Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

Au-iClick mirrors the mechanism of copper catalyzed azide-alkyne cycloaddition (CuAAC).

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Synthesis of **3-R** (R = NO_2, OMe, F)

A general procedure was followed for the iClick reaction between $PPh_3Au\text{-}N_3$ (**1**) and $PPh_3Au\text{-}C{\equiv}C\text{-}Ph\text{-}R$ (**2-R**, R = H, NO_2, F, OMe) to yield **3-R**. Complex **1** (0.04 mmol) was taken up in $CDCl_3$ (0.3 mL) and added to a solution of **2-R** (0.04 mmol) also in $CDCl_3$ (0.3 mL). The reaction mixture was transferred to a sealable NMR tube and the reaction progress was monitored via $^{31}P\{^1H\}$ and ^1H NMR spectroscopy. The reactions all proceed quantitatively by NMR and can be isolated by removing all the volatiles in vacuo and then triturating with pentane.

Synthesis and characterization of **3-NO_2**.

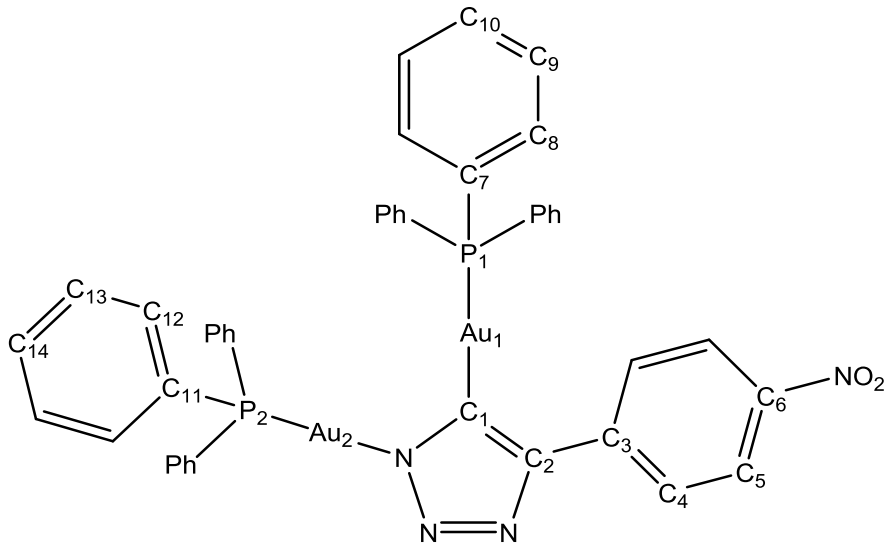

Figure S1. Atom labeling scheme for NMR chemical shift assignments for complex **3-NO_2**.

3-NO_2: 94% Yield (41 mg, 0.037 mmol). ^1H NMR (300 MHz, $CDCl_3$): δ 8.59 (d, $^3J_{HH}$ = 8.5 Hz, 2H, C4-*H*), 8.11 (d, $^3J_{HH}$ = 8.5 Hz, 2H, C5-*H*), 7.47 (m, 18H, aromatic), 7.30 (m, 12H, aromatic). $^{13}C\{^1H\}$ NMR (indirect detection through ^1H-^{13}C gHMBC and ^1H-^{13}C gHSQC (500 MHz, $CDCl_3$)): δ 149.7 (C2), 145.3 (C6), 143.5 (C3), 134.2 (C7, C8, C11, C12), 131.7 (C10), 131.6 (C14), 129.1 (C9, C13), 125.9 (C4), 123.7 (C5). $^{31}P\{^1H\}$ NMR (121.4 MHz, $CDCl_3$): δ 44.39 (s, P1), 32.08 (s, P2). Anal. Calcd. for $C_{44}H_{34}Au_2P_2N_4O_2$: C, 47.75; H, 3.10; N, 5.06. Found: C, 47.91; H, 3.26; N, 5.16.

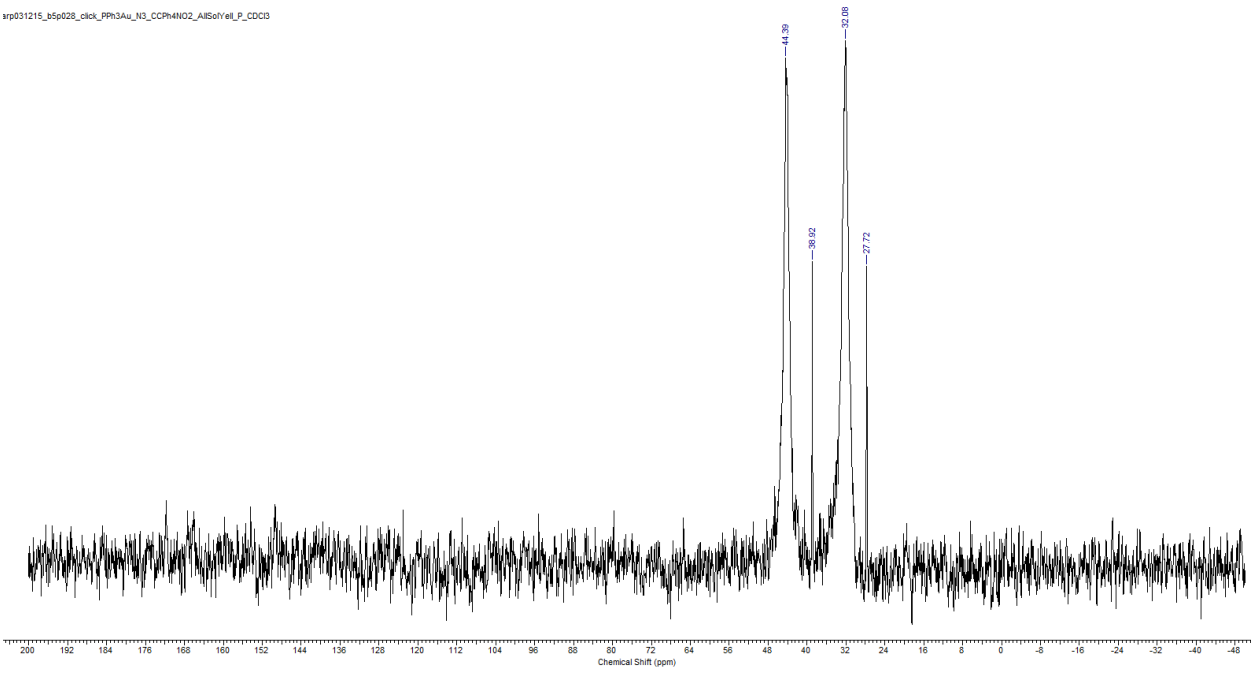

Figure S2. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 121.4 MHz) spectrum of **3-NO_2**.

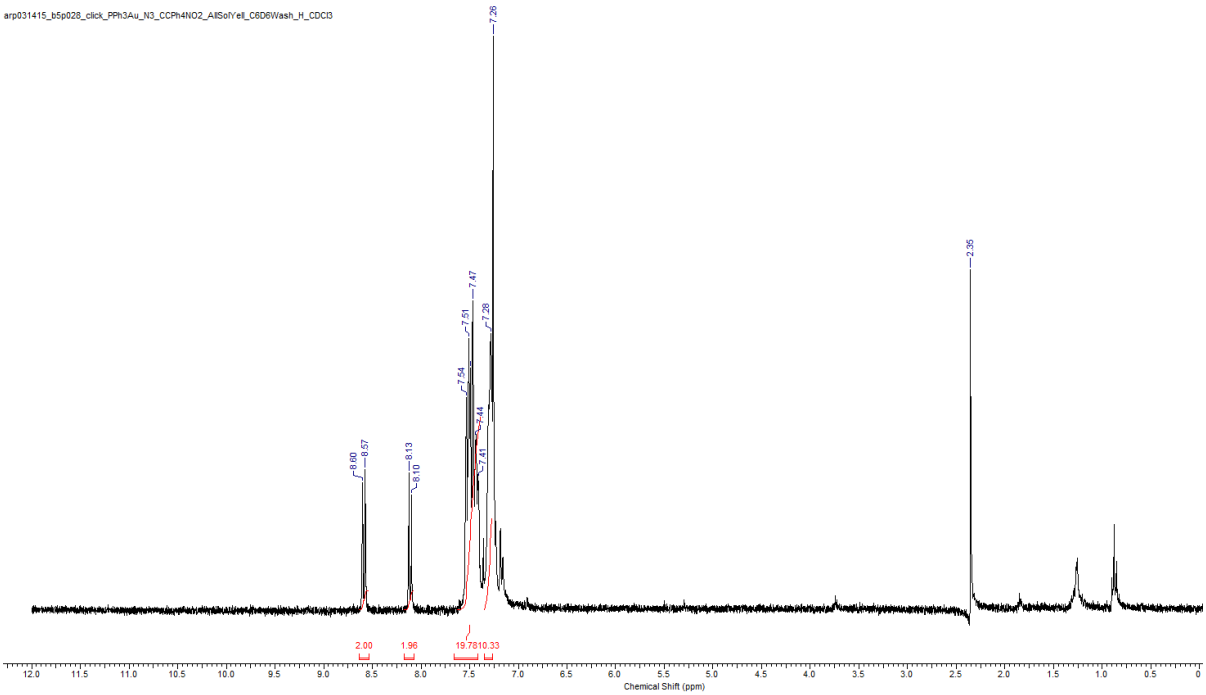

Figure S3. ^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **3-NO_2**.

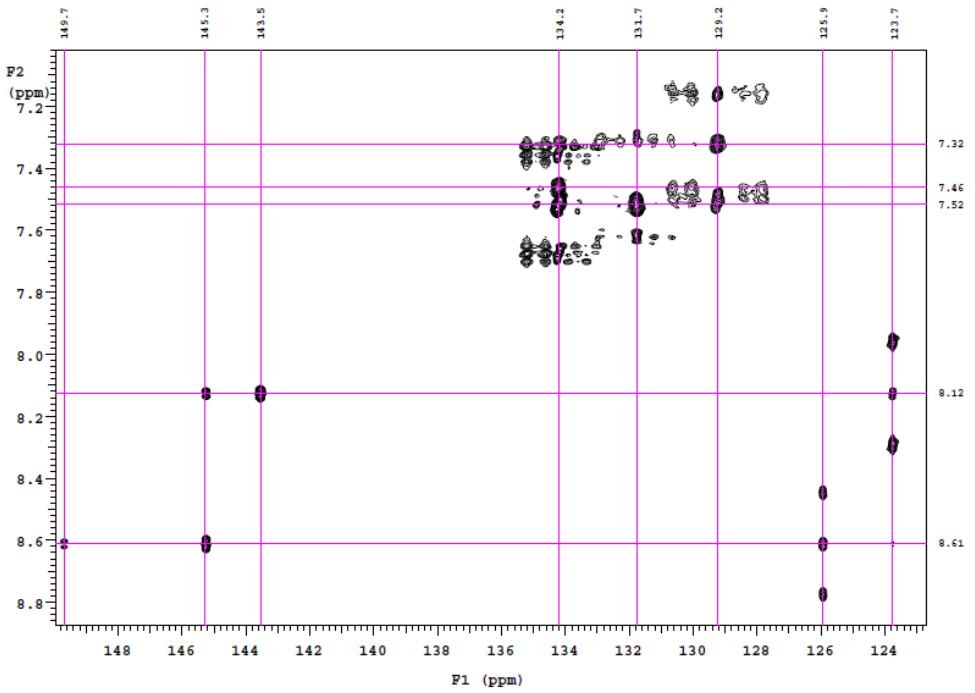

Figure S4. ^{1}H-^{13}C gHMBC spectrum (500 MHz, $CDCl_3$) of **3-NO_2.**

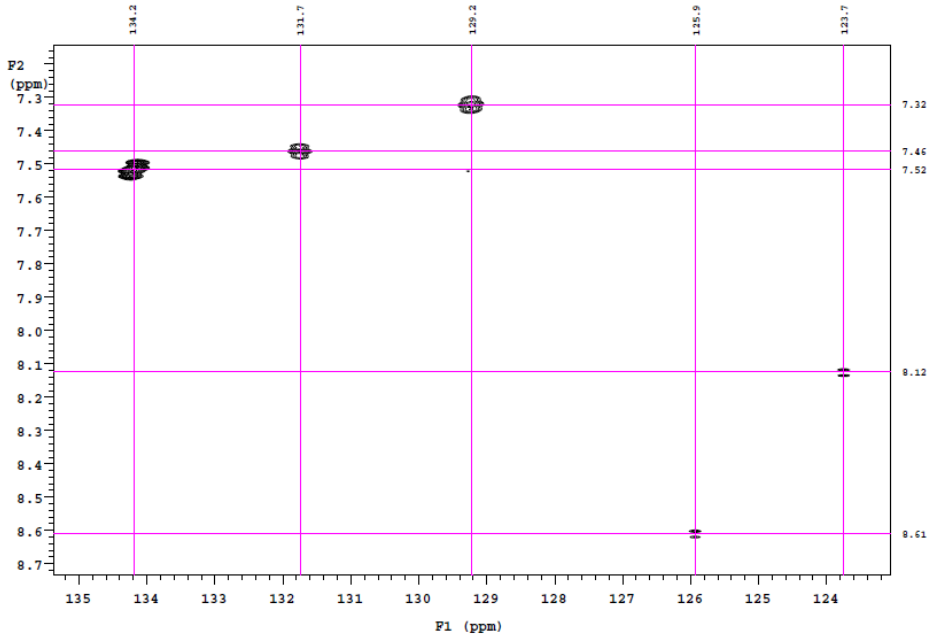

Figure S5. ^{1}H-^{13}C gHMBC spectrum (500 MHz, $CDCl_3$) of **3-NO_2.**

Synthesis and characterization of **3-OMe**.

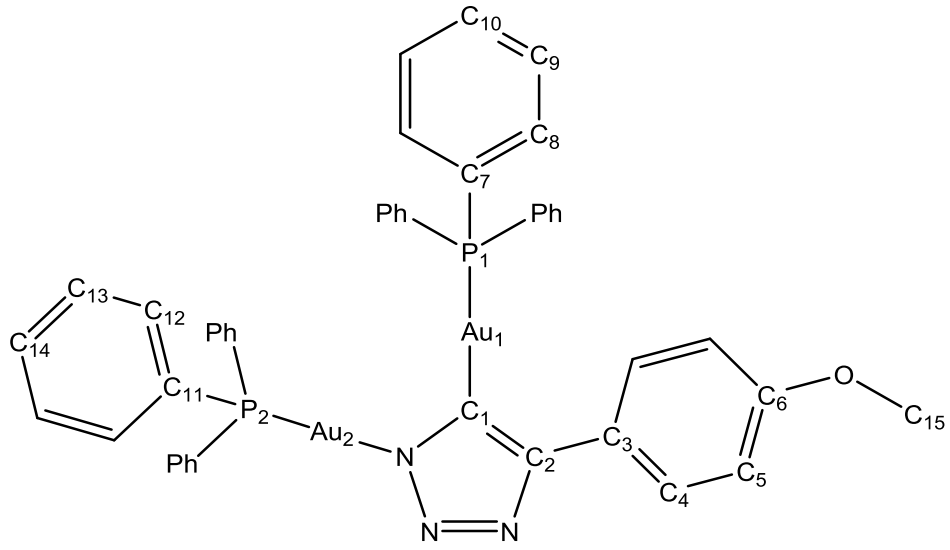

Figure S6. Atom labeling scheme for NMR chemical shift assignments for complex **3-OMe**.

3-OMe: 90% Yield (39 mg, 0.036 mmol). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.32 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H, C4-*H*), 7.46 (m, 18H, aromatic), 7.30 (m, 12H, aromatic), 6.84 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H, C5-*H*), 3.81 (s, 3H, OCH_3). ^{13}C{^{1}H} NMR shifts (indirect detection through ^{1}H-^{13}C gHMBC and ^{1}H-^{13}C gHSQC (500 MHz, $CDCl_3$)): δ 157.8 (C6), 151.2 (C2), 134.2 (C7, C8, C11, C12), 131.6 (C10, C14), 129.6 (C3), 129.1 (C9, C13), 127.6 (C4), 113.4 (C5), 55.3 (C15). ^{31}P{^{1}H} NMR (121.4 MHz, CDCl3): δ 44.58 (s, P1), 31.81 (s, P2). Anal. Calcd. for $C_{45}H_{37}Au_2P_2N_3O$: C, 49.51; H, 3.42; N, 3.85. Found: C, 49.79; H, 3.25; N, 3.65.

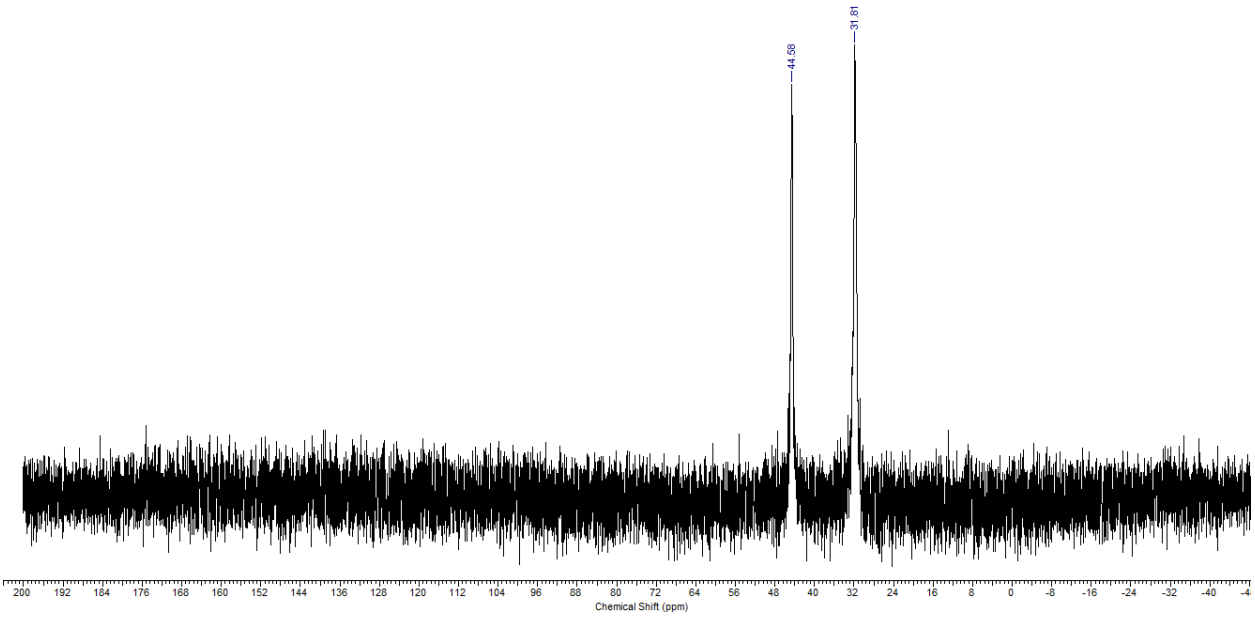

Figure S7. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 121.4 MHz) spectrum of **3-OMe**.

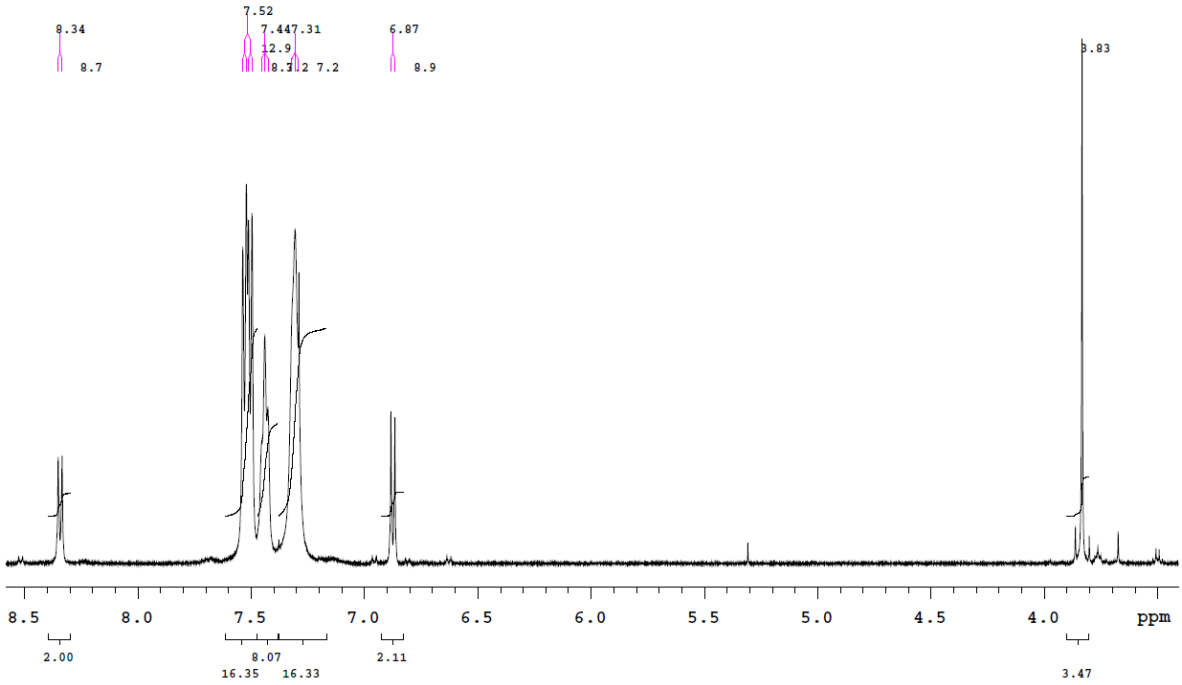

Figure S8. ^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **3-OMe**.

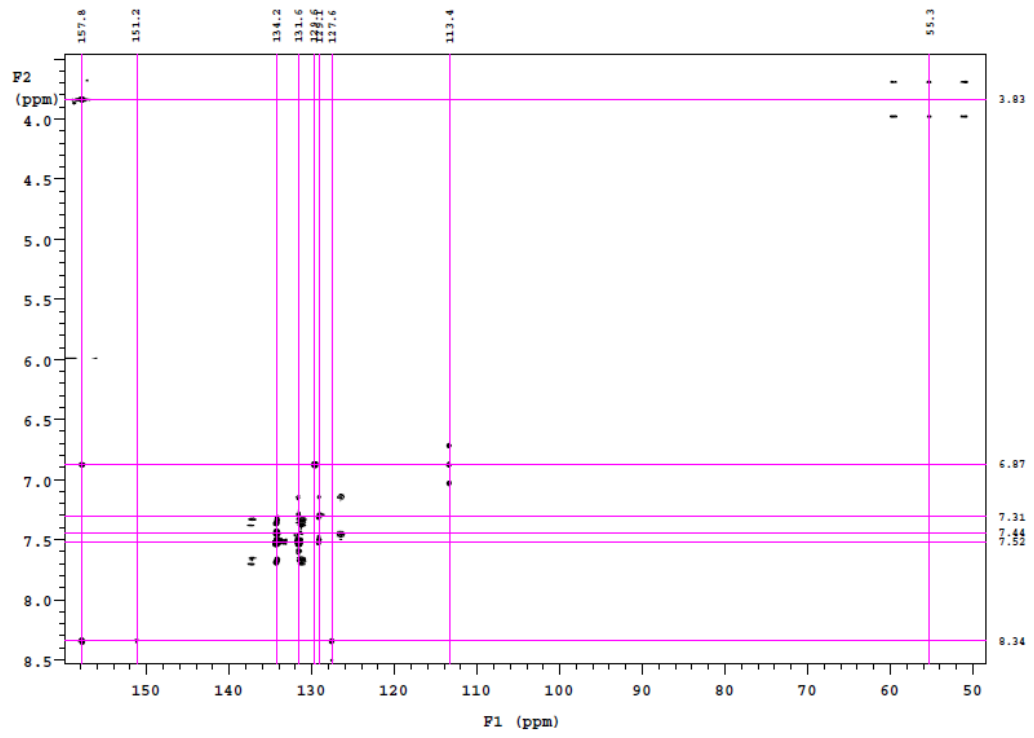

Figure S9. ^{1}H-^{13}C gHMBC spectrum ($CDCl_3$, 500 MHz) of **3-OMe**.

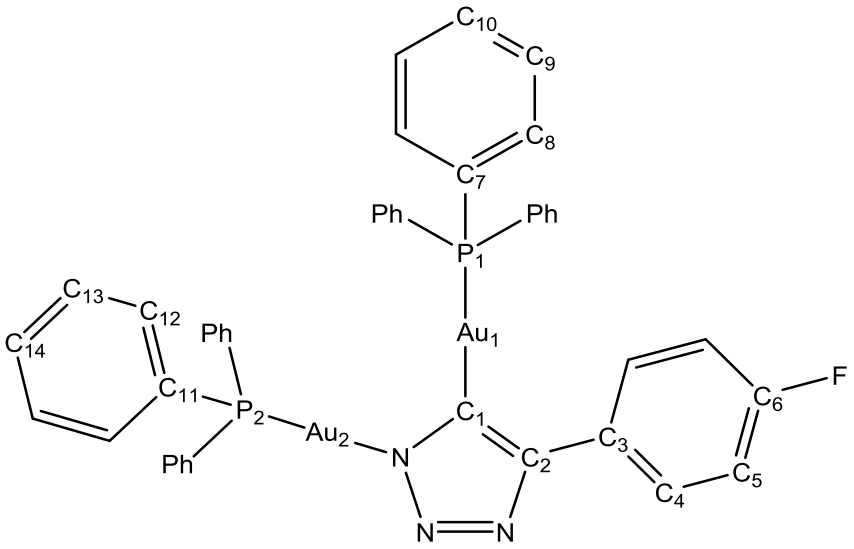

Figure S10. Atom labeling scheme for NMR chemical shift assignments for complex **3-F**.

3-F: 89% Yield (38 mg, 0.035 mmol). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.34 (dd, $^{3}J_{HH}$ = 8.6 Hz, $^{4}J_{HF}$ =6.1 Hz 2H, C4-*H*), 7.45 (m, 18H, aromatic), 7.30 (m, 12H, aromatic), 6.95 (dd, $^{3}J_{HF}$ = 8.6 Hz, $^{3}J_{HH}$ = 8.6 Hz, 2H, C5-*H*). ^{13}C{^{1}H} NMR shifts (indirect detection through ^{1}H-^{13}C gHMBC and ^{1}H-^{13}C gHSQC (500 MHz, $CDCl_3$)): δ 161.4 (C6), 150.6 (C2), 132.9 (C3), 132.4 (C7, C8, C11, C12), 131.6 (C10, C14), 129.1 (C9, C13), 127.8 (C4), 114.5 (C5). ^{31}P{^{1}H} NMR (121.4 MHz, $CDCl_3$): δ 44.50 (s, P1), 31.77 (s, P2). ^{19}F{^{1}H} NMR (282.2 MHz, $CDCl_3$): δ -118.8 (s, F). Anal. Calcd. for $C_{44}H_{34}Au_2P_2N_3F$: C, 48.79; H, 2.97; N, 3.80. Found: C, 48.95; H, 3.17; N, 3.89.

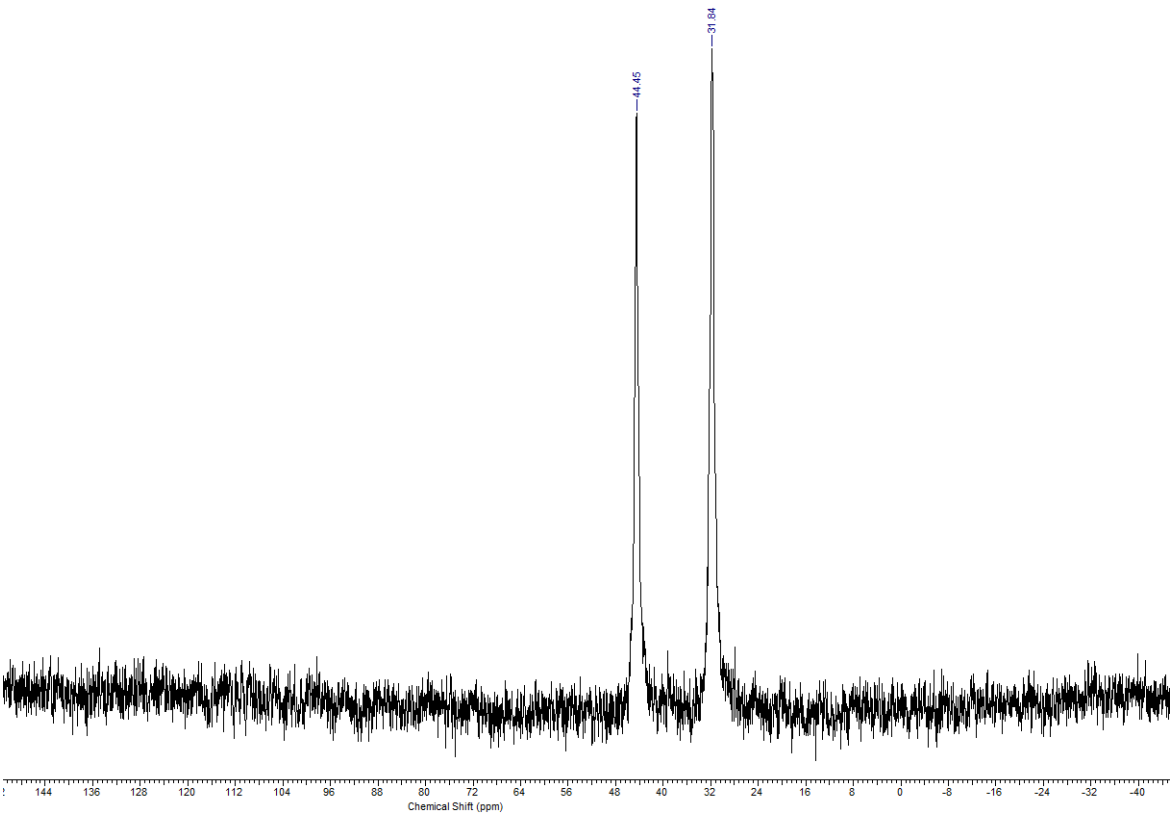

Figure S11. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 121.4 MHz) spectrum of **3-F**.

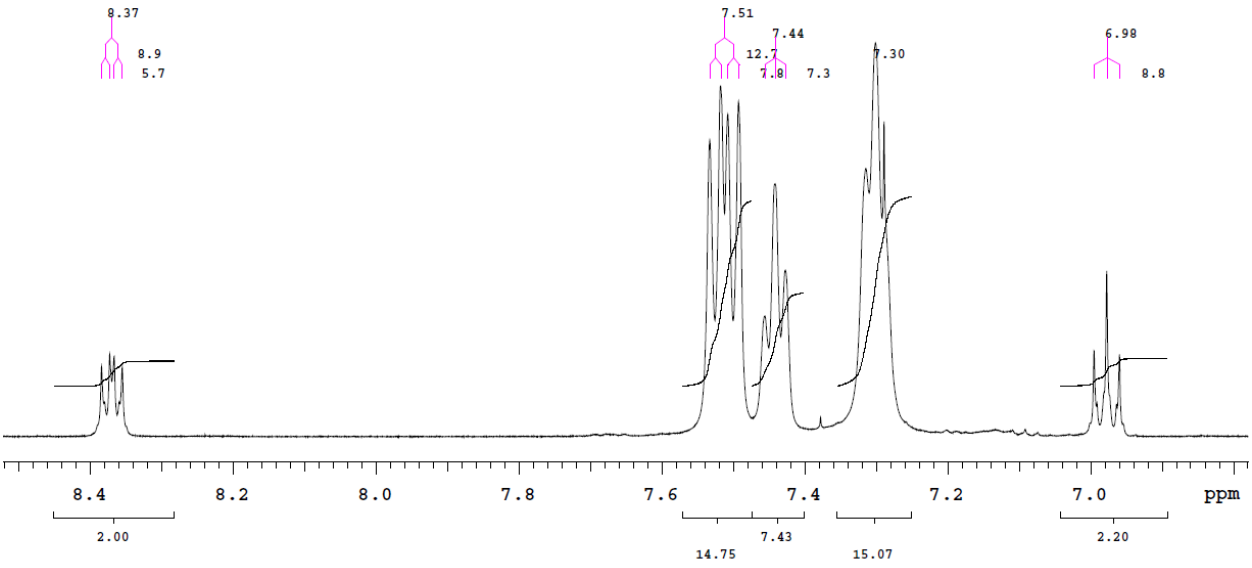

Figure S12. ^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **3-F**.

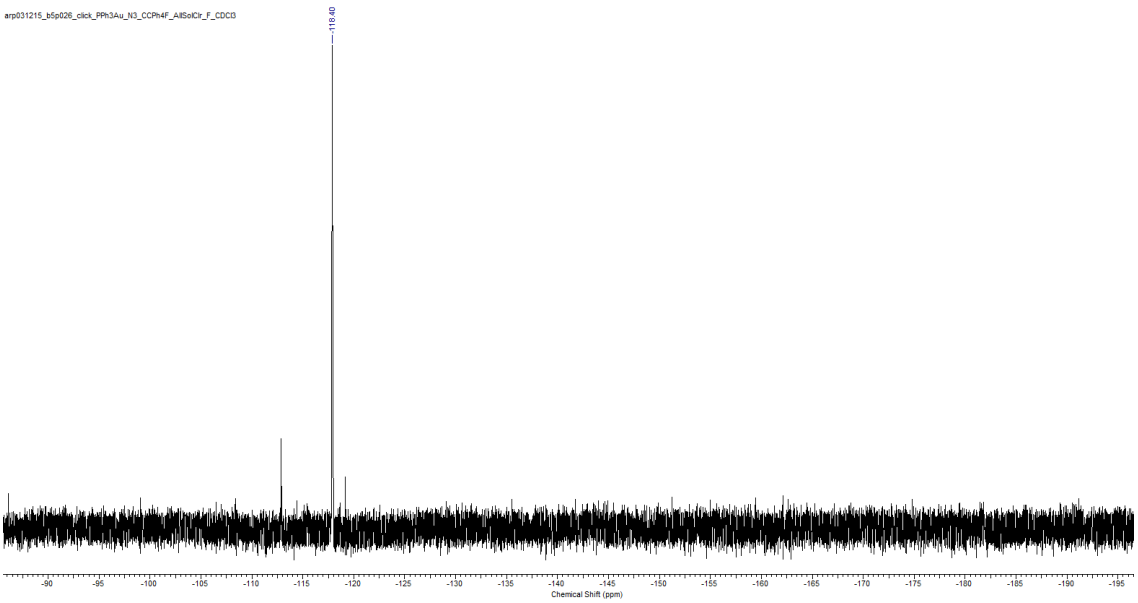

Figure S13. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 282.2 MHz) spectrum of **3-F**.

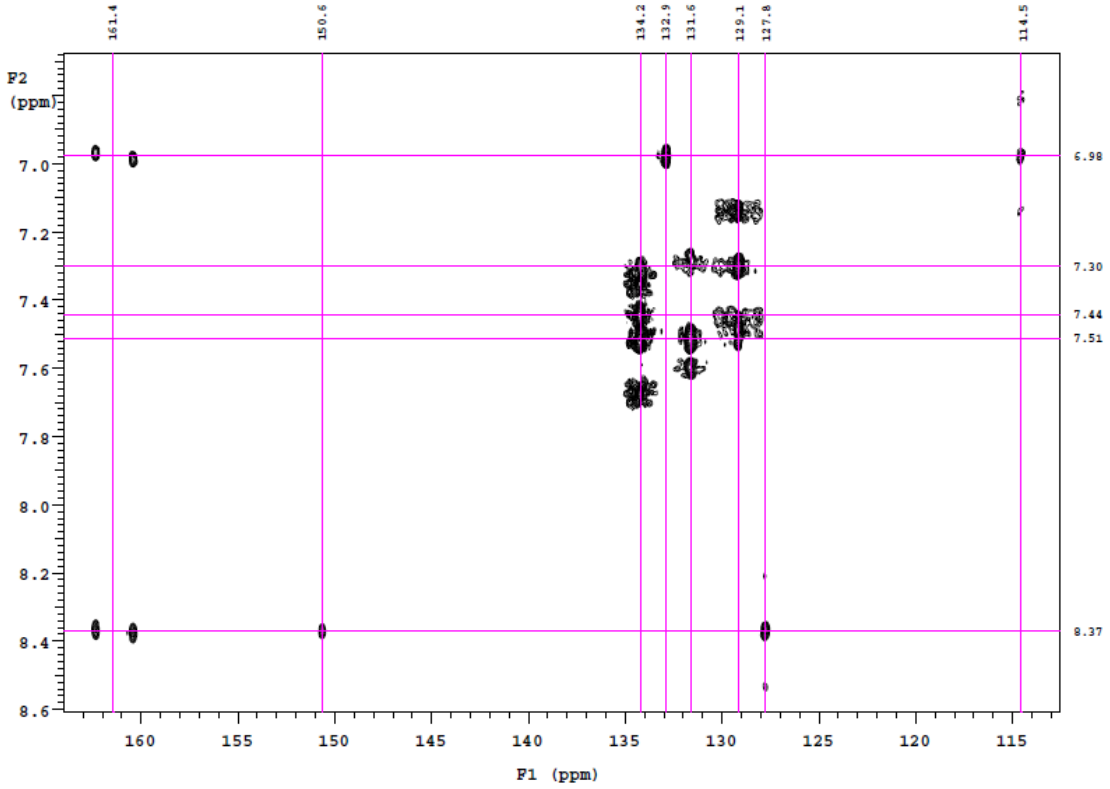

Figure S14. ^{1}H-^{13}C gHMBC spectrum ($CDCl_3$, 500 MHz) of **3-F**.

General guidelines for kinetic experiments

All kinetic experiments were performed using $CDCl_3$ stock solutions spiked with hexamethyldisiloxane (HMDSO) as an internal standard (0.005 M) against which the product integrations could be referenced. For each set of experiments, a fresh stock solution of azide and acetylide was prepared. To minimize the time a sample was mixed before spectra were collected, a NMR tube charged with a premeasured volume of Au(I)-acetylide stock solution was brought to the NMR instrument and the azide stock solution added to the tube directly prior to loading the sample into the magnet. A lock was already established on the NMR instrument with a similar sample, but to ensure accurate integrations, new lock and shims were established for each sample. Two steady state scans were executed to stabilize the magnetization prior to collection of each spectrum. If a third stock solution needed to be added to the tube (triphenylphosphine), it was mixed with the azide solution directly prior to mixing the azide with the acetylide.

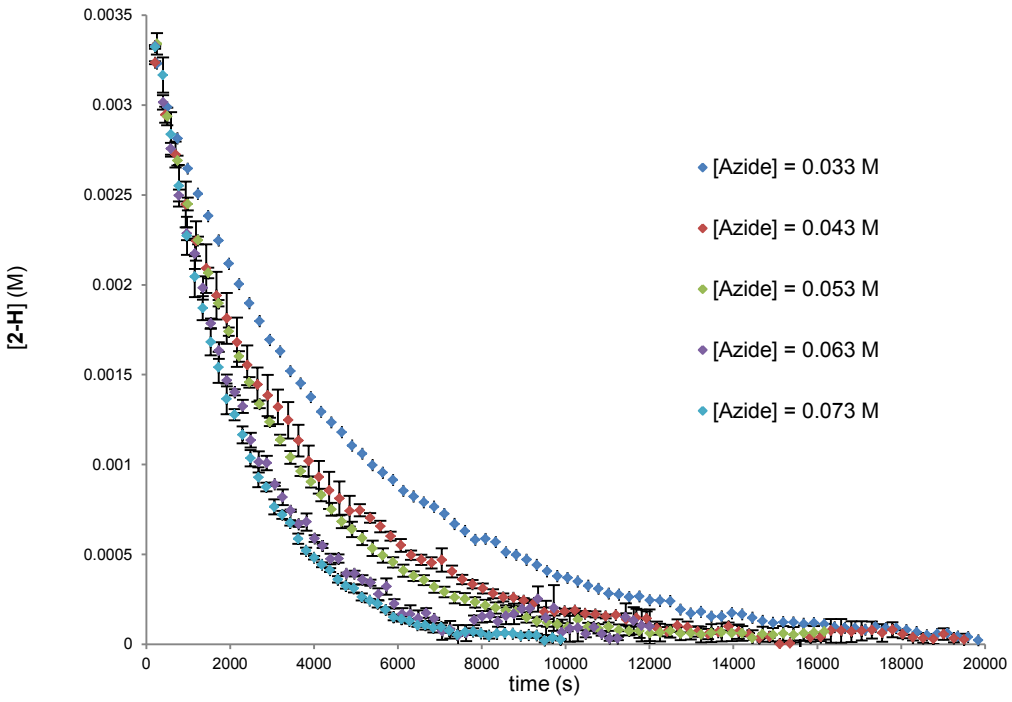

Figure S15. Concentration of **2-H** (0.0033 M) as a function of time under varying excess concentrations of **1**.

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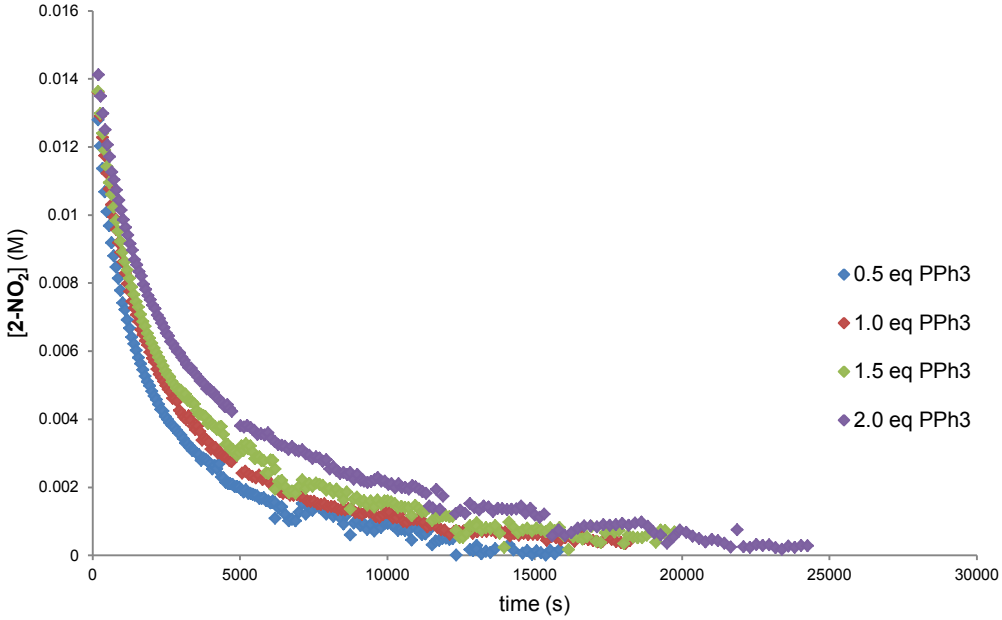

Figure S16. Concentration of **2-NO$_2$** as a function of time when equal concentrations of **1** and **2-NO$_2$** are reacted in the presence of free PPh_3.

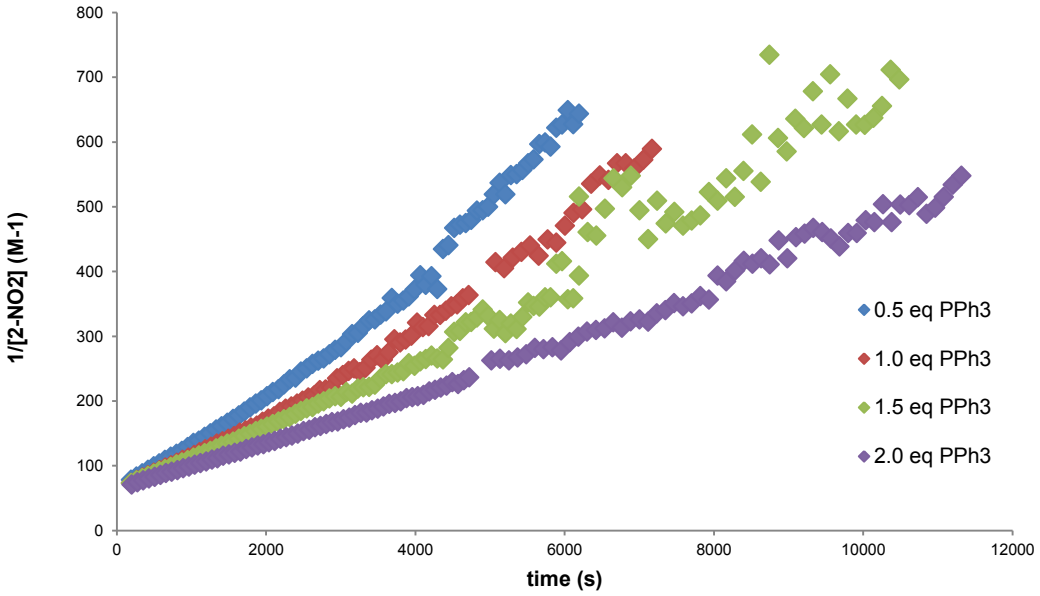

Figure S17. [**2-NO$_2$**]$^{-1}$ as a function of time when equal concentrations of **1** and **2-NO$_2$** are reacted in the presence of free PPh_3.

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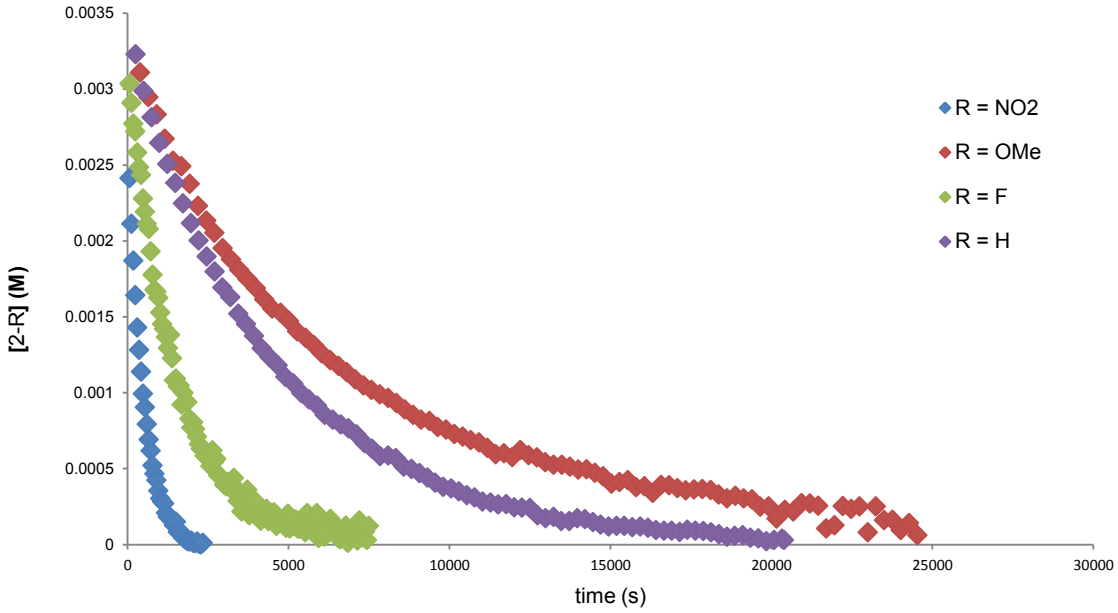

Figure S18. Plot of the [**2-R**] as a function of time under pseudo-first-order conditions of 10-fold excess [**1**].

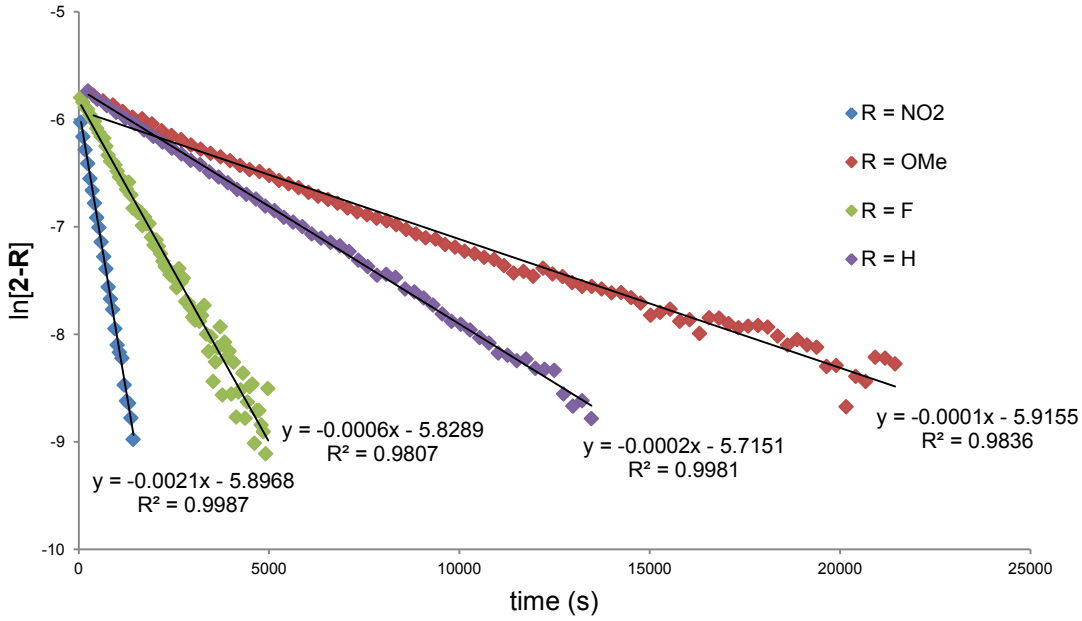

Figure S19. Plot of the ln[**2-R**] as a function of time under pseudo-first-order conditions of 10-fold excess [**1**].

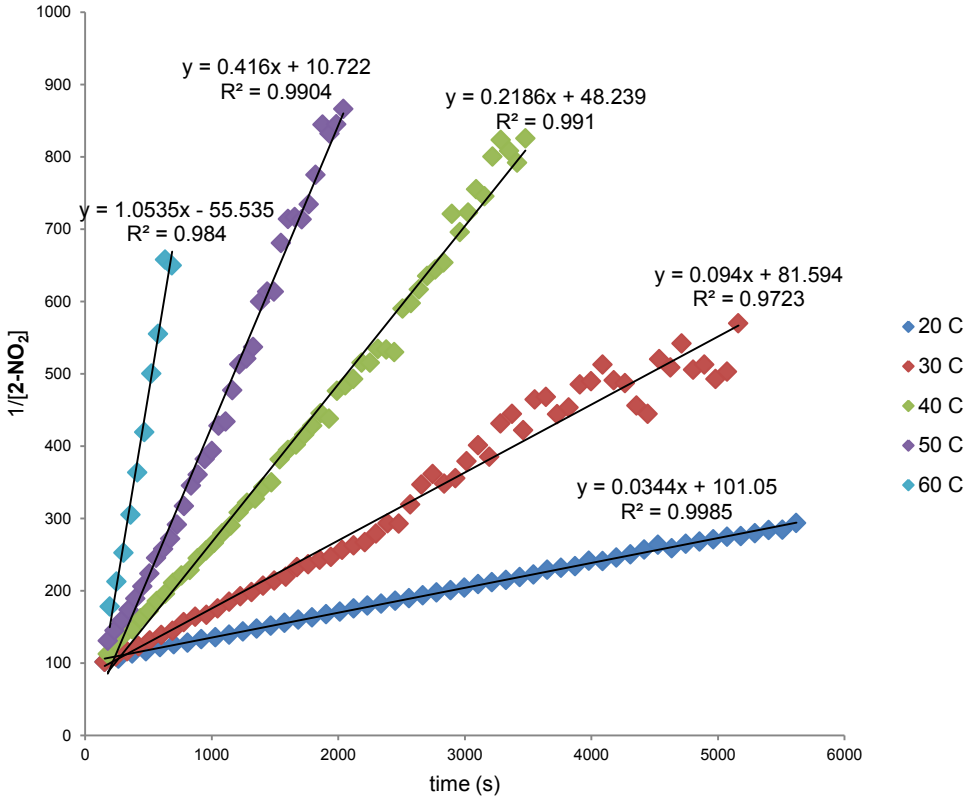

Figure S20. $[\mathbf{2\text{-}NO_2}]^{-1}$ as a function of time when equal concentrations of **1** and **2-NO$_2$** are reacted at temperatures ranging from 20-60 °C.

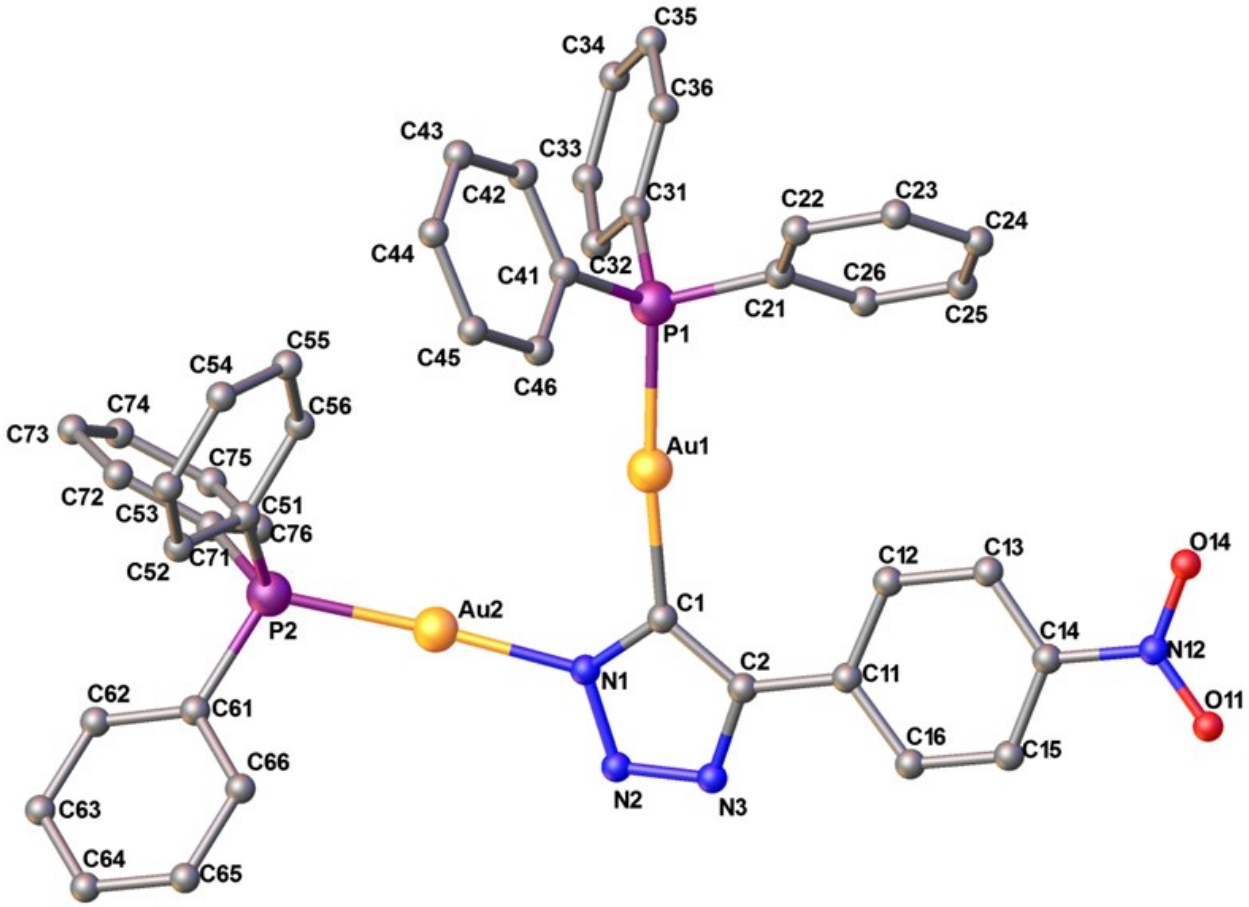

Figure S21. Molecular structure of **3-NO$_2$** with ellipsoids presented at 50% probability and hydrogen atoms, and two chloroform lattice molecules are removed for clarity.

X-Ray experimental details for **3-NO$_2$**:

X-Ray Intensity data were collected at 100 K on a Bruker **SMART** diffractometer using MoKα radiation (λ = 0.71073 Å) and an APEXII CCD area detector. Raw data frames were read by program SAINT[1] and integrated using 3D profiling algorithms. The resulting data were reduced to produce hkl reflections and their intensities and estimated standard deviations. The data were corrected for Lorentz and polarization effects and numerical absorption corrections were applied based on indexed and measured faces.

The structure was solved and refined in SHELXTL6.1, using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. There are two chloroform solvent molecules in the asymmetric unit, one of chloroform is partially disordered over two of the chlorine atoms. In this case, atom C81 should also be disordered but it is to a lesser extent which did not allow for its resolution. In the final cycle of refinement, 10806 reflections (of which 9294 are observed with $I > 2\sigma$ (I)) were used to refine 570 parameters and the resulting R_1, wR_2 and S (goodness of fit) were 2.13%, 4.96% and 0.981, respectively. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized.

Table S1. Crystal data and structure refinement for **3-NO_2**.

Identification code	apow6	
Empirical formula	$C_{46}H_{36}Au_2Cl_6N_4O_2P_2$	
Formula weight	1345.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 13.1709(4) Å	α= 104.570(2)°.
	b = 13.9693(4) Å	β= 113.005(1)°.
	c = 15.1962(4) Å	γ = 101.240(2)°.
Volume	2352.00(12) $Å^3$	
Z	2	
Density (calculated)	1.900 Mg/m^3	
Absorption coefficient	6.682 mm^{-1}	
F(000)	1292	
Crystal size	0.35 x 0.06 x 0.05 mm^3	
Theta range for data collection	1.56 to 27.50°.	
Index ranges	-17≤h≤17, -18≤k≤18, -19≤l≤19	
Reflections collected	79139	
Independent reflections	10806 [R(int) = 0.0712]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.7142 and 0.2013	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10806 / 0 / 570	
Goodness-of-fit on F^2	0.981	
Final R indices [I>2sigma(I)]	R1 = 0.0213, wR2 = 0.0496 [9294]	
R indices (all data)	R1 = 0.0274, wR2 = 0.0515	
Largest diff. peak and hole	1.577 and -1.305 $e.Å^{-3}$	

$R1 = \sum (||F_o| - |F_c||) / ||F_o|$ $wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$

$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$w= 1/[\sigma^2(F_o^2)+(m*p)^2+n*p]$, $p = [\max(F_o^2,0)+ 2* F_c^2]/3$, m & n are constants.

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Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **3-NO_2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	X	Y	Z	U(eq)
Au1	8956(1)	2052(1)	9540(1)	11(1)
Au2	9105(1)	3314(1)	12082(1)	11(1)
P1	7769(1)	2004(1)	7944(1)	12(1)
P2	8318(1)	4541(1)	12455(1)	13(1)
O11	13672(2)	-799(2)	9186(2)	33(1)
O14	12289(2)	-831(2)	7799(2)	27(1)
N1	9997(2)	2354(2)	11781(2)	11(1)
N2	10837(2)	2190(2)	12552(2)	15(1)
N3	11437(2)	1727(2)	12171(2)	14(1)
N12	12804(2)	-574(2)	8745(2)	22(1)
C1	10060(2)	1987(2)	10891(2)	11(1)
C2	10981(2)	1590(2)	11150(2)	12(1)
C11	11464(2)	1067(2)	10526(2)	12(1)
C12	10874(3)	715(2)	9447(2)	15(1)
C13	11312(3)	186(2)	8857(2)	16(1)
C14	12354(3)	20(2)	9349(2)	16(1)
C15	12977(3)	375(2)	10412(2)	19(1)
C16	12523(3)	883(2)	10987(2)	16(1)
C21	8218(2)	1344(2)	7027(2)	13(1)
C22	8452(3)	1769(2)	6368(2)	16(1)
C23	8836(3)	1238(3)	5722(2)	20(1)
C24	8988(3)	291(3)	5736(2)	21(1)
C25	8758(3)	-137(2)	6401(2)	18(1)
C26	8379(3)	381(2)	7044(2)	17(1)
C31	6254(3)	1221(2)	7431(2)	14(1)
C32	5879(3)	962(3)	8103(2)	22(1)
C33	4753(3)	312(3)	7743(3)	27(1)
C34	3976(3)	-54(3)	6710(3)	26(1)
C35	4328(3)	219(3)	6039(3)	23(1)
C36	5471(3)	838(2)	6395(2)	18(1)
C41	7811(3)	3272(2)	7826(2)	13(1)
C42	6869(3)	3438(2)	7117(2)	18(1)
C43	6974(3)	4419(3)	7040(2)	20(1)
C44	8012(3)	5247(2)	7679(2)	18(1)
C45	8942(3)	5093(2)	8397(2)	17(1)
C46	8851(3)	4107(2)	8474(2)	16(1)
C51	8210(3)	5297(2)	11627(2)	14(1)
C52	8736(3)	6377(2)	12011(2)	18(1)

C53	8683(3)	6911(3)	11337(3)	21(1)
C54	8094(3)	6374(3)	10295(2)	22(1)
C55	7555(3)	5296(3)	9903(2)	24(1)
C56	7617(3)	4755(3)	10566(2)	21(1)
C61	9261(3)	5494(2)	13750(2)	15(1)
C62	8829(3)	6013(3)	14357(2)	23(1)
C63	9590(4)	6777(3)	15319(2)	28(1)
C64	10782(3)	7014(3)	15677(2)	27(1)
C65	11225(3)	6492(3)	15092(2)	26(1)
C66	10452(3)	5720(2)	14120(2)	20(1)
C71	6873(3)	4085(2)	12344(2)	16(1)
C72	6168(3)	4722(3)	12270(3)	24(1)
C73	5101(3)	4378(3)	12252(3)	28(1)
C74	4717(3)	3403(3)	12297(3)	27(1)
C75	5399(3)	2770(3)	12351(3)	24(1)
C76	6479(3)	3103(2)	12372(2)	17(1)
C81	6209(4)	7320(3)	1409(3)	38(1)
Cl1	5163(1)	6888(1)	1796(1)	30(1)
Cl2	7411(1)	8382(1)	2457(1)	41(1)
Cl3	5606(1)	7687(1)	357(1)	51(1)
Cl1'	5384(18)	5941(16)	464(16)	96(4)
Cl2'	6780(20)	7960(20)	2157(19)	96(4)
Cl3'	5030(20)	7902(19)	195(18)	96(4)
C82	6490(3)	7421(3)	5575(3)	30(1)
Cl4	6055(1)	6119(1)	5473(1)	61(1)
Cl5	6558(1)	7482(1)	4449(1)	32(1)
Cl6	5537(1)	8066(1)	5792(1)	42(1)

Table S3. Bond lengths [Å] for **3-NO_2**.

Bond	Length	Bond	Length
Au1-C1	2.036(3)	C35-C36	1.389(4)
Au1-P1	2.2907(7)	C41-C42	1.396(4)
Au2-N1	2.028(2)	C41-C46	1.397(4)
Au2-P2	2.2347(8)	C42-C43	1.388(4)
P1-C31	1.814(3)	C43-C44	1.390(4)
P1-C41	1.816(3)	C44-C45	1.384(4)
P1-C21	1.830(3)	C45-C46	1.397(4)
P2-C71	1.811(3)	C51-C52	1.389(4)
P2-C51	1.819(3)	C51-C56	1.398(4)
P2-C61	1.821(3)	C52-C53	1.400(4)
O11-N12	1.225(4)	C53-C54	1.374(5)
O14-N12	1.240(3)	C54-C55	1.388(5)
N1-C1	1.363(3)	C55-C56	1.392(4)
N1-N2	1.367(3)	C61-C66	1.380(4)
N2-N3	1.322(3)	C61-C62	1.391(4)
N3-C2	1.371(3)	C62-C63	1.390(5)
N12-C14	1.454(4)	C63-C64	1.383(5)
C1-C2	1.391(4)	C64-C65	1.381(5)
C2-C11	1.464(4)	C65-C66	1.406(4)
C11-C16	1.403(4)	C71-C76	1.387(4)
C11-C12	1.407(4)	C71-C72	1.398(4)
C12-C13	1.386(4)	C72-C73	1.381(5)
C13-C14	1.381(4)	C73-C74	1.386(5)
C14-C15	1.390(4)	C74-C75	1.373(5)
C15-C16	1.374(4)	C75-C76	1.392(4)
C21-C22	1.385(4)	C81-Cl2'	1.10(3)
C21-C26	1.407(4)	C81-Cl3	1.741(4)
C22-C23	1.392(4)	C81-Cl1	1.759(4)
C23-C24	1.381(5)	C81-Cl2	1.780(4)
C24-C25	1.394(4)	C81-Cl1'	1.88(2)
C25-C26	1.376(4)	C81-Cl3'	2.34(2)
C31-C36	1.386(4)	Cl1'-Cl1'#1	2.43(4)
C31-C32	1.388(4)	C82-Cl4	1.744(4)
C32-C33	1.384(4)	C82-Cl6	1.764(4)
C33-C34	1.382(5)	C82-Cl5	1.770(4)
C34-C35	1.376(5)		

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond Angles [°] for **3-NO_2**.

Bond	Length	Bond	Length
C1-Au1-P1	174.44(8)	C24-C23-C22	120.3(3)
N1-Au2-P2	172.64(7)	C23-C24-C25	120.0(3)
C31-P1-C41	108.24(14)	C26-C25-C24	120.2(3)
C31-P1-C21	103.75(13)	C25-C26-C21	119.9(3)
C41-P1-C21	105.59(13)	C36-C31-C32	118.8(3)
C31-P1-Au1	113.75(10)	C36-C31-P1	122.8(2)
C41-P1-Au1	115.5(1)	C32-C31-P1	118.4(2)
C21-P1-Au1	109.05(10)	C33-C32-C31	120.7(3)
C71-P2-C51	106.13(14)	C34-C33-C32	119.9(3)
C71-P2-C61	107.26(14)	C35-C34-C33	120.0(3)
C51-P2-C61	104.82(14)	C34-C35-C36	120.1(3)
C71-P2-Au2	116.56(11)	C31-C36-C35	120.4(3)
C51-P2-Au2	110.47(10)	C42-C41-C46	119.4(3)
C61-P2-Au2	110.85(10)	C42-C41-P1	123.2(2)
C1-N1-N2	110.1(2)	C46-C41-P1	117.4(2)
C1-N1-Au2	127.02(19)	C43-C42-C41	120.3(3)
N2-N1-Au2	121.35(17)	C42-C43-C44	120.4(3)
N3-N2-N1	108.3(2)	C45-C44-C43	119.7(3)
N2-N3-C2	108.1(2)	C44-C45-C46	120.5(3)
O11-N12-O14	122.7(3)	C45-C46-C41	119.8(3)
O11-N12-C14	119.1(3)	C52-C51-C56	119.5(3)
O14-N12-C14	118.2(3)	C52-C51-P2	122.4(2)
N1-C1-C2	104.5(2)	C56-C51-P2	118.0(2)
N1-C1-Au1	123.4(2)	C51-C52-C53	120.0(3)
C2-C1-Au1	132.2(2)	C54-C53-C52	120.2(3)
N3-C2-C1	109.1(2)	C53-C54-C55	120.2(3)
N3-C2-C11	119.9(3)	C54-C55-C56	120.0(3)
C1-C2-C11	131.0(3)	C55-C56-C51	120.0(3)
C16-C11-C12	117.9(3)	C66-C61-C62	119.6(3)
C16-C11-C2	120.7(3)	C66-C61-P2	117.7(2)
C12-C11-C2	121.3(3)	C62-C61-P2	122.7(2)
C13-C12-C11	121.2(3)	C63-C62-C61	120.4(3)
C14-C13-C12	118.6(3)	C64-C63-C62	119.7(3)
C14-C13-H13A	120.7	C65-C64-C63	120.6(3)
C13-C14-C15	122.0(3)	C64-C65-C66	119.4(3)
C13-C14-N12	119.6(3)	C61-C66-C65	120.3(3)
C15-C14-N12	118.4(3)	C76-C71-C72	119.6(3)
C16-C15-C14	118.7(3)	C76-C71-P2	119.2(2)
C15-C16-C11	121.5(3)	C72-C71-P2	121.1(2)
C22-C21-C26	119.6(3)	C73-C72-C71	119.8(3)
C22-C21-P1	123.3(2)	C72-C73-C74	120.5(3)
C26-C21-P1	117.0(2)	C75-C74-C73	119.7(3)
C21-C22-C23	119.9(3)	C74-C75-C76	120.7(3)

C71-C76-C75	119.7(3)		
Cl2'-C81-Cl3	116.6(12)		
Cl2'-C81-Cl1	93.0(13)	Cl2'-C81-Cl3'	112.2(14)
Cl3-C81-Cl1	111.2(2)	Cl3-C81-Cl3'	16.8(6)
Cl2'-C81-Cl2	16.5(12)	Cl1-C81-Cl3'	96.1(6)
Cl3-C81-Cl2	110.7(2)	Cl2-C81-Cl3'	111.4(6)
Cl1-C81-Cl2	109.4(2)	Cl1'-C81-Cl3'	88.6(9)
Cl2'-C81-Cl1'	158.1(14)	C81-Cl1'-Cl1'#1	167.3(16)
Cl3-C81-Cl1'	85.3(6)	Cl4-C82-Cl6	111.5(2)
Cl1-C81-Cl1'	77.6(6)	Cl4-C82-Cl5	110.0(2)
Cl2-C81-Cl1'	157.3(7)	Cl6-C82-Cl5	109.98(18)

Table S-5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3-NO_2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au1	11(1)	12(1)	8(1)	5(1)	3(1)	5(1)
Au2	13(1)	12(1)	9(1)	4(1)	5(1)	5(1)
P1	12(1)	13(1)	9(1)	6(1)	2(1)	4(1)
P2	14(1)	14(1)	11(1)	5(1)	6(1)	5(1)
O11	32(1)	37(2)	38(2)	12(1)	20(1)	23(1)
O14	30(1)	24(1)	24(1)	-1(1)	17(1)	4(1)
N1	15(1)	9(1)	7(1)	2(1)	4(1)	3(1)
N2	18(1)	17(1)	10(1)	7(1)	5(1)	9(1)
N3	15(1)	17(1)	9(1)	6(1)	3(1)	6(1)
N12	21(2)	14(1)	29(2)	4(1)	15(1)	3(1)
C1	14(1)	8(1)	9(1)	4(1)	4(1)	3(1)
C2	12(1)	10(1)	10(1)	4(1)	3(1)	2(1)
C11	12(1)	10(1)	13(1)	5(1)	5(1)	3(1)
C12	16(2)	15(2)	14(2)	7(1)	6(1)	6(1)
C13	20(2)	14(2)	12(1)	3(1)	7(1)	2(1)
C14	19(2)	11(1)	20(2)	4(1)	12(1)	3(1)
C15	17(2)	20(2)	20(2)	9(1)	7(1)	8(1)
C16	15(2)	18(2)	12(1)	5(1)	3(1)	6(1)
C21	10(1)	13(1)	10(1)	2(1)	1(1)	2(1)
C22	15(2)	17(2)	13(1)	7(1)	3(1)	4(1)
C23	22(2)	25(2)	17(2)	10(1)	11(1)	4(1)
C24	20(2)	24(2)	18(2)	4(1)	11(1)	7(1)
C25	16(2)	16(2)	16(2)	3(1)	4(1)	4(1)
C26	18(2)	15(2)	12(1)	5(1)	4(1)	2(1)
C31	13(1)	14(2)	17(2)	8(1)	5(1)	6(1)
C32	19(2)	29(2)	18(2)	14(1)	7(1)	9(1)
C33	20(2)	38(2)	32(2)	22(2)	15(2)	10(2)
C34	14(2)	28(2)	31(2)	12(2)	7(2)	6(1)
C35	17(2)	24(2)	21(2)	4(1)	4(1)	5(1)
C36	18(2)	19(2)	16(2)	5(1)	7(1)	6(1)
C41	16(2)	12(1)	12(1)	4(1)	8(1)	5(1)
C42	15(2)	17(2)	14(2)	6(1)	1(1)	5(1)
C43	20(2)	25(2)	20(2)	15(1)	6(1)	12(1)
C44	26(2)	17(2)	21(2)	11(1)	14(1)	11(1)
C45	19(2)	15(2)	16(2)	5(1)	8(1)	3(1)
C46	15(2)	19(2)	14(1)	8(1)	6(1)	6(1)
C51	13(1)	18(2)	15(2)	9(1)	7(1)	6(1)
C52	16(2)	20(2)	16(2)	7(1)	6(1)	5(1)
C53	20(2)	18(2)	28(2)	12(1)	10(1)	7(1)
C54	22(2)	30(2)	22(2)	18(2)	11(1)	12(2)

C55	29(2)	30(2)	13(2)	9(1)	10(1)	8(2)
C56	29(2)	18(2)	14(2)	5(1)	9(1)	5(1)
C61	24(2)	13(1)	10(1)	6(1)	7(1)	7(1)
C62	30(2)	22(2)	17(2)	8(1)	12(2)	10(2)
C63	53(2)	18(2)	15(2)	6(1)	18(2)	15(2)
C64	47(2)	16(2)	8(2)	5(1)	4(2)	4(2)
C65	26(2)	23(2)	18(2)	9(1)	1(1)	5(2)
C66	27(2)	17(2)	16(2)	6(1)	8(1)	8(1)
C71	16(2)	20(2)	11(1)	4(1)	7(1)	5(1)
C72	26(2)	22(2)	31(2)	14(2)	16(2)	12(2)
C73	25(2)	32(2)	38(2)	16(2)	19(2)	15(2)
C74	20(2)	29(2)	34(2)	12(2)	15(2)	6(2)
C75	20(2)	24(2)	28(2)	12(2)	10(2)	5(1)
C76	18(2)	19(2)	16(2)	7(1)	8(1)	8(1)
C81	39(2)	32(2)	40(2)	8(2)	22(2)	8(2)
Cl1	32(1)	35(1)	37(1)	24(1)	20(1)	16(1)
Cl2	31(1)	33(1)	46(1)	-1(1)	17(1)	7(1)
Cl3	74(1)	48(1)	31(1)	20(1)	26(1)	6(1)
C82	29(2)	26(2)	21(2)	14(2)	-1(2)	2(2)
Cl4	66(1)	31(1)	48(1)	24(1)	-6(1)	-6(1)
Cl5	35(1)	36(1)	20(1)	11(1)	7(1)	14(1)
Cl6	37(1)	66(1)	28(1)	22(1)	13(1)	20(1)