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Supporting Information for

1,3-dipolar cycloaddition between a metal-azide (Ph_3PAuN_3) and a metal-acetylide ($Ph_3PAuC{\equiv}CPh$): an inorganic version of a click reaction.

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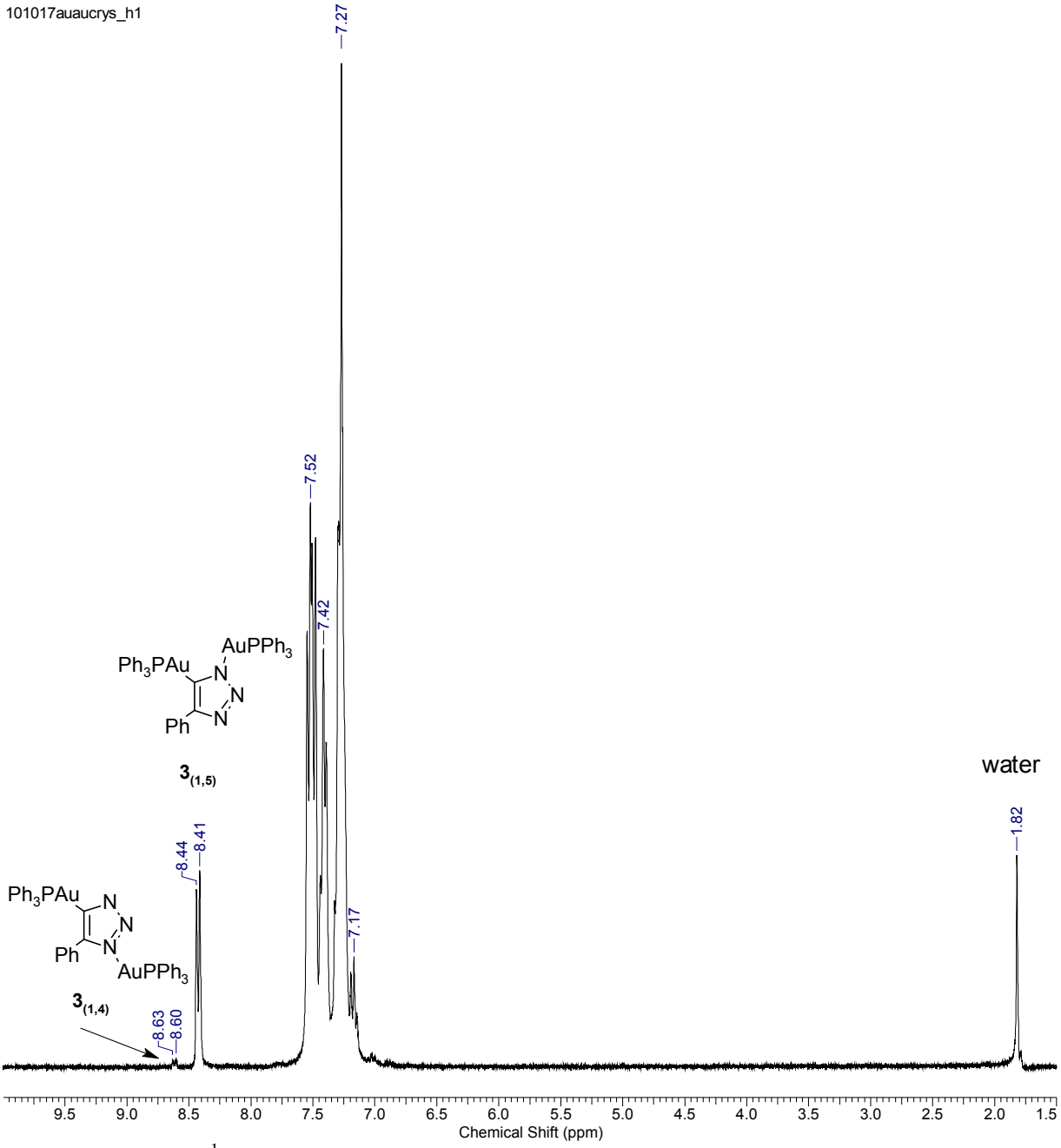

Figure S1. ^{1}H NMR spectrum of $\mathbf{3_{(1,5)}}$ (major) and $\mathbf{3_{(1,4)}}$ (minor) in $CDCl_3$ at 25 °C

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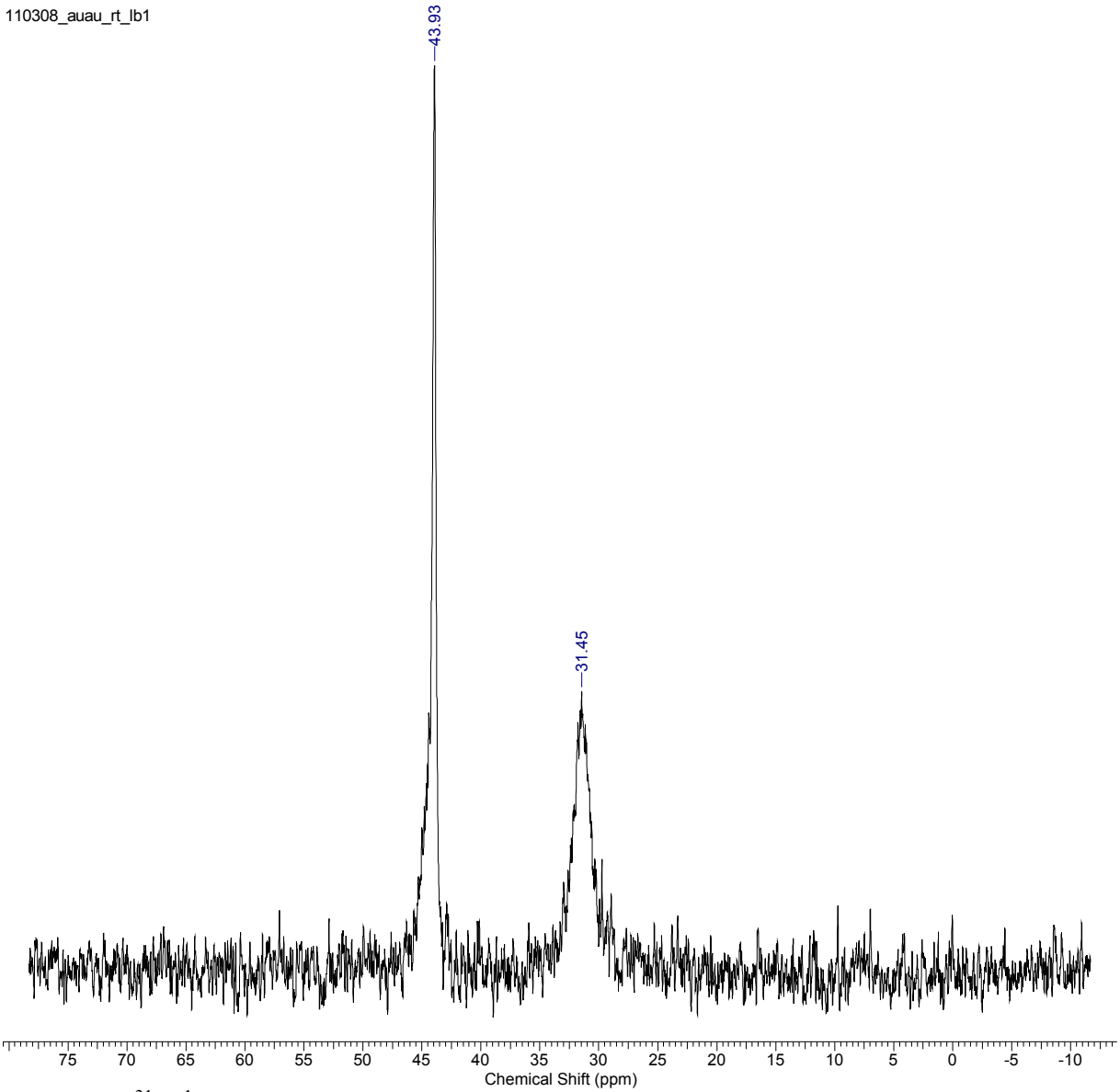

Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of $\mathbf{3_{(1,5)}}$ (major) and $\mathbf{3_{(1,4)}}$ (minor) in $CDCl_3$ at 25°C. $\mathbf{3_{(1,4)}}$ (minor) resonances hidden under $\mathbf{3_{(1,5)}}$ (major).

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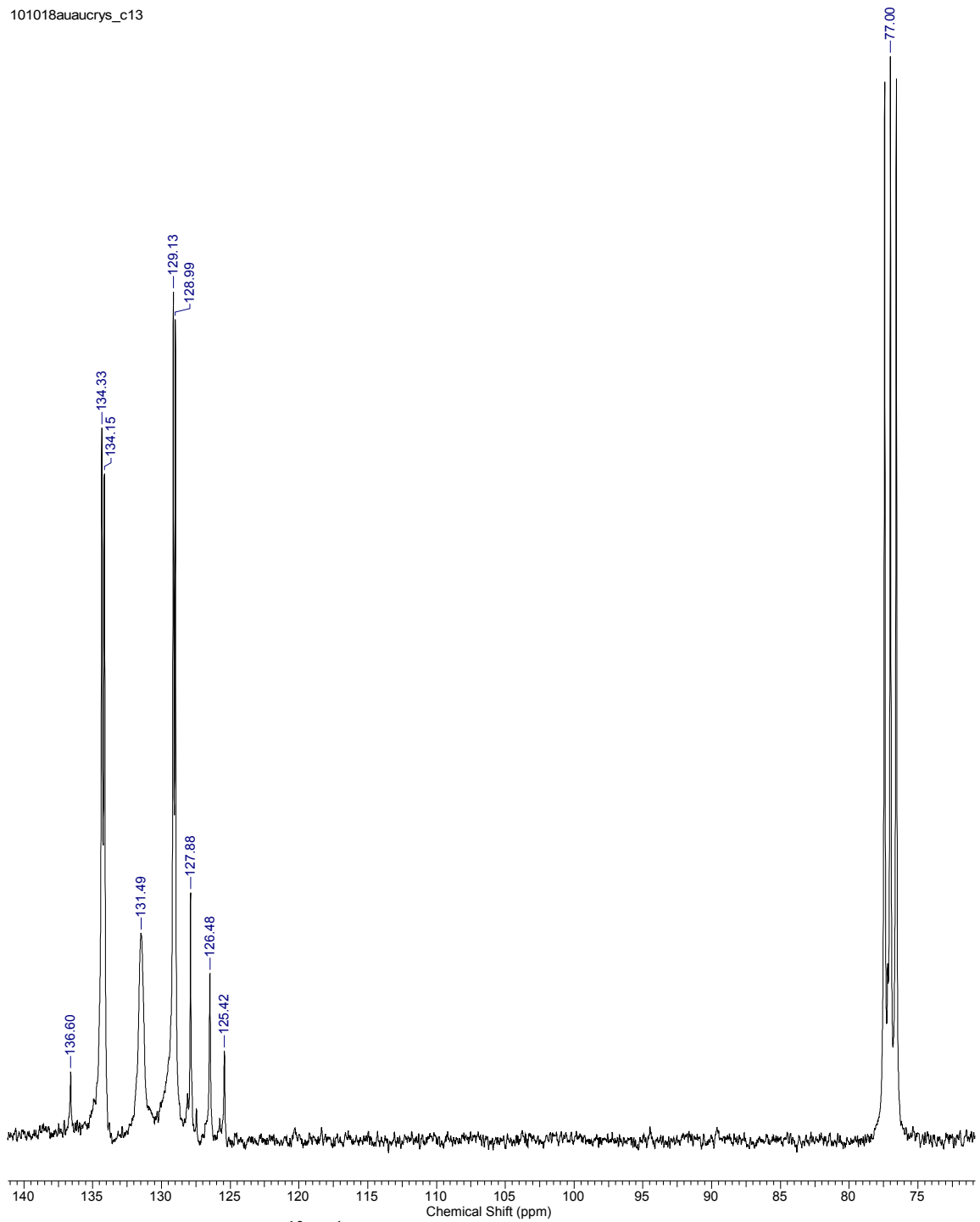

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{3_{(1,5)}}$ in $CDCl_3$ at 25°C

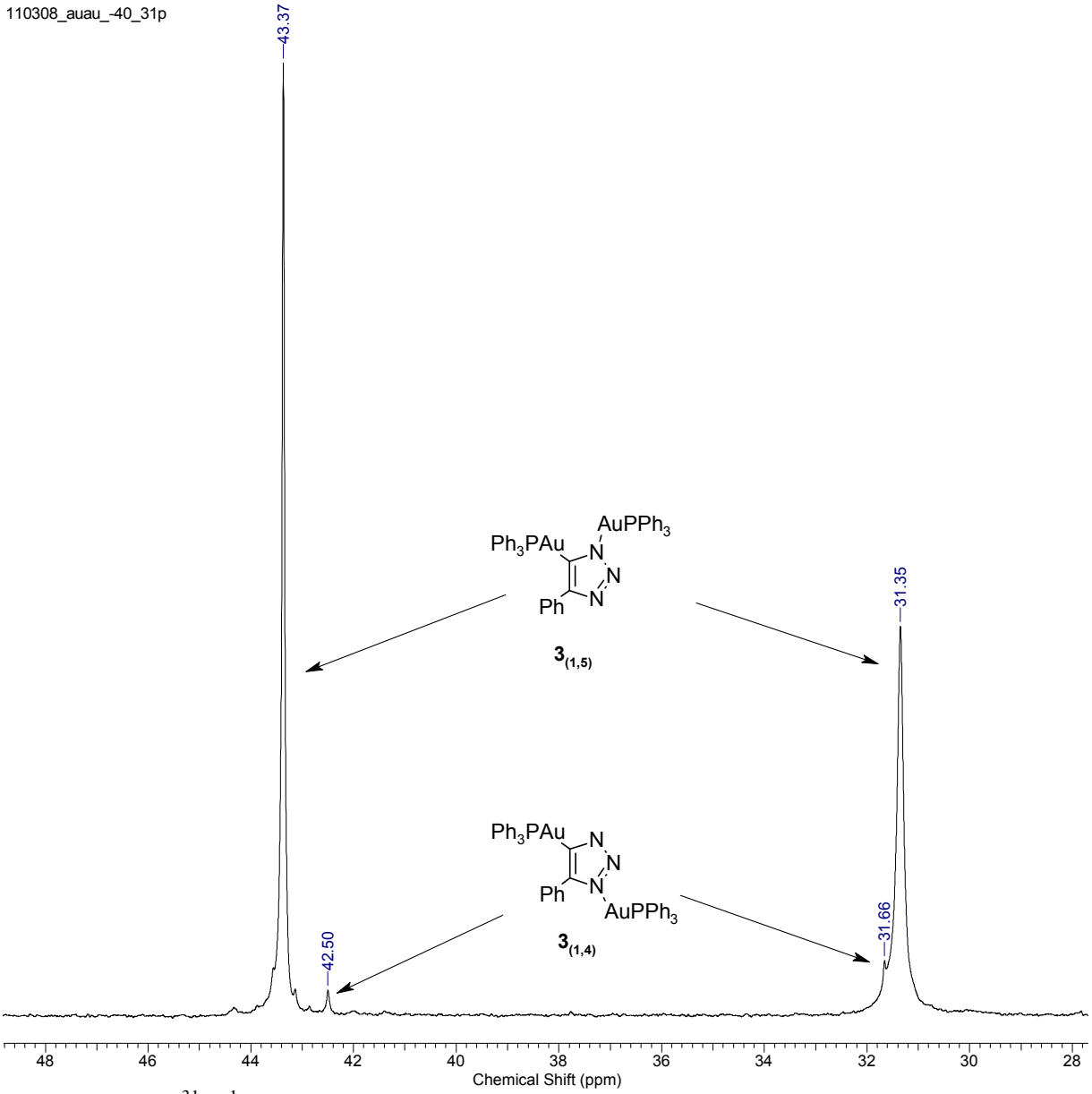

Figure S4. $^{31}P\{^{1}H\}$ NMR spectrum of $\mathbf{3_{(1,5)}}$ (major) and $\mathbf{3_{(1,4)}}$ (minor) in $CDCl_3$ at -40°C

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IR Spectrum.

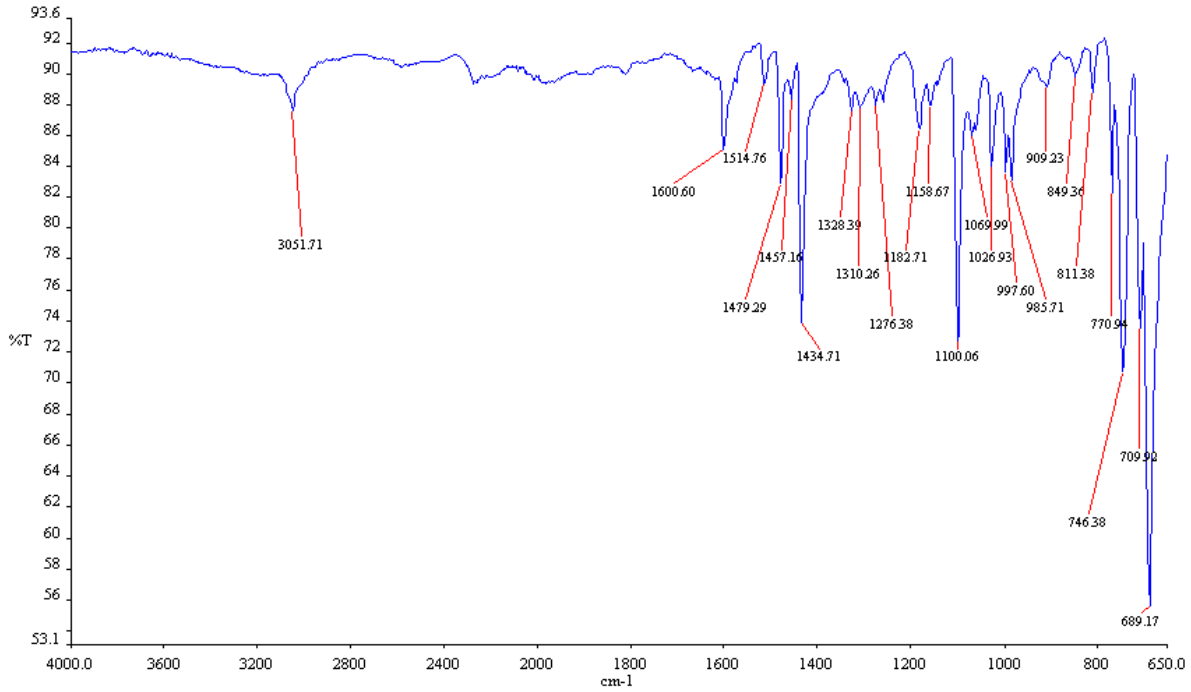

Figure S5. IR spectrum (neat) of $\mathbf{3}_{(1,5)}$ (major) and $\mathbf{3}_{(1,4)}$ (minor).

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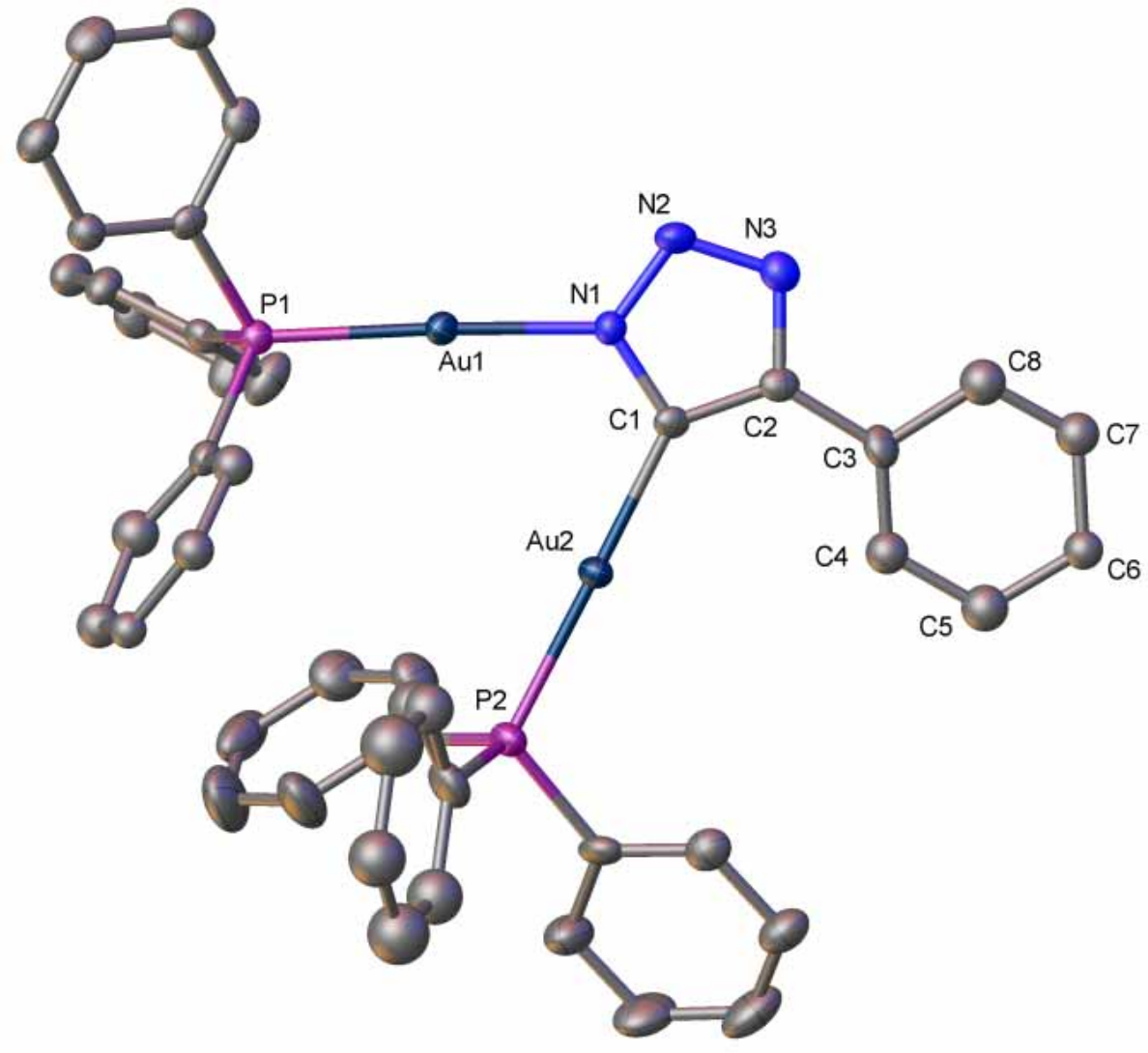

Figure S6. Molecular structure of $\mathbf{3}_{(1,5)}$ with ellipsoids drawn at the 50% probability level. Two lattice molecules of benzene, disordered atoms, and hydrogen atoms are removed for clarity.

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $\mathbf{3_{(1,5)}}$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Au1	8914(1)	5890(1)	3253(1)	19(1)
Au2	8468(1)	5595(1)	4198(1)	21(1)
P1	8059(1)	6682(1)	2920(1)	19(1)
P2	7329(1)	6217(1)	4476(1)	27(1)
N1	9633(2)	5158(2)	3574(1)	20(1)
N2	10267(2)	4683(2)	3452(1)	28(1)
N3	10514(2)	4236(2)	3737(1)	28(1)
C1	9453(3)	5018(2)	3941(1)	18(1)
C2	10022(3)	4430(3)	4039(1)	21(1)
C3	10111(3)	4014(3)	4390(1)	25(1)
C4	9562(7)	4050(8)	4675(3)	29(3)
C5	9657(7)	3636(8)	5001(3)	34(3)
C6	10293(7)	3069(8)	5028(4)	25(3)
C7	10815(9)	2945(7)	4711(4)	30(4)
C8	10753(10)	3388(9)	4404(4)	33(4)
C4'	9782(6)	4390(7)	4735(3)	25(3)
C5'	9847(6)	4009(8)	5075(3)	32(3)
C6'	10228(7)	3316(8)	5104(4)	30(3)
C7'	10589(9)	2975(7)	4803(4)	31(3)
C8'	10536(9)	3355(8)	4438(4)	29(4)
C9	7056(3)	5810(3)	4930(1)	27(1)
C10	6202(3)	5729(3)	5055(2)	44(2)
C11	6043(4)	5396(4)	5400(2)	55(2)
C12	6722(4)	5145(4)	5621(2)	51(2)
C13	7564(3)	5234(3)	5505(2)	38(1)
C14	7729(3)	5565(3)	5157(1)	31(1)
C15	7538(3)	7231(2)	4558(1)	38(1)
C16	7101(8)	7607(3)	4845(2)	49(3)
C17	7308(12)	8371(3)	4935(2)	61(4)
C18	7952(10)	8760(3)	4738(2)	51(4)

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C19	8388(6)	8385(4)	4451(4)	62(5)
C20	8181(5)	7620(4)	4361(3)	41(5)
C16'	7358(18)	7658(9)	4912(6)	49(6)
C17'	7669(19)	8424(9)	4966(4)	46(6)
C18'	8250(20)	8724(10)	4711(5)	60(6)
C19'	8434(12)	8337(10)	4380(6)	51(8)
C20'	8057(16)	7605(9)	4319(5)	42(8)
C21	6341(3)	6148(3)	4206(2)	34(1)
C22	5706(4)	6716(4)	4190(2)	61(2)
C23	4951(4)	6592(5)	3991(2)	75(2)
C24	4816(3)	5920(4)	3801(2)	57(2)
C25	5428(3)	5343(4)	3812(2)	48(2)
C26	6184(3)	5459(3)	4014(2)	42(1)
C27	7690(3)	7506(3)	3190(1)	21(1)
C28	6876(7)	7739(8)	3238(4)	35(3)
C29	6655(7)	8402(8)	3454(4)	31(3)
C30	7316(8)	8862(7)	3584(3)	21(3)
C31	8153(9)	8664(7)	3518(3)	27(3)
C32	8363(8)	8009(7)	3328(4)	26(3)
C28'	6852(6)	7477(8)	3359(4)	23(3)
C29'	6579(8)	8106(9)	3569(4)	34(4)
C30'	7072(10)	8729(9)	3619(4)	37(4)
C31'	7899(12)	8748(10)	3464(5)	46(5)
C32'	8195(10)	8115(9)	3251(5)	36(4)
C33	8582(3)	7108(3)	2517(1)	19(1)
C34	8365(3)	7843(3)	2378(1)	24(1)
C35	8780(3)	8130(3)	2065(1)	29(1)
C36	9408(3)	7694(3)	1890(1)	33(1)
C37	9624(3)	6971(3)	2023(1)	31(1)
C38	9219(3)	6676(3)	2338(1)	25(1)
C39	7120(3)	6174(3)	2733(1)	20(1)
C40	6770(3)	6362(3)	2393(1)	23(1)
C41	6122(3)	5905(3)	2238(1)	30(1)

C42	5813(3)	5265(3)	2423(1)	29(1)
C43	6139(3)	5086(3)	2771(2)	38(1)
C44	6798(3)	5532(3)	2924(2)	36(1)
C45	4057(4)	3795(4)	2519(2)	57(2)
C46	3524(4)	4396(4)	2590(2)	58(2)
C47	3201(4)	4522(3)	2931(2)	59(2)
C48	3421(4)	4032(4)	3221(2)	66(2)
C49	3987(4)	3406(4)	3150(2)	58(2)
C50	4295(3)	3310(4)	2801(2)	52(2)
C51	7654(5)	7447(4)	1222(3)	44(4)
C52	7543(5)	6747(5)	1410(2)	36(3)
C53	6862(7)	6255(4)	1315(2)	42(3)
C54	6291(6)	6464(5)	1032(2)	40(4)
C55	6402(5)	7165(6)	844(2)	45(3)
C56	7083(5)	7656(4)	939(3)	37(5)
C51'	7545(5)	7313(6)	1200(3)	51(5)
C52'	7268(6)	6586(6)	1321(3)	57(4)
C53'	6457(7)	6308(4)	1217(3)	40(3)
C54'	5924(6)	6758(5)	991(2)	34(3)
C55'	6201(5)	7485(5)	869(2)	40(3)
C56'	7012(6)	7762(4)	974(3)	64(7)

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Table S2. Bond lengths (in Å) for $\mathbf{3}_{(1,5)}$.

Bond	Length	Bond	Length
Au1-N1	2.032(3)	C7'-C8'	1.465(19)
Au1-P1	2.2416(12)	C9-C14	1.386(7)
Au2-C1	2.035(4)	C9-C10	1.399(7)
Au2-P2	2.2846(12)	C10-C11	1.384(8)
P1-C27	1.807(5)	C11-C12	1.381(8)
P1-C33	1.808(4)	C12-C13	1.373(7)
P1-C39	1.819(4)	C13-C14	1.394(7)
P2 -C15	1.796(4)	C15-C20'	1.337(18)
P2 -C21	1.810(5)	C15-C16	1.39(1)
P2 -C9	1.820(5)	C15-C20	1.39(1)
N3-N2	1.332(5)	C15-C16'	1.49(2)
N3-C2	1.365(5)	C16-C17	1.39(1)
N1-N2	1.346(5)	C17-C18	1.39(1)
N1-C1	1.368(5)	C18-C19	1.39(1)
C1-C2	1.383(6)	C19-C20	1.39(1)
C2-C3	1.457(6)	C16'-C17'	1.415(14)
C3-C8'	1.319(14)	C17'-C18'	1.376(14)
C3-C4	1.327(11)	C18'-C19'	1.393(15)
C3-C8	1.463(16)	C19'-C20'	1.402(14)
C3-C4'	1.486(11)	C21-C22	1.384(6)
C4-C5	1.377(14)	C21-C26	1.390(7)
C5-C6	1.385(16)	C22-C23	1.382(7)
C6-C7	1.410(17)	C23-C24	1.357(8)
C7-C8	1.34(2)	C24-C25	1.370(7)
C4'-C5'	1.387(13)	C25-C26	1.387(7)

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C5'-C6'	1.330(15)	C27-C32'	1.323(15)
C6'-C7'	1.349(17)	C27-C28	1.329(11)
C27-C28'	1.429(12)	C42-C43	1.381(7)
C27-C32	1.439(13)	C43-C44	1.386(6)
C28-C29	1.419(14)	C45-C46	1.345(8)
C29-C30	1.372(16)	C45-C50	1.362(9)
C30-C31	1.356(17)	C46-C47	1.339(9)
C31-C32	1.354(16)	C47-C48	1.380(9)
C28'-C29'	1.385(15)	C48-C49	1.409(9)
C29'-C30'	1.324(18)	C49-C50	1.350(8)
C30'-C31'	1.39(2)	C51-C52	1.39(1)
C31'-C32'	1.41(2)	C51-C56	1.39(1)
C33-C38	1.388(6)	C52-C53	1.39(1)
C33-C34	1.400(6)	C53-C54	1.39(1)
C34-C35	1.383(6)	C54-C55	1.39(1)
C35-C36	1.375(7)	C55-C56	1.39(1)
C36-C37	1.373(7)	C51'-C52'	1.39(1)
C37-C38	1.387(6)	C51'-C56'	1.39(1)
C39-C40	1.373(6)	C52'-C53'	1.39(1)
C39-C44	1.392(6)	C53'-C54'	1.39(1)
C40-C41	1.385(6)	C54'-C55'	1.39(1)
C41-C42	1.370(6)	C55'-C56'	1.39(1)

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Table S3. Bond angles (°) for $\mathbf{3}_{(1,5)}$.

Bond	Angle	Bond	Angle
N1-Au1-P1	176.9(1)	C4-C3-C2	125.6(6)
C1-Au2-P2	177.99(12)	C8'-C3-C8	13.7(9)
C27-P1-C33	104.6(2)	C4-C3-C8	116.1(9)
C27-P1-C39	108.80(19)	C2-C3-C8	117.0(7)
C33-P1-C39	104.8(2)	C8'-C3-C4'	115.8(8)
C27-P1-Au1	111.98(15)	C4-C3-C4'	28.5(5)
C33-P1-Au1	114.18(14)	C2-C3-C4'	118.4(5)
C39-P1-Au1	111.97(15)	C8-C3-C4'	121.5(8)
C15-P2 -C21	107.6(2)	C3-C4-C5	124.1(9)
C15-P2 -C9	105.5(2)	C4-C5-C6	119.9(11)
C21-P2 -C9	105.0(2)	C5-C6-C7	116.9(11)
C15-P2 -Au2	112.77(16)	C8-C7-C6	122.4(13)
C21-P2 -Au2	112.54(18)	C7-C8-C3	119.5(13)
C9-P2 -Au2	112.88(15)	C5'-C4'-C3	120.1(9)
N2-N3-C2	107.9(4)	C6'-C5'-C4'	121.5(11)
N2-N1-C1	110.7(3)	C5'-C6'-C7'	120.6(12)
N2-N1-Au1	126.0(3)	C6'-C7'-C8'	120.0(12)
C1-N1-Au1	122.8(3)	C3-C8'-C7'	121.6(12)
N3-N2-N1	108.0(4)	C14-C9-C10	119.1(5)
N1-C1-C2	104.1(4)	C14-C9-P2	117.9(4)
N1-C1-Au2	120.2(3)	C10-C9-P2	123.0(4)
C2-C1-Au2	135.6(3)	C11-C10-C9	119.7(5)
N3-C2-C1	109.3(4)	C12-C11-C10	120.5(5)
N3-C2-C3	121.0(4)	C13-C12-C11	120.5(6)
C1-C2-C3	129.6(4)	C12-C13-C14	119.4(5)

C8'-C3-C4	105.0(8)	C9-C14-C13	120.8(5)
C8'-C3-C2	125.4(7)	C20'-C15-C16	122.9(8)
C20'-C15-C20	10.0(12)	C28-C27-C28'	25.9(6)
C16-C15-C20	120.0(6)	C32'-C27-C32	16.8(8)
C20'-C15-C16'	114.9(11)	C28-C27-C32	117.0(8)
C16-C15-C16'	18.4(9)	C28'-C27-C32	121.8(7)
C20-C15-C16'	109.2(7)	C32'-C27-P1	121.6(7)
C20'-C15-P2	117.9(8)	C28-C27-P1	127.1(6)
C16-C15-P2	119.0(4)	C28'-C27-P1	119.1(6)
C20-C15-P2	120.7(4)	C32-C27-P1	115.4(6)
C16'-C15-P2	125.7(7)	C27-C28-C29	122.7(9)
C15-C16-C17	120.(7)	C30-C29-C28	118.0(9)
C18-C17-C16	120.0(9)	C31-C30-C29	120.1(10)
C19-C18-C17	120.0(9)	C32-C31-C30	121.7(11)
C18-C19-C20	120.0(9)	C31-C32-C27	120(1)
C19-C20-C15	120.0(8)	C29'-C28'-C27	118.7(10)
C17'-C16'-C15	120.8(13)	C30'-C29'-C28'	122.0(12)
C18'-C17'-C16'	118.5(13)	C29'-C30'-C31'	119.4(14)
C17'-C18'-C19'	121.5(14)	C30'-C31'-C32'	119.7(14)
C18'-C19'-C20'	118.4(15)	C27-C32'-C31'	120.8(13)
C15-C20'-C19'	125.4(15)	C38-C33-C34	119.2(4)
C22-C21-C26	117.3(5)	C38-C33-P1	117.9(3)
C22-C21-P2	124.8(5)	C34-C33-P1	122.9(3)
C26-C21-P2	117.9(4)	C35-C34-C33	120.0(4)
C23-C22-C21	120.5(6)	C36-C35-C34	120.2(5)
C24-C23-C22	121.3(6)	C37-C36-C35	120.4(5)
C23-C24-C25	119.7(6)	C36-C37-C38	120.3(5)
C24-C25-C26	119.4(6)	C37-C38-C33	120.0(4)

C25-C26-C21	121.8(5)	C40-C39-C44	119.0(4)
C32'-C27-C28	107.2(9)	C40-C39-P1	121.9(3)
C32'-C27-C28'	119.3(9)	C44-C39-P1	118.8(4)
C39-C40-C41	120.4(4)	C53-C52-C51	120.0(7)
C42-C41-C40	120.8(5)	C52-C53-C54	120.0(8)
C41-C42-C43	119.3(4)	C53-C54-C55	120.0(8)
C42-C43-C44	120.2(5)	C54-C55-C56	120.0(8)
C43-C44-C39	120.2(5)	C55-C56-C51	120.1(8)
C46-C45-C50	119.5(7)	C52'-C51'-C56'	120.0(6)
C47-C46-C45	121.7(7)	C51'-C52'-C53'	120.0(6)
C46-C47-C48	119.9(6)	C54'-C53'-C52'	120.0(6)
C47-C48-C49	118.8(6)	C55'-C54'-C53'	120.0(6)
C50-C49-C48	118.7(6)	C56'-C55'-C54'	120.0(6)
C49-C50-C45	121.4(6)	C55'-C56'-C51'	120.0(6)
C52-C51-C56	120.0(8)		

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Table S4. Anisotropic displacement parameters ($Å^2 x10^3$) for $\mathbf{3_{(1,5)}}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ...+ 2 h k a^* b^* U^{12}]$.

	U11	U22	U33	U23	U13	U12
Au1	19(1)	22(1)	17(1)	0(1)	-1(1)	2(1)
Au2	22(1)	21(1)	19(1)	-1(1)	2(1)	5(1)
P1	19(1)	20(1)	19(1)	0(1)	0(1)	1(1)
P2	32(1)	27(1)	24(1)	2(1)	6(1)	12(1)
N1	22(2)	21(2)	18(2)	1(2)	0(2)	4(2)
N2	29(2)	36(3)	19(2)	-4(2)	4(2)	8(2)
N3	25(2)	31(3)	29(3)	0(2)	0(2)	4(2)
C1	17(2)	20(3)	16(2)	-4(2)	-2(2)	-2(2)
C2	17(2)	26(3)	20(3)	-3(2)	1(2)	-3(2)
C3	17(2)	27(3)	31(3)	4(2)	-2(2)	2(2)
C9	34(3)	24(3)	22(3)	-4(2)	11(2)	5(2)
C10	41(3)	62(4)	28(3)	3(3)	7(2)	10(3)
C11	43(4)	85(5)	35(4)	7(3)	16(3)	-2(3)
C12	64(4)	64(4)	25(3)	9(3)	4(3)	-13(3)
C13	47(3)	42(3)	25(3)	3(3)	2(2)	-4(3)
C14	34(3)	31(3)	27(3)	-1(2)	1(2)	-1(2)
C15	40(3)	30(3)	43(4)	-2(3)	0(3)	16(2)
C21	32(3)	45(3)	25(3)	9(3)	4(2)	13(2)
C22	60(4)	68(5)	56(5)	-14(4)	-11(3)	38(3)
C23	58(5)	100(6)	66(5)	-2(5)	-21(4)	43(4)
C24	29(3)	111(6)	32(4)	17(4)	-2(3)	8(4)
C25	32(3)	66(4)	47(4)	1(3)	3(3)	0(3)
C26	26(3)	54(4)	46(4)	0(3)	-1(3)	10(3)
C27	22(2)	24(3)	17(3)	3(2)	-1(2)	3(2)
C33	19(2)	23(3)	15(2)	-3(2)	-4(2)	-4(2)
C34	24(3)	25(3)	23(3)	0(2)	0(2)	1(2)
C35	32(3)	29(3)	25(3)	4(2)	-2(2)	-5(2)
C36	27(3)	42(3)	30(3)	5(3)	2(2)	-11(2)
C37	24(3)	36(3)	34(3)	-4(3)	3(2)	-1(2)

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C38	20(2)	26(3)	28(3)	2(2)	-6(2)	-5(2)
C39	20(2)	17(2)	23(3)	-2(2)	1(2)	2(2)
C40	20(2)	29(3)	20(3)	5(2)	0(2)	-3(2)
C41	23(2)	41(3)	26(3)	0(3)	-3(2)	-1(2)
C42	22(3)	33(3)	32(3)	-3(3)	-6(2)	-6(2)
C43	37(3)	41(3)	36(3)	10(3)	-5(3)	-18(3)
C44	39(3)	43(3)	26(3)	10(3)	-8(2)	-14(3)
C45	56(4)	47(4)	68(5)	-2(4)	14(3)	-14(3)
C46	55(4)	41(4)	78(6)	15(4)	2(4)	-7(3)
C47	45(4)	33(4)	98(6)	-4(4)	15(4)	9(3)
C48	71(5)	68(5)	58(5)	-13(4)	20(4)	-10(4)
C49	59(4)	48(4)	65(5)	16(4)	-17(4)	5(3)
C50	31(3)	45(4)	80(6)	-17(4)	6(3)	5(3)

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Computational Results for $\mathbf{3}_{(1,5)'}$.

Table S5. Optimized Cartesian coordinates of ground-state (singlet) for $\mathbf{3}_{(1,5)'}$.

Atom	x	y	z
Au	3.13414	-0.50824	-0.12262
Au	-3.1182	-0.53687	0.00241
P	5.42199	-0.15626	0.03395
P	-5.4768	-0.14276	0.01235
N	-0.61742	-2.20306	-0.14505
N	1.09665	-0.87802	-0.21797
N	0.69437	-2.17095	-0.22824
C	0.00288	-0.06645	-0.10413
C	-1.10297	-0.92136	-0.05757
C	0.09247	1.39864	-0.06948
C	0.95307	2.10346	-0.93354
C	1.03565	3.49634	-0.88894
C	0.25346	4.22122	0.0136
C	-0.61287	3.53672	0.87043
C	-0.68992	2.14434	0.83298
C	-5.91906	1.64342	0.01789
C	-7.04495	2.15246	0.68227
C	-7.33119	3.51873	0.63698
C	-6.49876	4.38745	-0.07097
C	-5.37225	3.88908	-0.7297
C	-5.07873	2.52632	-0.68116
C	-6.32574	-0.84244	-1.46235
C	-7.46026	-0.25348	-2.04098
C	-8.06834	-0.84089	-3.15225
C	-7.55017	-2.01851	-3.69487
C	-6.41668	-2.60632	-3.12886
C	-5.80222	-2.01972	-2.0222
C	-6.35486	-0.86439	1.4596
C	-7.67905	-1.3248	1.39691
C	-8.29609	-1.85073	2.53359
C	-7.59838	-1.92331	3.74087
C	-6.27752	-1.4749	3.80933
C	-5.65567	-0.95371	2.67445
C	5.88167	1.61643	-0.09362
C	7.11208	2.03318	-0.62514
C	7.42779	3.39183	-0.68134
C	6.52032	4.34304	-0.2105
C	5.29125	3.93521	0.31247

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C	4.96893	2.57899	0.36766
C	6.11015	-0.74971	1.62962
C	7.18882	-0.11658	2.26506
C	7.69091	-0.62316	3.46548
C	7.12198	-1.76176	4.03903
C	6.04354	-2.39273	3.41448
C	5.53429	-1.88791	2.2182
C	6.37937	-1.01757	-1.2754
C	7.66141	-1.54001	-1.04726
C	8.35813	-2.1665	-2.08254
C	7.78291	-2.27718	-3.34966
C	6.50422	-1.76513	-3.58159
C	5.80208	-1.1431	-2.54968
H	1.53634	1.55049	-1.6648
H	1.70148	4.01637	-1.57409
H	0.31409	5.30632	0.04552
H	-1.22478	4.08839	1.58033
H	-1.34892	1.61425	1.51396
H	-7.69305	1.48654	1.24408
H	-8.2039	3.90273	1.15863
H	-6.72217	5.45055	-0.10224
H	-4.71282	4.56127	-1.2716
H	-4.18823	2.14547	-1.17465
H	-7.86233	0.66931	-1.63301
H	-8.9442	-0.37462	-3.5957
H	-8.02297	-2.47179	-4.56206
H	-6.00094	-3.5152	-3.55474
H	-4.90622	-2.4667	-1.5988
H	-8.22515	-1.28579	0.45903
H	-9.32047	-2.20857	2.47283
H	-8.07917	-2.33751	4.62306
H	-5.72478	-1.54246	4.74225
H	-4.61968	-0.62825	2.72318
H	7.81799	1.30128	-1.00644
H	8.38083	3.70563	-1.09838
H	6.76683	5.40019	-0.25973
H	4.57413	4.67014	0.66661
H	4.00144	2.2693	0.75343
H	7.62925	0.77659	1.83217
H	8.52326	-0.12343	3.95347
H	7.51192	-2.15151	4.97534
H	5.58885	-3.27151	3.86266

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H	4.68199	-2.37033	1.74639
H	8.11183	-1.47102	-0.06167
H	9.3483	-2.57272	-1.89495
H	8.3252	-2.76995	-4.15194
H	6.04589	-1.86095	-4.56174
H	4.79843	-0.76625	-2.72856

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Table S6. Optimized Cartesian coordinates of ground-state (singlet) for $\mathbf{3}_{(1,4)}'$.

Atom	x	y	z
Au	-1.82905	1.43078	-0.00219
Au	1.80779	0.57941	-0.01463
P	-3.64515	-0.01271	-0.02323
P	2.67095	-1.64619	0.03194
N	0.66983	4.71031	0.03241
N	-0.25841	2.76217	0.00994
N	-0.488	4.10199	0.04587
C	1.08321	2.50081	-0.03233
C	1.66763	3.77544	-0.02028
C	3.07652	4.19284	-0.041
C	4.1148	3.32287	-0.42138
C	5.44403	3.74601	-0.42721
C	5.77158	5.0539	-0.06228
C	4.74874	5.93288	0.30498
C	3.42113	5.51019	0.31626
C	4.50421	-1.69995	0.15092
C	5.27954	-2.69228	-0.46774
C	6.66901	-2.68684	-0.3285
C	7.2948	-1.69385	0.42761
C	6.52977	-0.69946	1.04164
C	5.14198	-0.69716	0.90056
C	2.06152	-2.65286	1.44506
C	2.82407	-3.67318	2.03472
C	2.30272	-4.41835	3.094
C	1.01878	-4.15238	3.5745
C	0.25681	-3.13279	2.99973
C	0.77702	-2.38223	1.9448
C	2.25686	-2.62159	-1.47466
C	1.99567	-3.9997	-1.44581
C	1.6991	-4.68572	-2.62579
C	1.6622	-4.00425	-3.84419
C	1.9143	-2.62984	-3.88052
C	2.2033	-1.94001	-2.70249
C	-3.76769	-1.04331	1.49495
C	-4.24013	-2.36394	1.47533
C	-4.337	-3.09353	2.6624
C	-3.96546	-2.51205	3.87628
C	-3.48846	-1.19838	3.90239
C	-3.38389	-0.46813	2.71818

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C	-5.24227	0.88438	-0.13682
C	-6.42828	0.37446	0.41409
C	-7.62381	1.08287	0.28255
C	-7.64473	2.30342	-0.39564
C	-6.46652	2.82029	-0.93858
C	-5.26797	2.1185	-0.80713
C	-3.61676	-1.19425	-1.42861
C	-4.78912	-1.68816	-2.021
C	-4.71137	-2.60508	-3.0709
C	-3.46716	-3.0346	-3.53713
C	-2.29585	-2.54062	-2.95837
C	-2.36889	-1.6201	-1.91269
H	3.86991	2.3092	-0.72856
H	6.22563	3.05225	-0.73031
H	6.80712	5.38534	-0.07066
H	4.98703	6.95614	0.58689
H	2.62465	6.1905	0.59912
H	4.80264	-3.46168	-1.06769
H	7.26132	-3.45699	-0.8153
H	8.37651	-1.68941	0.53057
H	7.01138	0.084	1.61971
H	4.55335	0.09176	1.3618
H	3.82895	-3.87839	1.67751
H	2.90348	-5.20264	3.54667
H	0.61775	-4.73163	4.40193
H	-0.73775	-2.91075	3.37638
H	0.19166	-1.5723	1.51737
H	2.01448	-4.53749	-0.50279
H	1.4974	-5.753	-2.59102
H	1.43574	-4.54077	-4.76178
H	1.88034	-2.0919	-4.82386
H	2.37954	-0.86767	-2.73202
H	-4.52351	-2.82748	0.53526
H	-4.70171	-4.11675	2.63611
H	-4.04383	-3.08086	4.79886
H	-3.19151	-0.74233	4.84261
H	-2.99761	0.54778	2.74079
H	-6.41783	-0.56579	0.95766
H	-8.53651	0.68327	0.71609
H	-8.57547	2.85579	-0.49148
H	-6.47411	3.7767	-1.4533
H	-4.34885	2.53606	-1.20994
H	-5.76069	-1.34895	-1.67444
H	-5.62411	-2.97785	-3.52768

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H	-3.41093	-3.745	-4.3575
H	-1.32411	-2.8597	-3.32432
H	-1.45576	-1.21808	-1.48139

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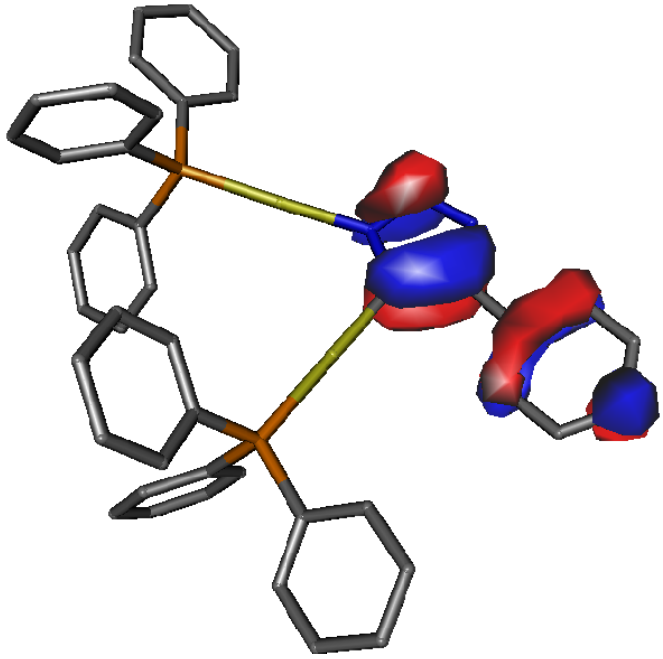

Figure S7. Highest occupied molecular orbital for $\mathbf{3}_{(1,5)}$'.

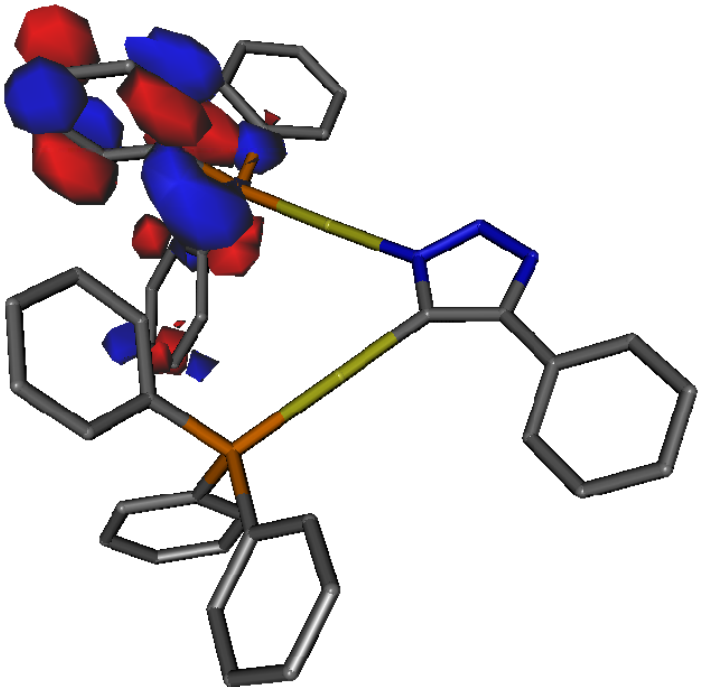

Figure S8. Lowest unoccupied molecular orbital for $\mathbf{3}_{(1,5)}$'.

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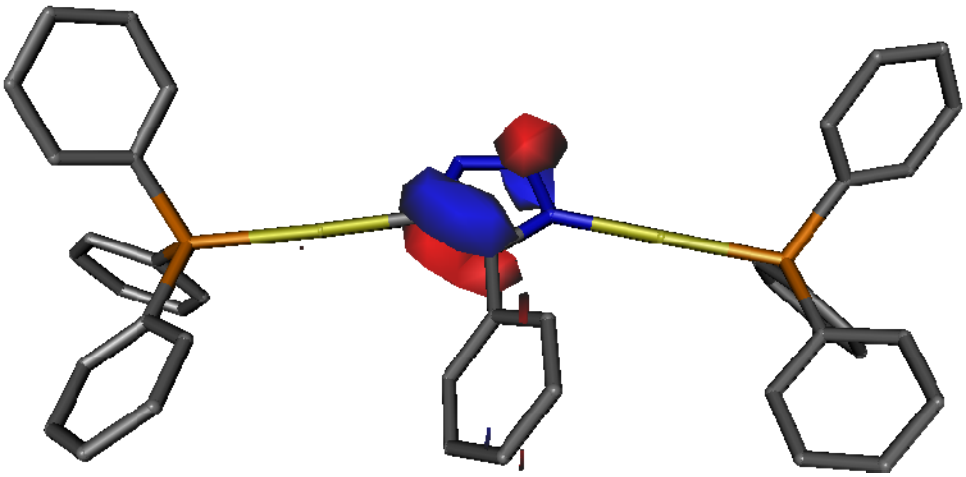

Figure S9. Highest occupied molecular orbital for **3**$_{(1,4)}$'.

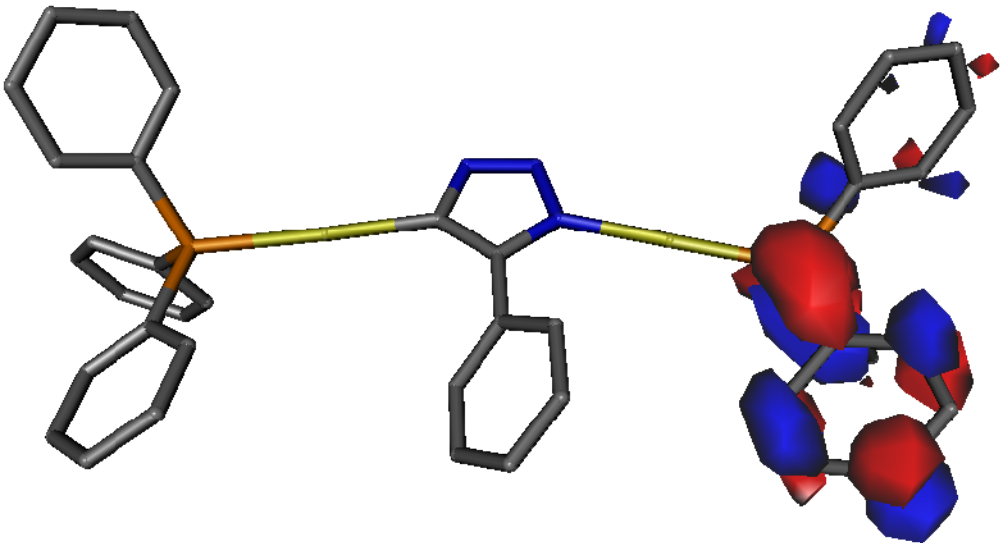

Figure S10. Lowest unoccupied molecular orbital picture for **3**$_{(1,4)}$'.

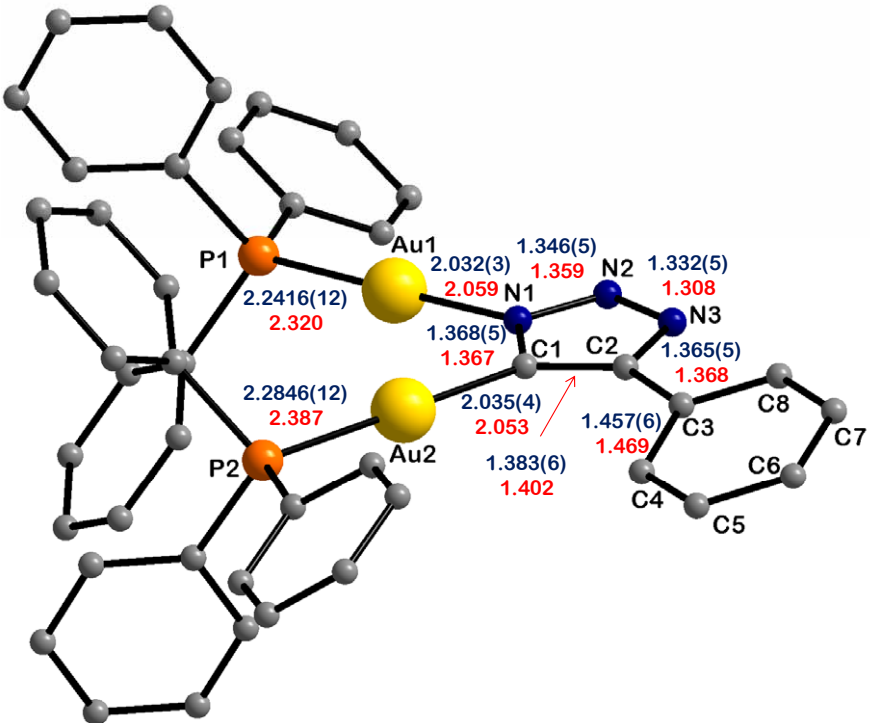

Figure S11. Geometry optimized structure of $\mathbf{3}_{(1,5)}$' including metrical parameters (crystallographically obtained bond length in blue and calculated bond length in red).

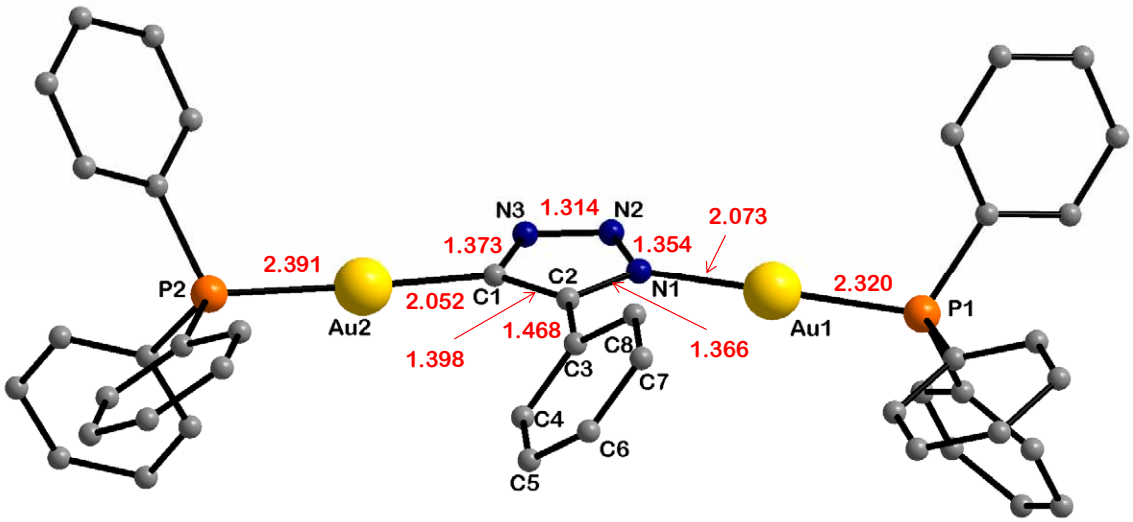

Figure S12. Geometry optimized structure of $\mathbf{3}_{(1,4)}$' including calculated bond lengths in red.