angles (deg) and torsion angles (deg) between the light-on and the light-off stages at 177 K

Bond length					
Au1–P1	−0.0065(5)	C121–C122	−0.003(3)	C213–C214	−0.005(4)
Au1–P2	−0.0076(5)	C121–C126	−0.005(3)	C214–C215	−0.006(4)
Au1–Cl1	−0.0052(5)	C122–C123	−0.004(3)	C215–C216	−0.010(3)
P1–C111	−0.0039(18)	C123–C124	+0.001(4)	C221–C222	−0.007(3)
P1–C121	−0.0050(19)	C124–C125	−0.008(5)	C221–C226	−0.002(3)
P1–C131	−0.0097(18)	C125–C126	−0.003(4)	C222–C223	−0.002(3)
P2–C211	−0.008(2)	C131–C136	−0.010(3)	C223–C224	−0.003(4)
P2–C221	−0.005(2)	C131–C132	−0.002(3)	C224–C225	−0.004(3)
P2–C231	−0.004(2)	C132–C133	−0.008(3)	C225–C226	−0.007(3)
C111–C116	−0.004(2)	C133–C134	−0.003(3)	C231–C232	−0.003(3)
C111–C112	−0.011(3)	C134–C135	−0.003(3)	C231–C236	−0.011(3)
C112–C113	−0.005(3)	C135–C136	−0.006(3)	C232–C233	−0.006(4)
C113–C114	−0.005(3)	C211–C216	−0.002(3)	C233–C234	−0.001(5)
C114–C115	−0.003(3)	C211–C212	−0.014(3)	C234–C235	−0.005(4)
C115–C116	+0.001(3)	C212–C213	−0.003(3)	C235–C236	−0.006(4)

Bond angle					
P1–Au1–P2	−0.05(16)	C113–C112–C111	+0.09(18)	C231–C236–C235	−0.1(2)
P1–Au1–Cl1	+0.07(16)	C114–C115–C116	−0.05(18)	C233–C234–C235	−0.3(3)
P2–Au1–Cl1	−0.02(17)	C114–C113–C112	+0.22(19)	C234–C235–C236	+0.4(3)
C121–P1–Au1	+0.18(7)	C115–C114–C113	−0.24(18)	C234–C233–C232	−0.2(3)
C111–P1–Au1	−0.03(6)	C121–C122–C123	+0.4(2)	C236–C231–C232	+0.1(2)
C131–P1–Au1	−0.12(6)	C121–C126–C125	−0.0(2)	Au1–P1–C111–C112	−0.03(14)
C211–P2–Au1	+0.09(7)	C122–C121–C126	−0.2(2)	Au1–P1–C111–C116	−0.05(17)
C221–P2–Au1	−0.09(6)	C124–C125–C126	+0.2(3)	Au1–P1–C121–C122	−0.1(2)
C231–P2–Au1	−0.11(7)	C124–C123–C122	−0.4(3)	Au1–P1–C121–C126	+0.2(2)
C111–P1–C121	−0.07(9)	C125–C124–C123	0.0(2)	Au1–P1–C131–C132	+0.07(16)
C111–P1–C131	+0.10(8)	C133–C132–C131	−0.1(2)	Au1–P1–C131–C136	−0.25(16)
C121–P1–C131	−0.07(9)	C133–C134–C135	+0.1(2)	Au1–P2–C211–C212	+0.37(19)
C221–P2–C211	−0.03(9)	C134–C133–C132	−0.1(2)	Au1–P2–C211–C216	+0.14(17)
C231–P2–C211	+0.01(9)	C135–C136–C131	+0.1(2)	Au1–P2–C221–C222	+0.04(15)
C231–P2–C221	+0.14(9)	C136–C131–C132	+0.20(18)	Au1–P2–C221–C226	+0.16(19)

C112–C111–P1	0.00(14)	C136–C135–C134	−0.2(2)	Au1–P2–C231–C232	−0.1(3)
C116–C111–P1	−0.14(14)	C211–C212–C213	0.0(2)	Au1–P2–C231–C236	−0.4(2)
C122–C121–P1	+0.21(16)	C212–C211–C216	−0.06(19)	P1–Au1–P2–C211	−0.05(7)
C126–C121–P1	+0.01(17)	C214–C213–C212	−0.1(2)	P1–Au1–P2–C221	−0.02(7)
C132–C131–P1	−0.17(15)	C214–C215–C216	−0.3(2)	P1–Au1–P2–C231	−0.04(8)
C136–C131–P1	−0.04(15)	C215–C216–C211	+0.3(2)	P2–Au1–P1–C111	−0.03(7)
C212–C211–P2	+0.01(16)	C215–C214–C213	+0.1(2)	P2–Au1–P1–C121	+0.02(7)
C216–C211–P2	+0.06(16)	C222–C223–C224	+0.1(2)	P2–Au1–P1–C131	−0.05(7)
C222–C221–P2	−0.11(16)	C222–C221–C226	+0.02(19)	Cl1–Au1–P1–C111	−0.02(7)
C226–C221–P2	+0.09(15)	C223–C222–C221	−0.1(2)	Cl1–Au1–P1–C121	+0.03(7)
C232–C231–P2	+0.03(17)	C224–C225–C226	0.0(2)	Cl1–Au1–P1–C131	−0.03(6)
C236–C231–P2	−0.09(17)	C225–C226–C221	+0.1(2)	Cl1–Au1–P2–C211	−0.06(7)
C111–C116–C115	−0.16(18)	C225–C224–C223	−0.1(2)	Cl1–Au1–P2–C221	−0.03(8)
C112–C111–C116	+0.12(17)	C231–C232–C233	+0.2(3)	Cl1–Au1–P2–C231	−0.06(7)

Torsion angle					
P1–C111–C112–C113	+0.17(17)	C211–P2–C221–C222	0.00(19)	C131–C132–C133–C134	0.0(4)
P1–C111–C116–C115	−0.13(16)	C211–P2–C221–C226	+0.12(17)	C132–C131–C136–C135	−0.4(3)
P1–C121–C122–C123	+0.1(3)	C211–P2–C231–C232	+0.0(3)	C132–C133–C134–C135	−0.3(4)
P1–C121–C126–C125	+0.1(3)	C211–P2–C231–C236	−0.4(2)	C133–C134–C135–C136	+0.2(3)
P1–C131–C132–C133	−0.04(18)	C221–P2–C211–C212	+0.31(18)	C134–C135–C136–C131	+0.1(3)
P1–C131–C136–C135	−0.01(17)	C221–P2–C211–C216	+0.1(2)	C136–C131–C132–C133	+0.3(3)
P2–C211–C212–C213	−0.1(2)	C221–P2–C231–C232	+0.1(3)	C211–C212–C213–C214	−0.2(4)
P2–C211–C216–C215	+0.39(19)	C221–P2–C231–C236	−0.3(2)	C212–C213–C214–C215	−0.1(4)
P2–C221–C222–C223	+0.27(18)	C231–P2–C211–C212	+0.45(19)	C212–C211–C216–C215	+0.1(3)
P2–C221–C226–C225	+0.02(18)	C231–P2–C211–C216	+0.22(19)	C213–C214–C215–C216	+0.5(4)
P2–C231–C232–C233	−0.2(3)	C231–P2–C221–C222	−0.1(2)	C214–C215–C216–C211	−0.5(4)
P2–C231–C236–C235	0.0(2)	C231–P2–C221–C226	+0.07(16)	C216–C211–C212–C213	+0.2(4)
C111–P1–C121–C126	+0.17(19)	C111–C112–C113–C114	−0.6(3)	C221–C222–C223–C224	−0.3(4)
C111–P1–C121–C122	−0.1(2)	C112–C111–C116–C115	−0.2(3)	C222–C223–C224–C225	+0.1(4)
C111–P1–C131–C136	−0.20(17)	C112–C113–C114–C115	+1.0(3)	C222–C221–C226–C225	+0.1(3)
C111–P1–C131–C132	+0.13(18)	C113–C114–C115–C116	−1.0(3)	C223–C224–C225–C226	+0.2(4)
C121–P1–C111–C112	−0.20(18)	C114–C115–C116–C111	+0.6(3)	C224–C225–C226–C221	−0.3(4)
C121–P1–C111–C116	−0.22(16)	C116–C111–C112–C113	+0.2(3)	C226–C221–C222–C223	+0.1(3)
C121–P1–C131–C132	+0.19(19)	C121–C122–C123–C124	−0.3(5)	C231–C232–C233–C234	+0.4(7)
C121–P1–C131–C136	−0.13(15)	C122–C123–C124–C125	+0.5(6)	C232–C233–C234–C235	−0.8(7)

C131–P1–C111–C112	−0.14(18)	C122–C121–C126–C125	+0.4(4)	C232–C231–C236–C235	−0.4(4)
C131–P1–C111–C116	−0.15(15)	C123–C124–C125–C126	−0.4(6)	C233–C234–C235–C236	+0.6(6)
C131–P1–C121–C122	−0.1(2)	C124–C125–C126–C121	−0.2(5)	C234–C235–C236–C231	0.0(5)
C131–P1–C121–C126	+0.3(2)	C126–C121–C122–C123	−0.1(4)	C236–C231–C232–C233	+0.2(5)

Table S3. Wavelengths of emission band (λ_{max}) and lifetimes (τ) at every temperature

Temperature / K	λ_{max} / nm	τ / μs
295	502.2	3.69
275	507.8	8.13
255	509.2	15.0
235	512.2	21.5
215	514.0	23.6
195	515.8	25.9
175	516.8	26.7
155	517.2	27.2
135	519.0	28.0
115	520.0	28.6
95	522.0	29.6
75	523.0	30.8