Coinage metal metallacycles involving a fluorinated 3,5-diarylpyrazolate

Jaspreet S. Lakhi,[†] Monika R. Patterson,[†] H. V. Rasika Dias*

Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, Texas 76019, United States

Supporting Information

NMR Spectra:

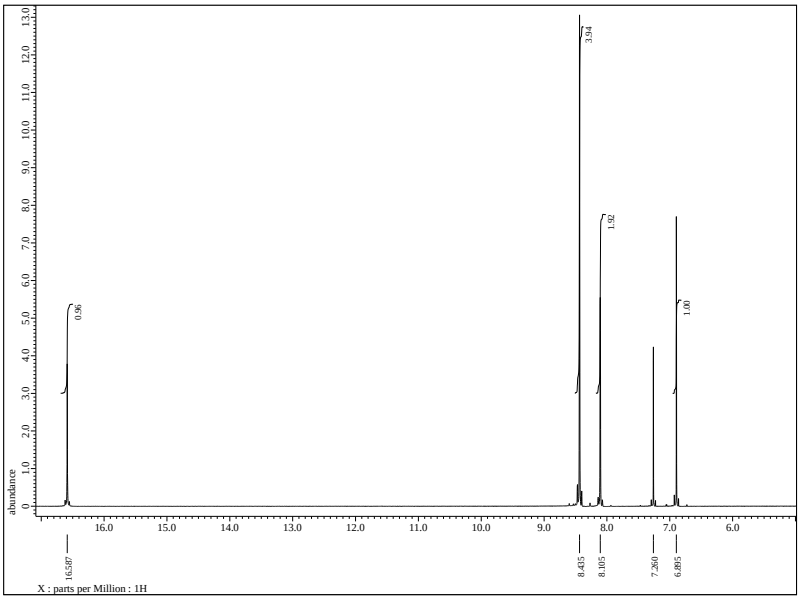


Figure S1: ^{1}H NMR spectrum of 1,3-bis(3,5-bis(trifluoromethyl)phenyl)-3-hydroxyprop-2-en-1-one.

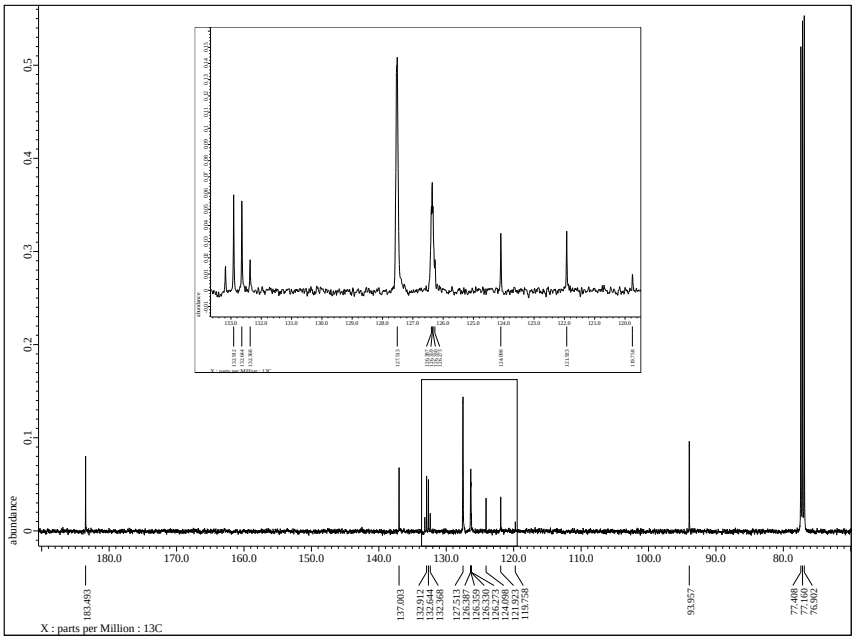


Figure S2: ^{13}C{^{1}H} NMR spectrum of 1,3-bis(3,5-bis(trifluoromethyl)phenyl)-3-hydroxyprop-2-en-1-one.

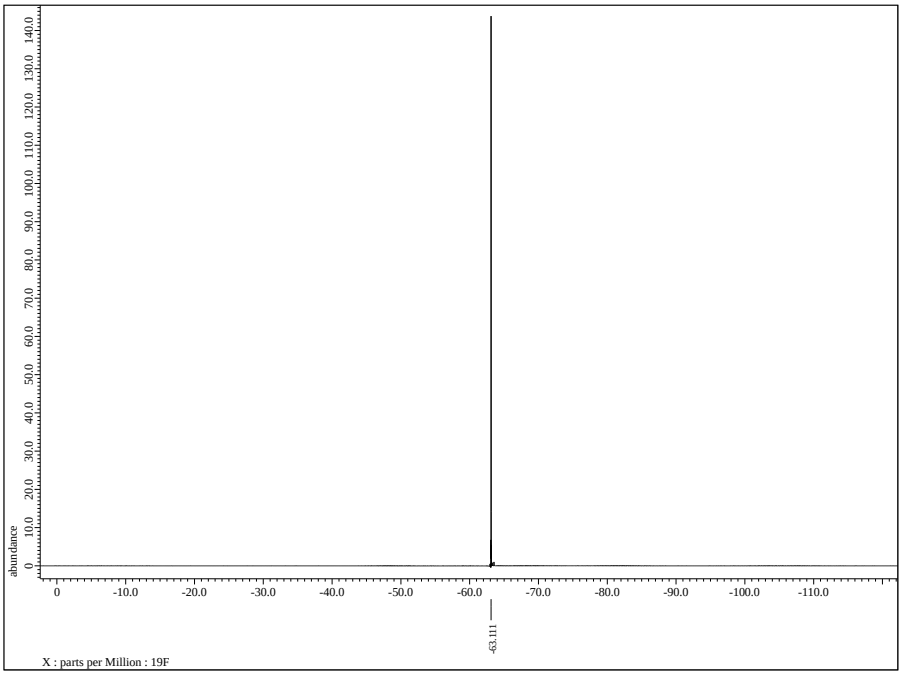


Figure S3: ^{19}F NMR spectrum of 1,3-bis(3,5-bis(trifluoromethyl)phenyl)-3-hydroxyprop-2-en-1-one.

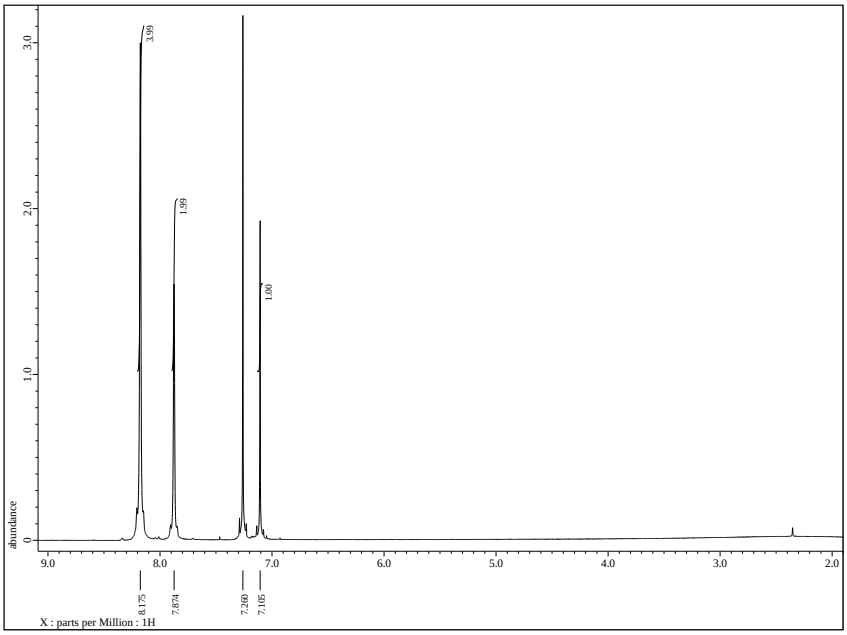


Figure S4: ^{1}H NMR spectrum of 3,5-(3,5-$(CF_3)_2$Ph)$_2$PzH.

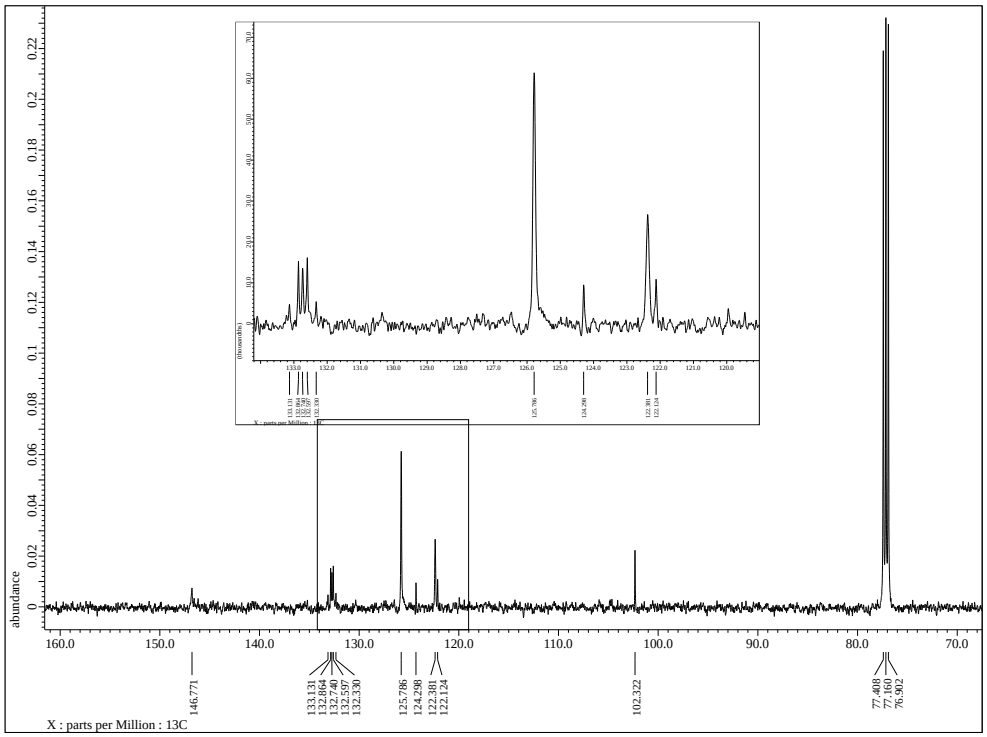


Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of 3,5-(3,5-$(CF_3)_2$Ph)$_2$PzH.

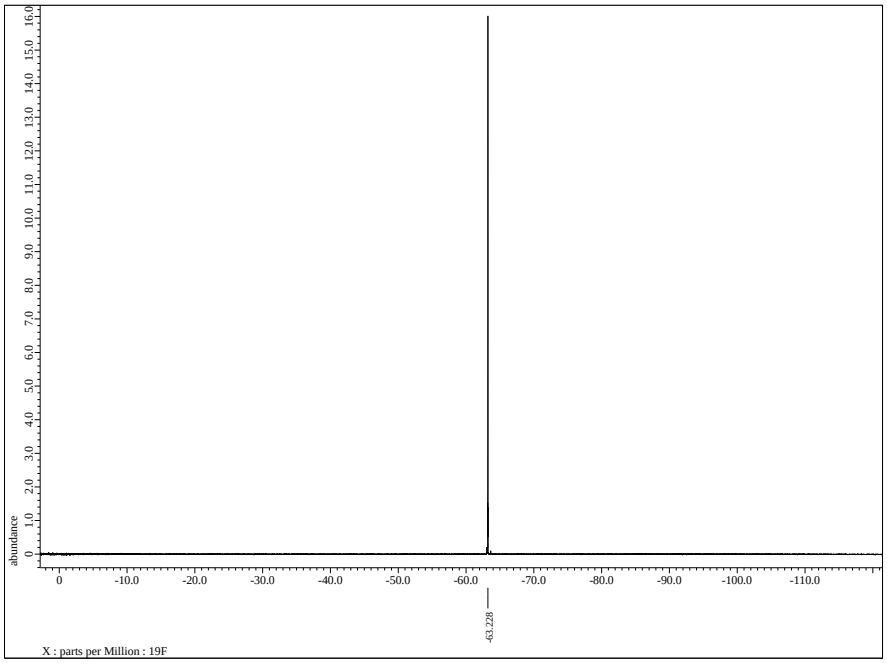


Figure S6: ^{19}F NMR spectrum of 3,5-(3,5-$(CF_3)_2$Ph)$_2$PzH.

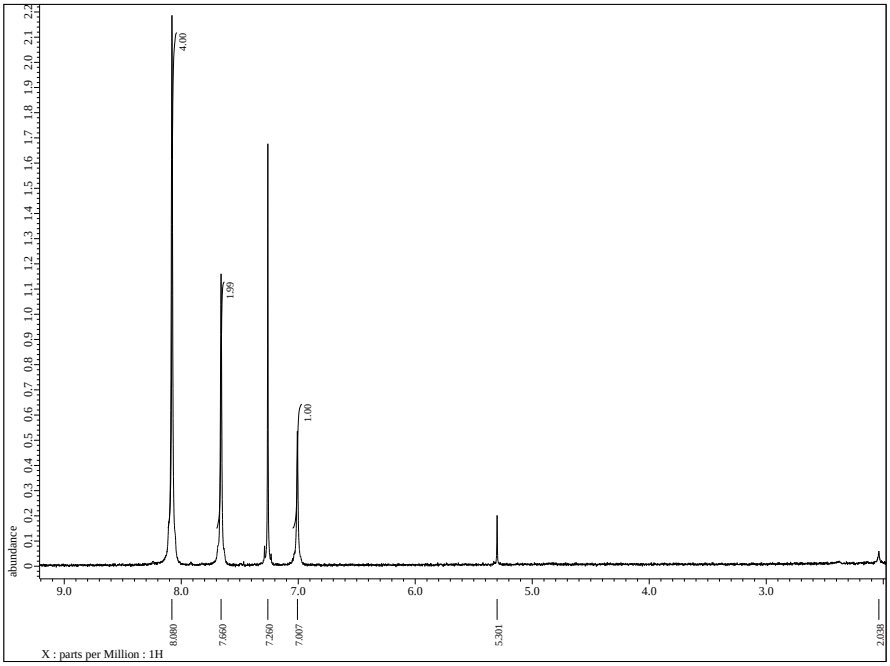


Figure S7: ^{1}H NMR spectrum of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Cu\}_3$.

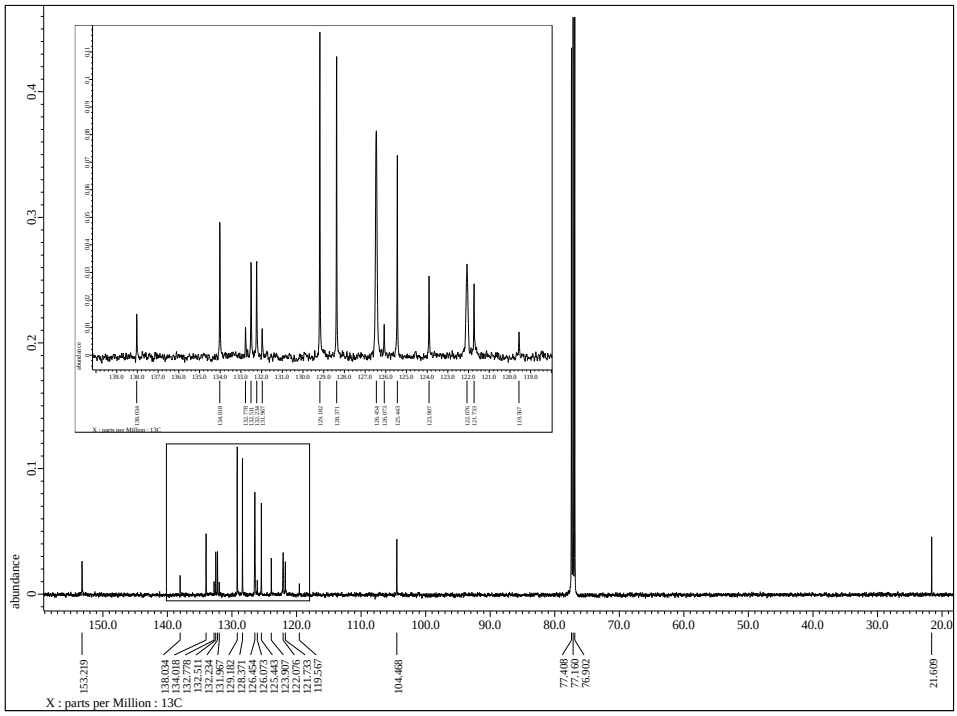


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Cu\}_3$. Data collected on a sample containing some toluene as toluene free materials is not very soluble in $CDCl_3$.

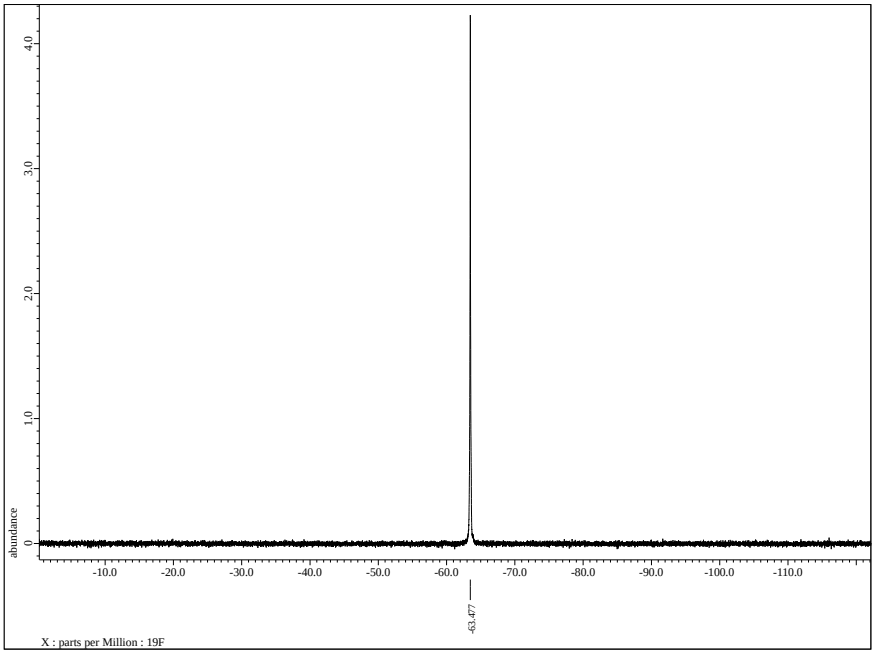


Figure S9: ^{19}F NMR spectrum of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Cu\}_3$.

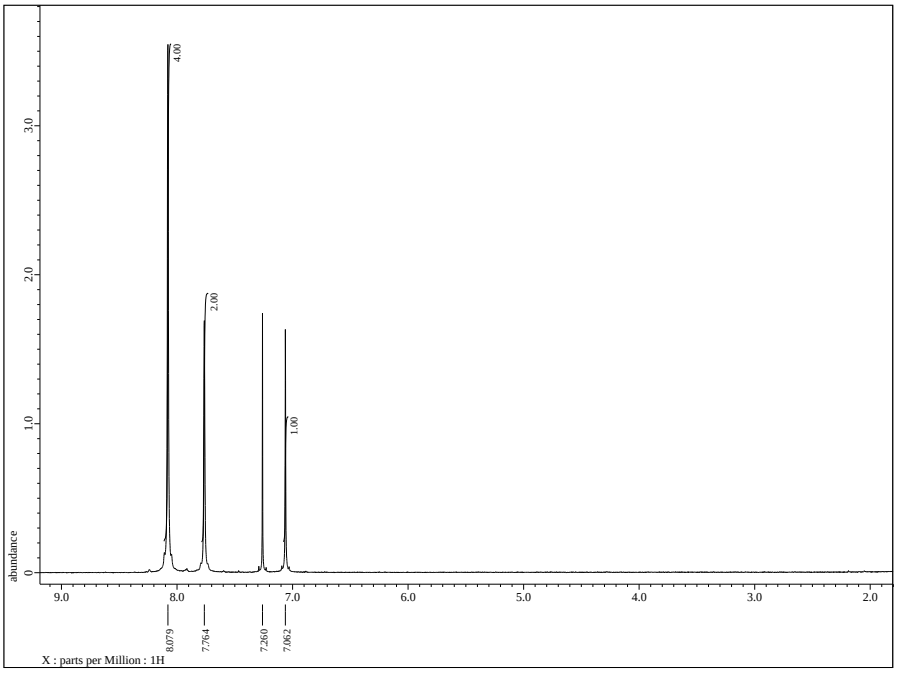


Figure S10: ^{1}H NMR spectrum of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Ag\}_3$.

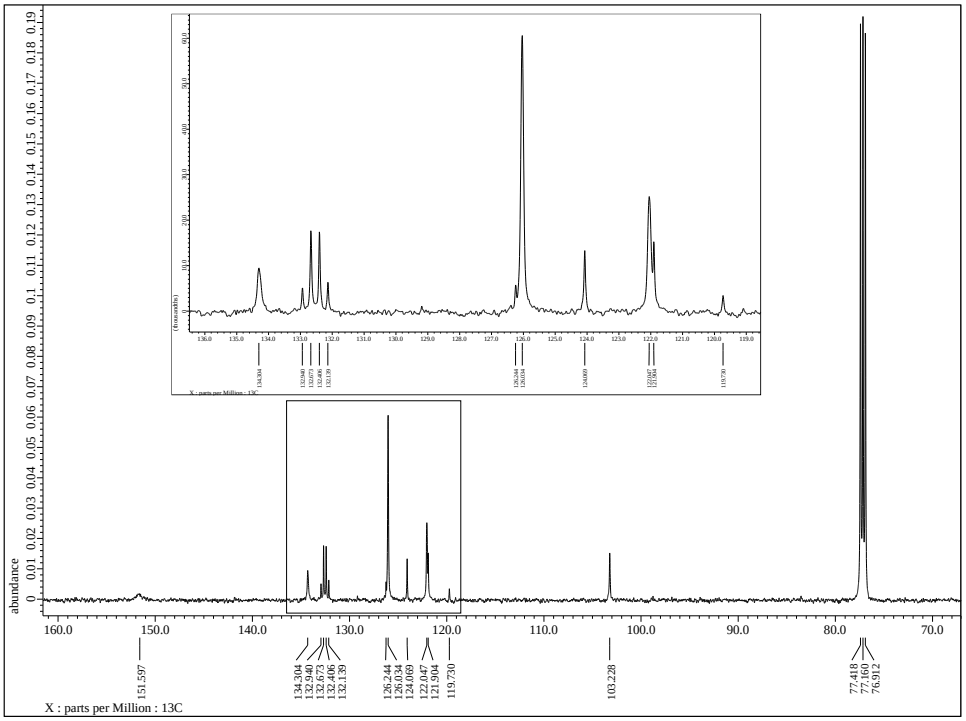


Figure S11: $^{13}C\{^{1}H\}$ NMR spectrum of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Ag\}_3$.

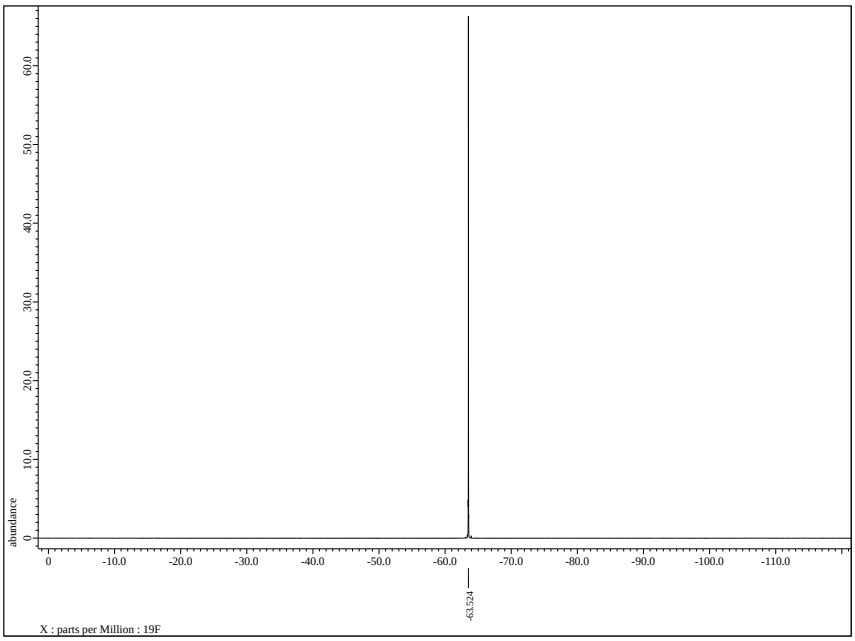


Figure S12: ^{19}F NMR spectrum of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Ag\}_3$.

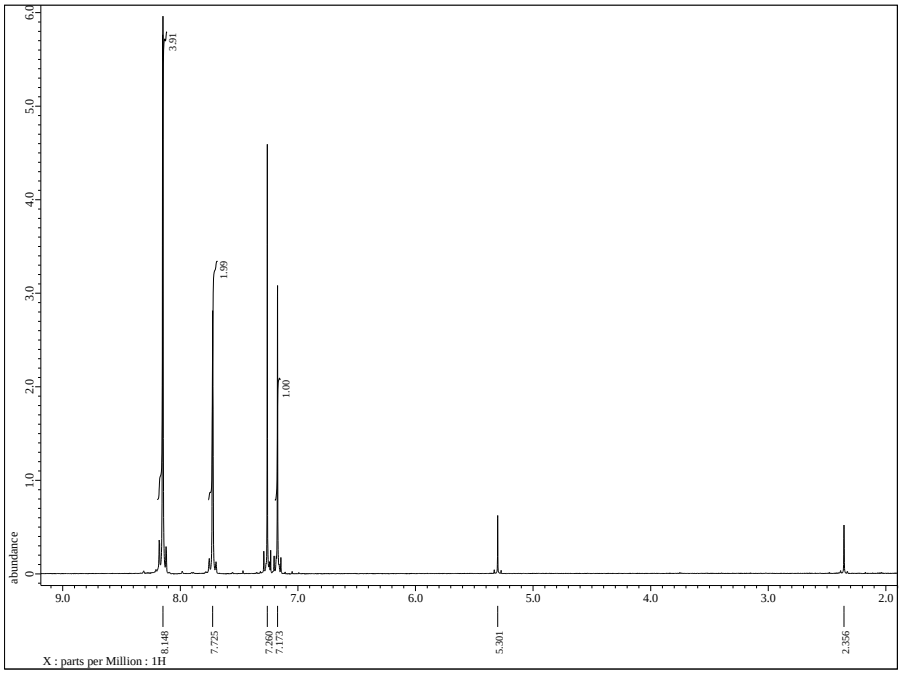


Figure S13: ^{1}H NMR spectrum of {[3,5-(3,5-$(CF_3)_2$Ph)$_2$Pz]Au}$_3$.

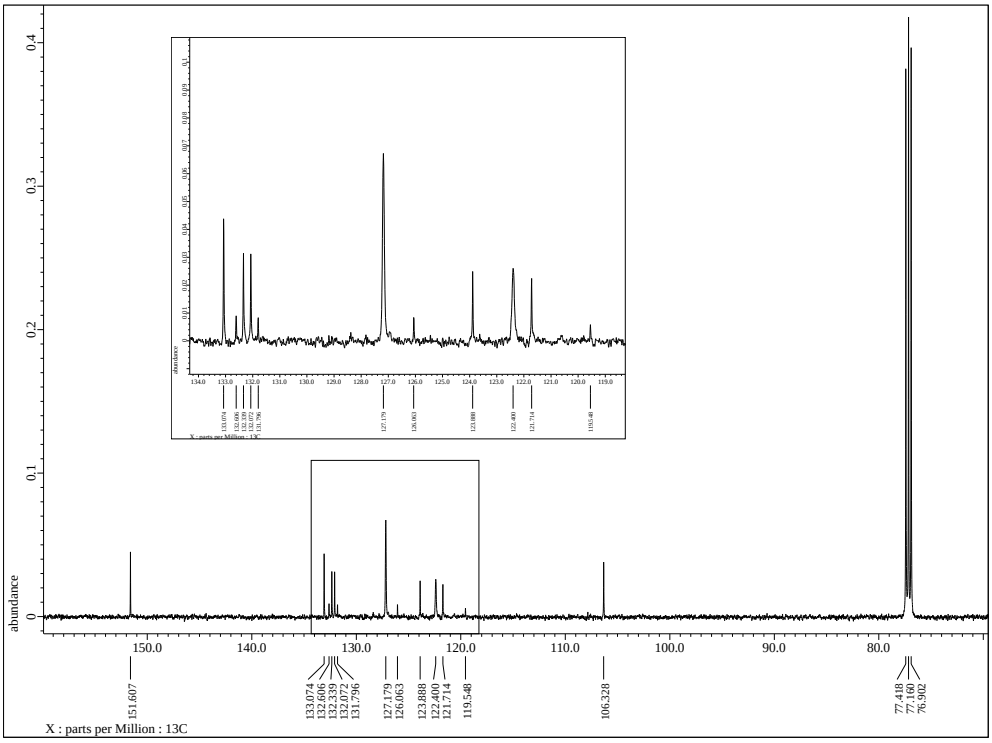


Figure S14: $^{13}C\{^{1}H\}$ NMR spectrum of {[3,5-(3,5-$(CF_3)_2$Ph)$_2$Pz]Au}$_3$.

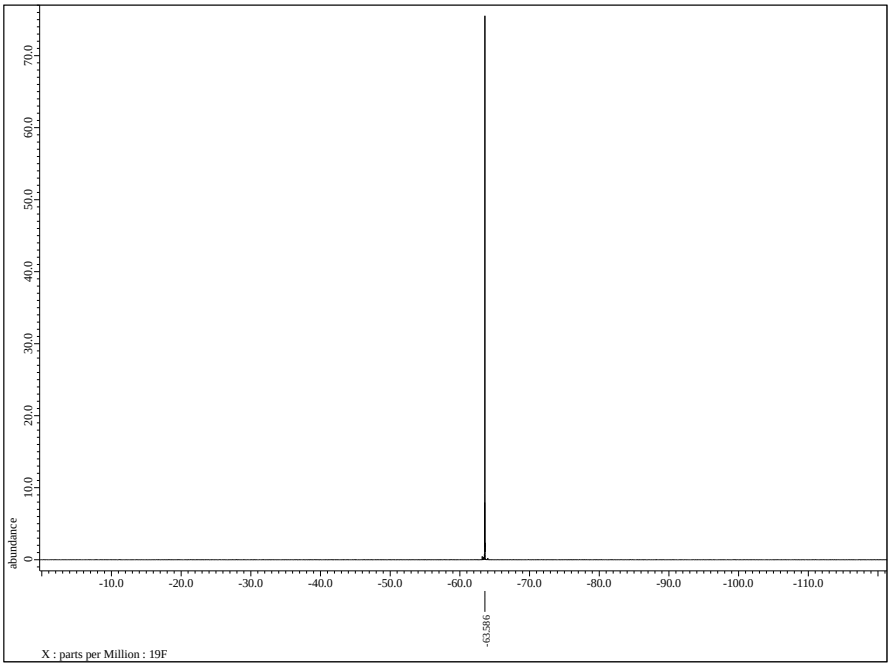


Figure S15: ^{19}F NMR spectrum of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Au\}_3$.

Luminescence Data:

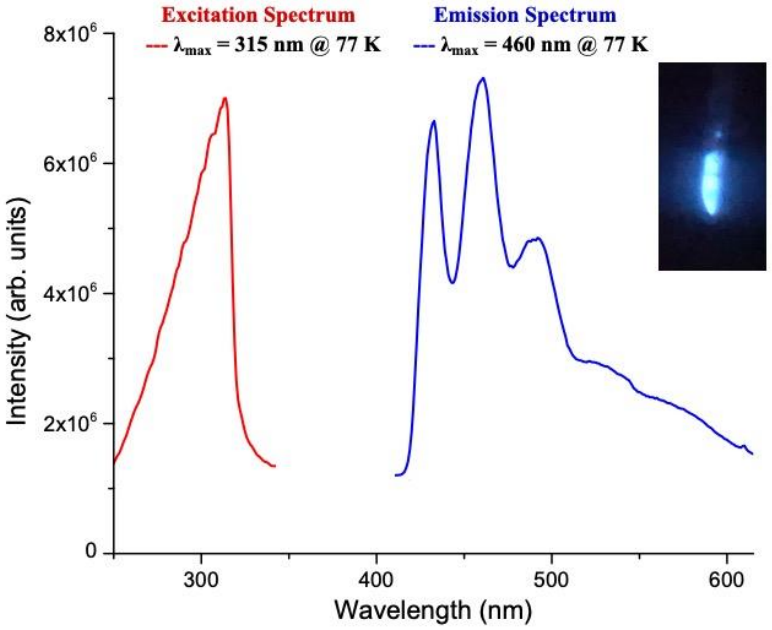


Figure S16: Luminescence Spectra of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Cu\}_3$ at 77 K.

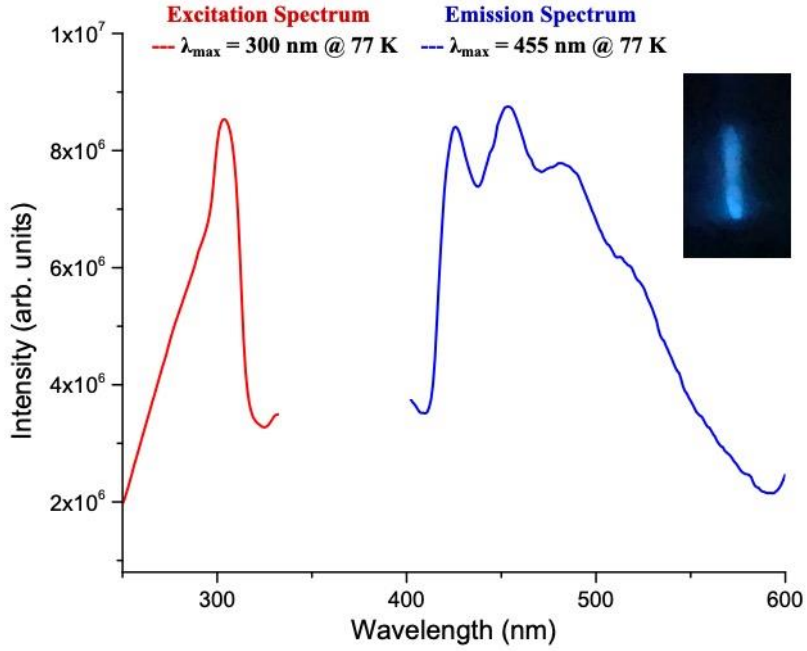


Figure S17: Luminescence Spectra of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Ag\}_3$ at 77 K.

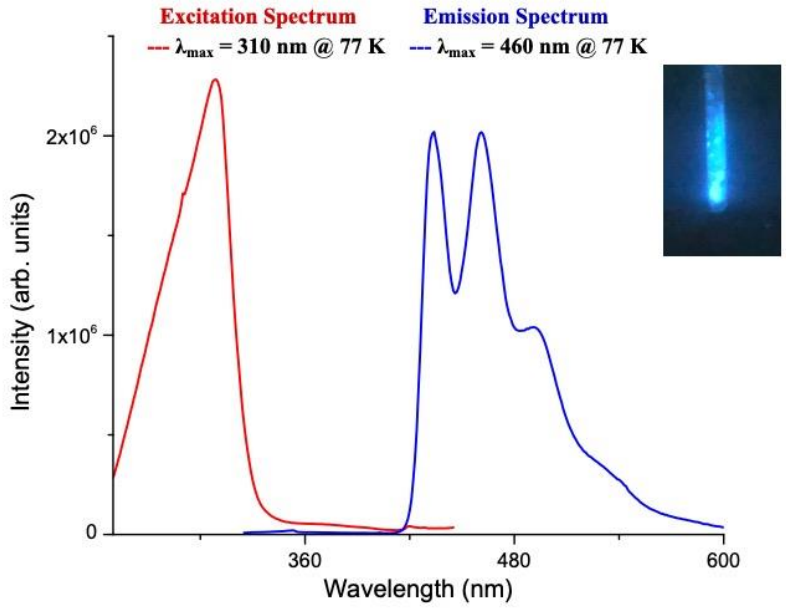


Figure S18: Luminescence Spectra of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Au\}_3$ at 77 K.

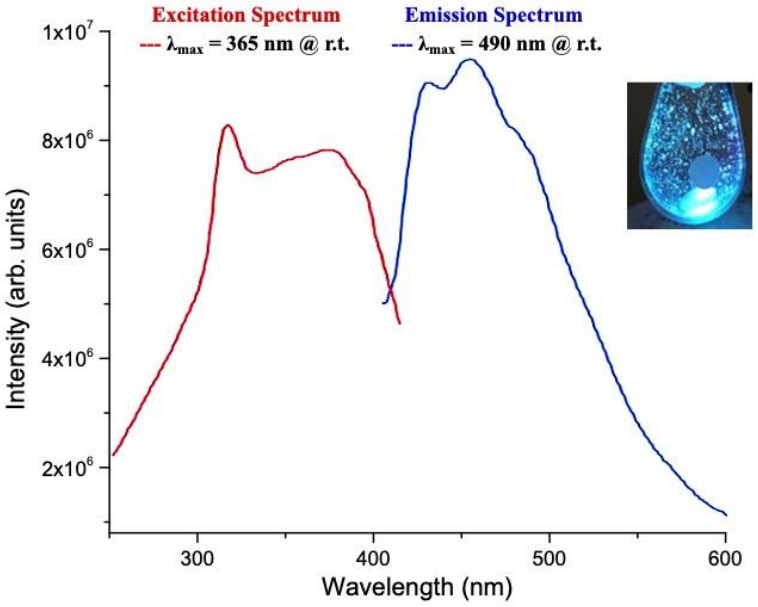
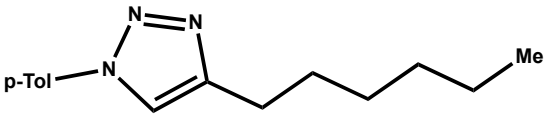


Figure S19: Luminescence Spectra of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Au\}_3$ at room temperature.

Table S1. Azide-alkyne cycloaddition results

Entry	Catalyst	Alkyne	Percent Conversion	Isolated Yield
1	$\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Cu\}_3$	1-Octyne	99 %	94 %
2	$\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Ag\}_3$	1-Octyne	0 %	N/A
3	$\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Au\}_3$	1-Octyne	0 %	N/A
4	$\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Cu\}_3$	Phenylacetylene	100 %	97 %

1-(*p*-tolyl)-4-hexyl-1*H*-1,2,3-triazole



^{1}H NMR ($CDCl_3$, 500 MHz): 7.67 (s, 1H), 7.55 (d, 2H, J = 6.87 Hz), 7.23 (d, 2H, J = 6.87 Hz), 2.73 (t, 2H, J = 7.45 Hz), 2.35 (s, 3H), 1.65-1.71 (m, 2H), 1.33-1.37 (m, 2H), 1.26-1.29 (m, 4H), 0.85 (t, 3H, J = 6.87 Hz). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 500 MHz): 149.0, 138.4, 135.0, 130.1, 120.2, 118.8, 31.6, 29.4, 29.0, 25.7, 22.6, 21.0, 14.1.

Reference: Devaborniny, P.; Ponduru, T.; Noonikara-Poyil, A.; Jayaranta, N.; Dias, H.V.R.; Acetylene and terminal alkyne complexes of copper(I) supported fluorinated pyrazolates: synthesis, structures, and transformations. *Dalton Transactions.* **2019**, *48*, 15782-15794.

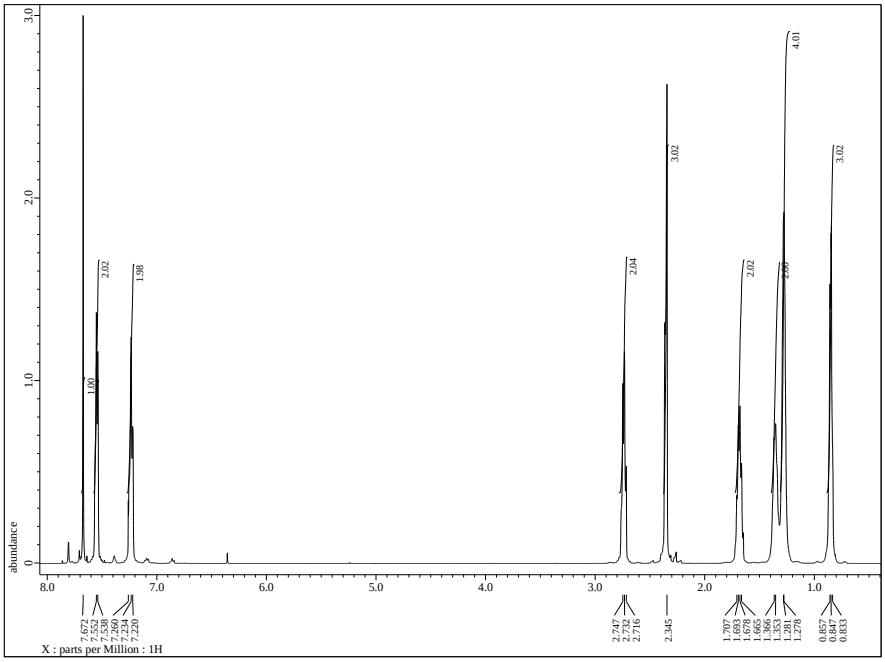


Figure S20: ^{1}H NMR spectrum of 1-(*p*-tolyl)-4-hexyl-1*H*-1,2,3-triazole in $CDCl_3$ at room temperature.

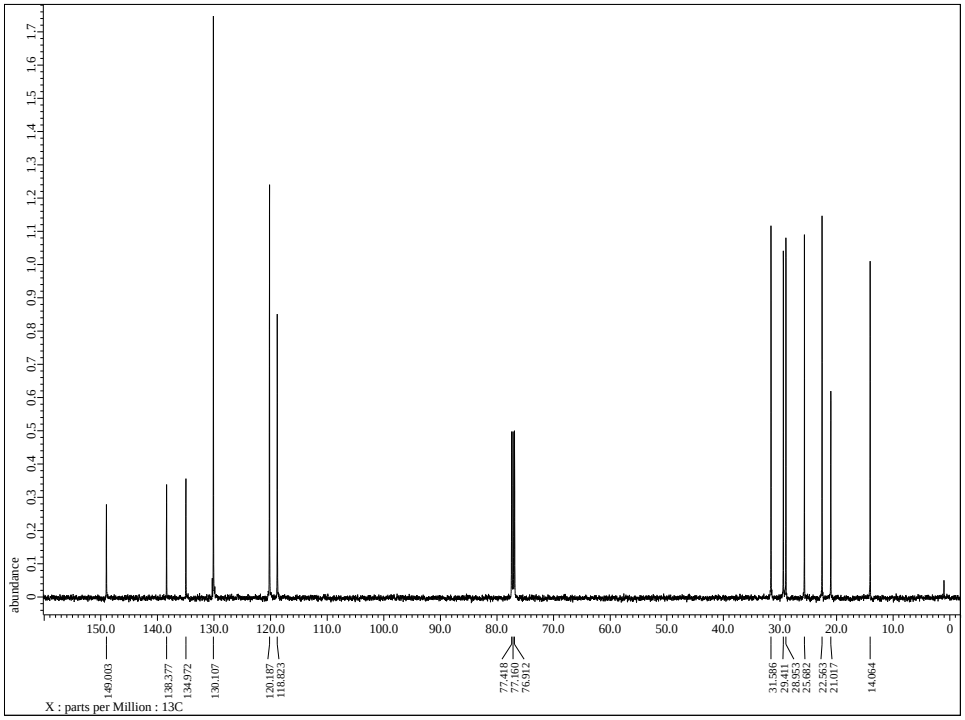
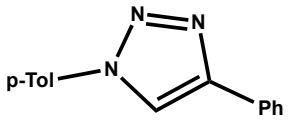


Figure S21: ^{13}C{^{1}H} NMR spectrum of 1-(*p*-tolyl)-4-hexyl-1*H*-1,2,3-triazole in $CDCl_3$ at room temperature.

1-(*p*-tolyl)-4-phenyl-1*H*-1,2,3-triazole



^{1}H NMR ($CDCl_3$, 500 MHz): 8.15 (s, 1H), 7.90 (d, 2H, J = 7.45 Hz), 7.65 (d, 2H, J = 8.60 Hz), 7.45 (t, 2H, J = 7.45 Hz), 7.30-7.36 (m, 3H), 2.42 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$, 500 MHz): 148.3, 139.0, 134.8, 130.4, 129.0, 128.4, 125.9, 120.5, 117.8, 21.2.

Reference: Meng, X.; Xu, X.; Gao, T.; Chen, B.; *Eur. J. Org. Chem.* **2010**, *2010*, 5409-5414.

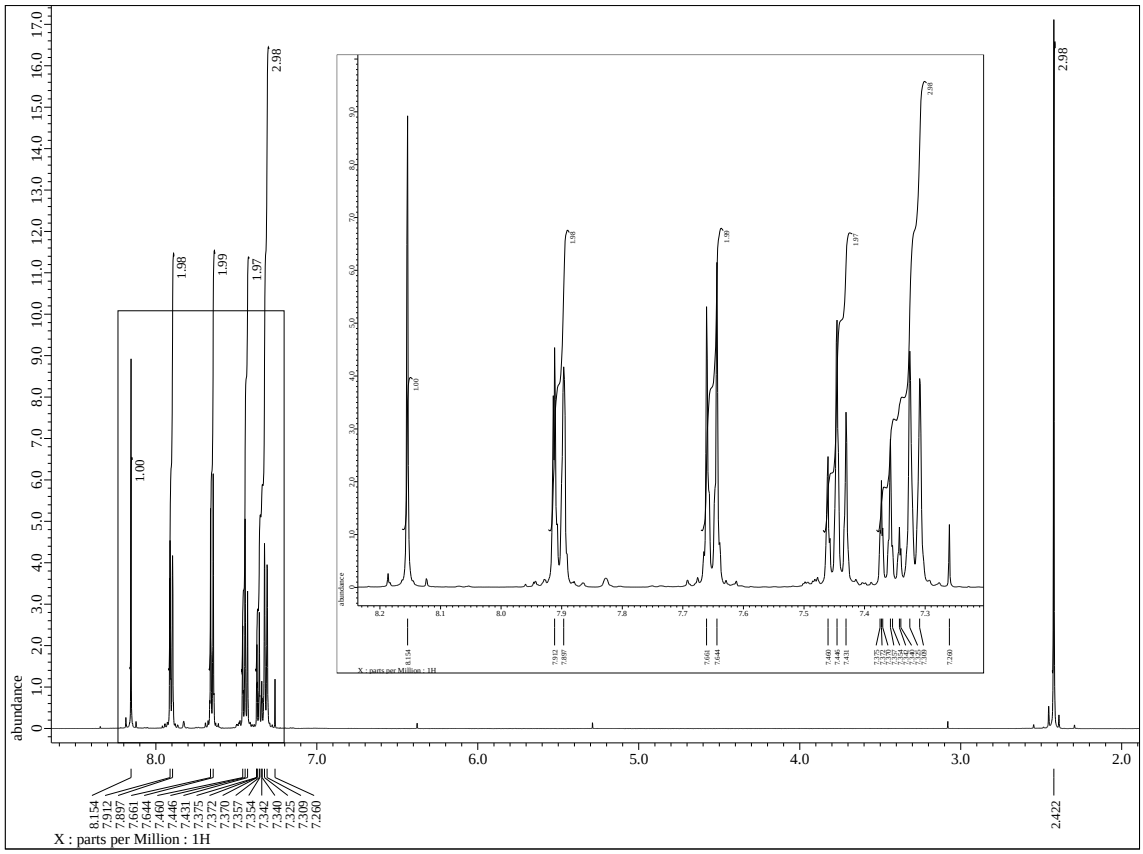


Figure S22: ^{1}H NMR spectrum of 1-(*p*-tolyl)-4-phenyl-1*H*-1,2,3-triazole in $CDCl_3$ at room temperature.

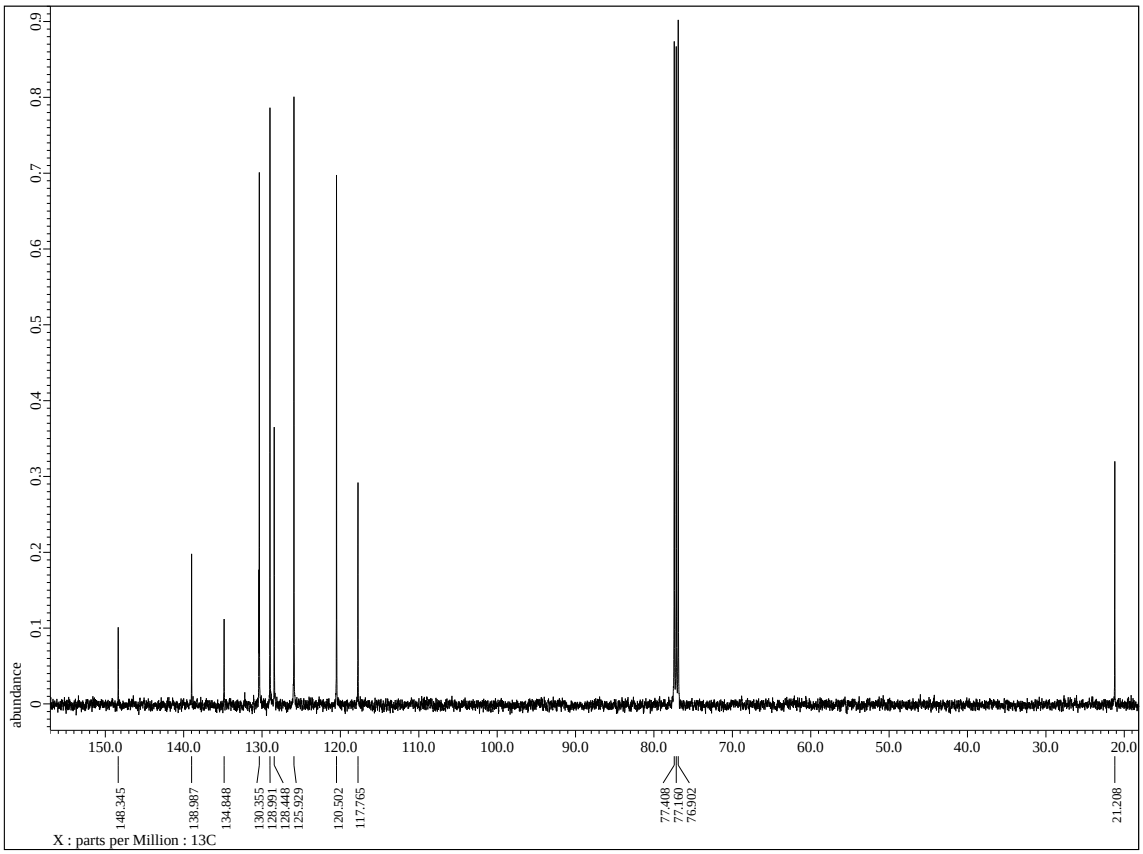


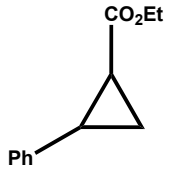
Figure S23: $^{13}C\{^{1}H\}$ NMR spectrum of 1-(*p*-tolyl)-4-phenyl-1*H*-1,2,3-triazole in $CDCl_3$ at room temperature.

Table S2. Copper catalyzed cyclopropanation reactions

Entry	Catalyst	EDA addition time (hours)	*trans:cis**	Cyclopropane yield %*
1	$\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Cu\}_3$	10	73:27	45
2	$\{[3,5\text{-}(CF_3)_2Pz]Cu\}_3$	10	61:39	37

*Calculated from ^{1}H NMR, using an internal standard of dimethylformamide.

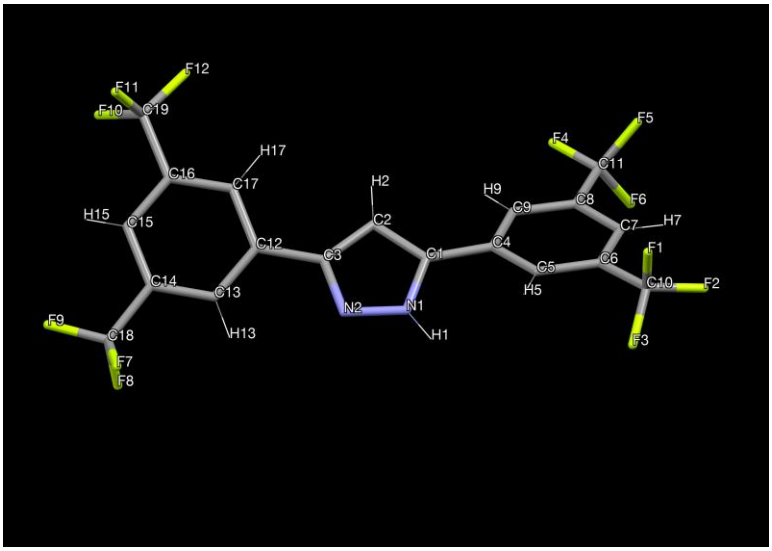
Ethyl-2-phenylcyclopropane-1-carboxylate:



cis: ^{1}H NMR ($CDCl_3$, 500 MHz): 7.29-7.19 (m, 5H), 3.89 (q, 2H, J = 7.0 Hz), 2.60 (app q, 1H, J = 8.5 Hz), 2.10 (ddd, 1H, J = 9.3, 8.6, 5.0 Hz), 1.73 (ddd, 1H, J = 6.5, 5.0, 4.6 Hz), 1.35 (ddd, 1H, J = 8.6, 8.3, 4.6 Hz), 0.99 (t, 3H, J = 7.0 Hz). ^{13}C NMR ($CDCl_3$, 500 MHz): 171.0, 136.6, 129.3, 127.9, 126.6, 60.1, 25.4, 21.8, 14.0, 11.1.

trans: ^{1}H NMR ($CDCl_3$, 500 MHz): 7.33-7.11 (m, 5H), 4.19 (q, 2H, J = 7.0 Hz), 2.54 (ddd, 1H, J = 9.2, 6.5, 4.0 Hz), 1.92 (ddd, 1H, J = 8.2, 5.3, 4.0 Hz), 1.62 (ddd, 1H, J = 9.2, 5.3, 4.6 Hz), 1.33 (ddd, 1H, J = 8.2, 6.6, 4.6 Hz), 1.30 (t, 3H, J = 7.0 Hz). ^{13}C NMR ($CDCl_3$, 500 MHz): 173.4, 140.1, 128.5, 126.5, 126.2, 60.7, 26.2, 24.2, 17.1, 14.3.

Reference: Barrett, A.; Braddock, D.; Lenoir, I.; Tone, H.; *J. Org. Chem.* **2001**, *66*, 8260-8263.



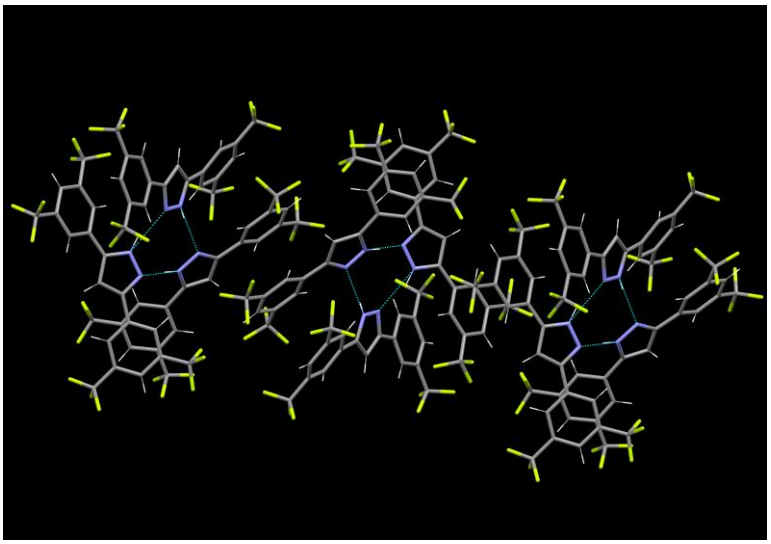


Figure S24. Top: Molecular structure and atom labelling scheme of 3,5-(3,5-$(CF_3)_2$Ph)$_2$PzH. Bottom: A view showing packing of hydrogen bonded 3,5-(3,5-$(CF_3)_2$Ph)$_2$PzH trimers

Table S3. Crystal data and structure refinement for 3,5-(3,5-$(CF_3)_2$Ph)$_2$PzH.

Identification code	Rad534
Empirical formula	$C_{19}H_8F_{12}N_2$
Formula weight	492.27
Temperature/K	99.99
Crystal system	trigonal
Space group	R-3
a/Å	17.7048(6)

b/Å	17.7048(6)
c/Å	31.8231(11)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	8638.8(7)
Z	18
ρ_{calc}g/cm^3	1.703
μ/mm^{-1}	0.184
F(000)	4392.0
Crystal size/mm^3	0.5 × 0.41 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.466 to 59.264
Index ranges	-24 ≤ h ≤ 24, -24 ≤ k ≤ 24, -44 ≤ l ≤ 44
Reflections collected	36951
Independent reflections	5428 [R_{int} = 0.0228, R_{sigma} = 0.0144]
Data/restraints/parameters	5428/0/300
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0332, wR_2 = 0.0889
Final R indexes [all data]	R_1 = 0.0342, wR_2 = 0.0900
Largest diff. peak/hole / e Å^{-3}	0.35/-0.41

Table S4. Bond Lengths for 3,5-(3,5-(CF$_3$)$_2$Ph)$_2$PzH.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C10	1.3346(17)	C3	C12	1.4691(16)
F2	C10	1.3187(17)	C4	C5	1.3944(16)
F3	C10	1.3388(16)	C4	C9	1.4013(16)
F4	C11	1.3247(17)	C5	C6	1.3907(17)
F5	C11	1.3371(18)	C6	C7	1.3871(17)
F6	C11	1.3237(19)	C6	C10	1.5001(17)
F7	C18	1.3388(16)	C7	C8	1.3939(17)
F8	C18	1.3420(17)	C8	C9	1.3834(17)
F9	C18	1.3321(16)	C8	C11	1.5007(18)
F10	C19	1.3301(18)	C12	C13	1.3977(16)
F11	C19	1.3356(18)	C12	C17	1.4001(16)
F12	C19	1.3238(18)	C13	C14	1.3888(17)
N1	N2	1.3478(14)	C14	C15	1.3885(18)
N1	C1	1.3563(15)	C14	C18	1.5039(18)
N2	C3	1.3434(15)	C15	C16	1.3953(18)
C1	C2	1.3905(16)	C16	C17	1.3862(17)
C1	C4	1.4656(16)	C16	C19	1.5074(18)

C2	C3	1.4071(16)	

Table S5. Bond Angles for 3,5-(3,5-$(CF_3)_2$Ph)$_2$PzH.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	N1	C1	112.37(10)	F5	C11	C8	111.59(12)
C3	N2	N1	105.30(10)	F6	C11	F4	106.99(13)
N1	C1	C2	106.48(10)	F6	C11	F5	105.72(13)
N1	C1	C4	121.14(11)	F6	C11	C8	111.80(12)
C2	C1	C4	132.38(11)	C13	C12	C3	119.70(11)
C1	C2	C3	104.97(9)	C13	C12	C17	118.99(11)
N2	C3	C2	110.88(10)	C17	C12	C3	121.31(11)
N2	C3	C12	118.78(10)	C14	C13	C12	120.17(11)
C2	C3	C12	130.34(11)	C13	C14	C18	118.24(11)
C5	C4	C1	120.33(11)	C15	C14	C13	121.22(11)
C5	C4	C9	119.19(11)	C15	C14	C18	120.52(11)
C9	C4	C1	120.46(10)	C14	C15	C16	118.29(11)
C6	C5	C4	120.14(11)	C15	C16	C19	117.74(11)
C5	C6	C10	119.20(11)	C17	C16	C15	121.34(11)
C7	C6	C5	120.99(11)	C17	C16	C19	120.91(12)
C7	C6	C10	119.74(11)	C16	C17	C12	119.95(11)
C6	C7	C8	118.48(11)	F7	C18	F8	105.64(12)
C7	C8	C11	117.90(11)	F7	C18	C14	111.95(10)
C9	C8	C7	121.40(11)	F8	C18	C14	111.27(12)
C9	C8	C11	120.68(11)	F9	C18	F7	108.07(12)
C8	C9	C4	119.75(11)	F9	C18	F8	106.46(11)
F1	C10	F3	105.30(11)	F9	C18	C14	113.01(11)
F1	C10	C6	111.26(12)	F10	C19	F11	106.25(13)
F2	C10	F1	106.72(13)	F10	C19	C16	111.43(12)
F2	C10	F3	107.88(14)	F11	C19	C16	111.19(12)
F2	C10	C6	112.96(12)	F12	C19	F10	108.45(13)
F3	C10	C6	112.27(11)	F12	C19	F11	106.50(13)
F4	C11	F5	107.36(14)	F12	C19	C16	112.69(12)
F4	C11	C8	112.97(11)				

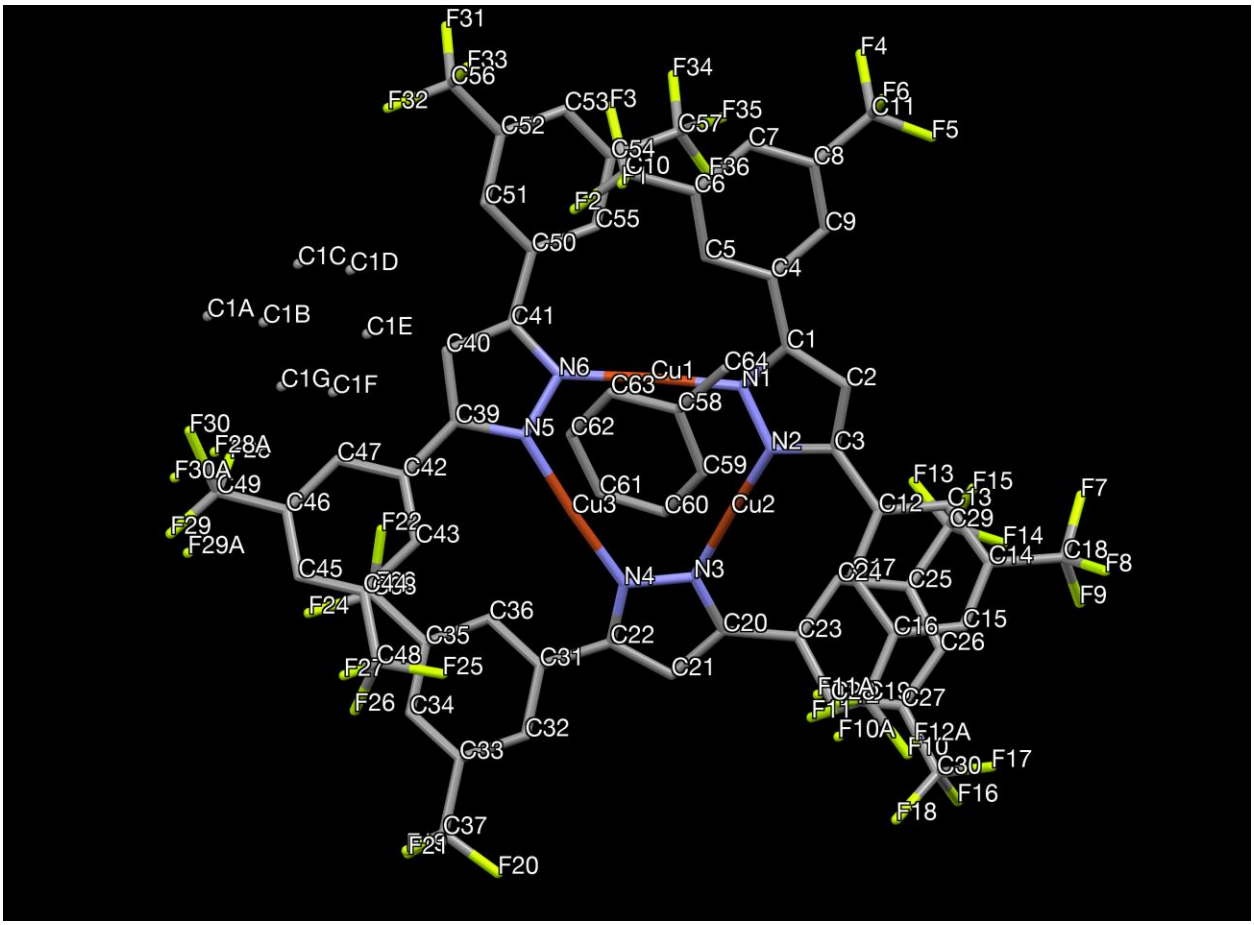


Figure S25. Molecular structure and atom labelling scheme of {[3,5-(3,5-$(CF_3)_2Ph)_2Pz$]Cu}$_3$•1.5(toluene)

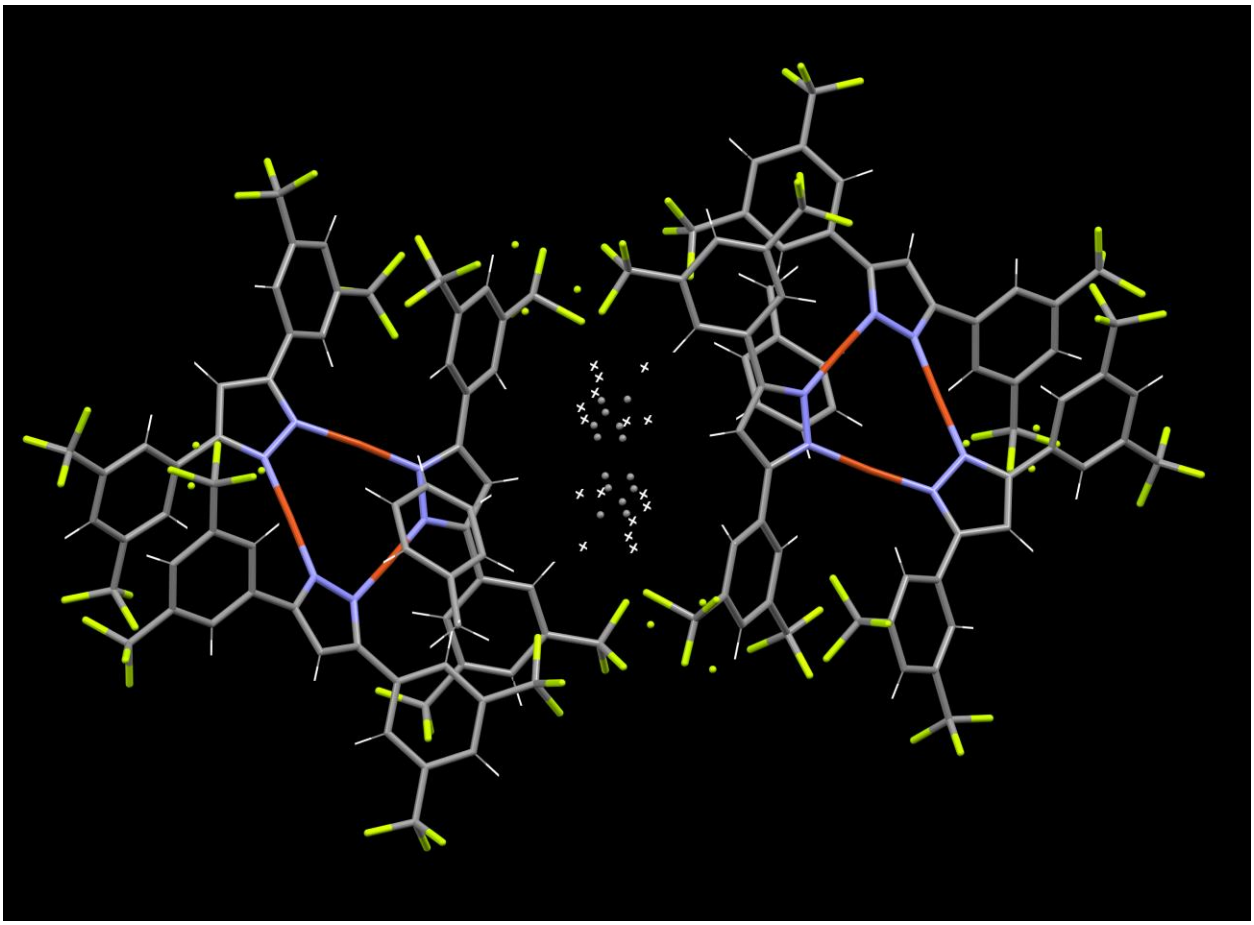


Figure S26. A view of packing two moieties of {[3,5-(3,5-$(CF_3)_2$Ph)$_2$Pz]Cu}$_3$•1.5(toluene)

Table S6. Crystal data and structure refinement for {[3,5-(3,5-$(CF_3)_2$Ph)$_2$Pz]Cu}$_3$•1.5(toluene).

Identification code	Rad539
Empirical formula	$C_{67.5}H_{33}Cu_3F_{36}N_6$
Formula weight	1802.62
Temperature/K	100.01
Crystal system	triclinic
Space group	P-1
a/Å	8.4054(10)
b/Å	19.555(2)
c/Å	21.674(2)
α/°	107.382(2)
β/°	91.600(2)
γ/°	98.226(2)
Volume/Å^3	3355.4(7)

Z	2
ρ_{calc}g/cm^3	1.784
μ/mm^{-1}	1.091
F(000)	1782.0
Crystal size/mm^3	0.3 × 0.07 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.654 to 52
Index ranges	$-10 \leq h \leq 10$, $-24 \leq k \leq 24$, $-26 \leq l \leq 26$
Reflections collected	30015
Independent reflections	13114 [R_{int} = 0.0440, R_{sigma} = 0.0620]
Data/restraints/parameters	13114/327/1104
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ (I)]	R_1 = 0.0864, wR_2 = 0.2395
Final R indexes [all data]	R_1 = 0.1105, wR_2 = 0.2592
Largest diff. peak/hole / e Å^{-3}	2.40/-0.97

Table S7. Bond Lengths for {[3,5-(3,5-(CF$_3$)$_2$Ph)$_2$Pz]Cu}$_3$•1.5(toluene).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	N1	1.869(7)	C14	C15	1.379(14)
Cu1	N6	1.867(7)	C14	C18	1.504(13)
Cu2	N2	1.848(7)	C15	C16	1.394(13)
Cu2	N3	1.843(7)	C16	C17	1.399(12)
Cu3	N4	1.849(7)	C16	C19	1.427(10)
Cu3	N5	1.854(7)	C19	F11A	1.382(12)
F1	C10	1.333(12)	C19	F12A	1.387(11)
F2	C10	1.331(11)	C19	F10A	1.315(12)
F3	C10	1.343(12)	C20	C21	1.411(11)
F4	C11	1.336(11)	C20	C23	1.462(11)
F5	C11	1.330(11)	C21	C22	1.385(11)
F6	C11	1.340(11)	C22	C31	1.478(11)
F7	C18	1.337(12)	C23	C24	1.403(12)
F8	C18	1.323(14)	C23	C28	1.387(12)
F9	C18	1.339(13)	C24	C25	1.391(12)
F10	C19	1.354(11)	C25	C26	1.390(14)
F11	C19	1.412(12)	C25	C29	1.500(13)
F12	C19	1.334(12)	C26	C27	1.383(13)
F13	C29	1.325(13)	C27	C28	1.392(12)
F14	C29	1.323(12)	C27	C30	1.500(13)
F15	C29	1.327(13)	C31	C32	1.399(11)
F16	C30	1.297(16)	C31	C36	1.396(12)
F17	C30	1.312(15)	C32	C33	1.406(11)

F18	C30	1.330(13)	C33	C34	1.370(13)
F19	C37	1.304(12)	C33	C37	1.495(12)
F20	C37	1.308(12)	C34	C35	1.386(12)
F21	C37	1.318(11)	C35	C36	1.390(11)
F22	C38	1.340(11)	C35	C38	1.505(12)
F23	C38	1.339(11)	C39	C40	1.393(12)
F24	C38	1.331(10)	C39	C42	1.456(11)
F25	C48	1.305(13)	C40	C41	1.377(11)
F26	C48	1.343(13)	C41	C50	1.482(11)
F27	C48	1.323(14)	C42	C43	1.389(12)
F28	C49	1.39(3)	C42	C47	1.402(11)
F29	C49	1.21(2)	C43	C44	1.402(11)
F30	C49	1.49(3)	C44	C45	1.378(13)
F31	C56	1.308(13)	C44	C48	1.491(13)
F32	C56	1.323(12)	C45	C46	1.391(13)
F33	C56	1.332(13)	C46	C47	1.393(12)
F34	C57	1.321(11)	C46	C49	1.490(12)
F35	C57	1.297(12)	C49	F29A	1.440(19)
F36	C57	1.310(12)	C49	F28A	1.26(3)
N1	N2	1.363(9)	C49	F30A	1.235(17)
N1	C1	1.346(10)	C50	C51	1.398(11)
N2	C3	1.347(10)	C50	C55	1.396(11)
N3	N4	1.368(9)	C51	C52	1.381(12)
N3	C20	1.335(11)	C52	C53	1.403(13)
N4	C22	1.346(11)	C52	C56	1.492(13)
N5	N6	1.373(9)	C53	C54	1.376(13)
N5	C39	1.356(10)	C54	C55	1.396(12)
N6	C41	1.352(10)	C54	C57	1.489(12)
C1	C2	1.390(11)	C58	C59	1.429(16)
C1	C4	1.478(10)	C58	C63	1.379(16)
C2	C3	1.375(11)	C58	C64	1.463(15)
C3	C12	1.483(11)	C59	C60	1.344(17)
C4	C5	1.385(11)	C60	C61	1.363(19)
C4	C9	1.394(11)	C61	C62	1.352(19)
C5	C6	1.396(12)	C62	C63	1.453(18)
C6	C7	1.396(13)	C1A	C1B	1.504(19)
C6	C10	1.488(13)	C1B	C1C	1.394(15)
C7	C8	1.374(12)	C1B	C1G	1.391(15)
C8	C9	1.395(11)	C1C	C1D	1.389(15)
C8	C11	1.496(12)	C1D	C1E	1.389(15)
C12	C13	1.386(12)	C1E	C1F	1.391(15)

C12	C17	1.390(12)	C1F	C1G	1.386(15)		
C13	C14	1.382(13)					

Table S8. Bond Angles for {[3,5-(3,5-$(CF_3)_2$Ph)$_2$Pz]Cu}$_3$•1.5(toluene).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N6	Cu1	N1	176.7(3)	F16	C30	F17	107.6(11)
N3	Cu2	N2	178.1(3)	F16	C30	F18	105.1(10)
N4	Cu3	N5	175.2(3)	F16	C30	C27	112.0(12)
N2	N1	Cu1	115.2(5)	F17	C30	F18	107.2(12)
C1	N1	Cu1	136.7(5)	F17	C30	C27	112.1(9)
C1	N1	N2	108.0(6)	F18	C30	C27	112.5(8)
N1	N2	Cu2	120.9(5)	C32	C31	C22	118.4(7)
C3	N2	Cu2	129.8(5)	C36	C31	C22	121.6(7)
C3	N2	N1	108.5(6)	C36	C31	C32	119.8(7)
N4	N3	Cu2	119.4(5)	C31	C32	C33	119.1(8)
C20	N3	Cu2	130.2(5)	C32	C33	C37	119.1(8)
C20	N3	N4	108.9(6)	C34	C33	C32	121.3(8)
N3	N4	Cu3	116.6(5)	C34	C33	C37	119.5(8)
C22	N4	Cu3	135.8(6)	C33	C34	C35	118.8(8)
C22	N4	N3	107.4(6)	C34	C35	C36	121.7(8)
N6	N5	Cu3	118.4(5)	C34	C35	C38	118.6(8)
C39	N5	Cu3	130.8(6)	C36	C35	C38	119.7(8)
C39	N5	N6	108.6(6)	C35	C36	C31	119.2(8)
N5	N6	Cu1	118.4(5)	F19	C37	F20	108.4(10)
C41	N6	Cu1	131.3(6)	F19	C37	F21	105.9(8)
C41	N6	N5	107.2(6)	F19	C37	C33	113.3(8)
N1	C1	C2	108.8(7)	F20	C37	F21	103.1(9)
N1	C1	C4	122.9(7)	F20	C37	C33	113.7(8)
C2	C1	C4	128.2(7)	F21	C37	C33	111.7(8)
C3	C2	C1	105.8(7)	F22	C38	C35	112.2(7)
N2	C3	C2	109.0(7)	F23	C38	F22	106.3(7)
N2	C3	C12	121.4(7)	F23	C38	C35	111.3(8)
C2	C3	C12	129.6(7)	F24	C38	F22	107.4(8)
C5	C4	C1	121.9(7)	F24	C38	F23	107.3(7)
C5	C4	C9	119.8(7)	F24	C38	C35	112.1(8)
C9	C4	C1	118.2(7)	N5	C39	C40	108.5(7)
C4	C5	C6	119.7(8)	N5	C39	C42	123.0(7)
C5	C6	C7	120.7(8)	C40	C39	C42	128.5(7)
C5	C6	C10	119.8(8)	C41	C40	C39	105.7(7)

C7	C6	C10	119.3(8)	N6	C41	C40	110.0(7)
C8	C7	C6	118.9(8)	N6	C41	C50	121.4(7)
C7	C8	C9	121.1(8)	C40	C41	C50	128.5(7)
C7	C8	C11	119.0(7)	C43	C42	C39	121.6(7)
C9	C8	C11	119.9(8)	C43	C42	C47	118.7(7)
C4	C9	C8	119.8(8)	C47	C42	C39	119.7(8)
F1	C10	F3	106.8(8)	C42	C43	C44	120.1(8)
F1	C10	C6	111.8(7)	C43	C44	C48	119.8(8)
F2	C10	F1	105.9(9)	C45	C44	C43	121.6(8)
F2	C10	F3	105.9(8)	C45	C44	C48	118.6(8)
F2	C10	C6	113.4(7)	C44	C45	C46	118.2(8)
F3	C10	C6	112.5(9)	C45	C46	C47	121.3(8)
F4	C11	F6	105.4(7)	C45	C46	C49	119.5(8)
F4	C11	C8	112.6(8)	C47	C46	C49	119.2(8)
F5	C11	F4	105.8(8)	C46	C47	C42	120.1(8)
F5	C11	F6	106.8(8)	F25	C48	F26	106.8(10)
F5	C11	C8	114.2(7)	F25	C48	F27	108.5(10)
F6	C11	C8	111.3(8)	F25	C48	C44	112.5(8)
C13	C12	C3	119.8(8)	F26	C48	C44	111.3(9)
C13	C12	C17	119.4(8)	F27	C48	F26	104.6(8)
C17	C12	C3	120.8(8)	F27	C48	C44	112.6(9)
C14	C13	C12	119.7(8)	F28	C49	F30	96(3)
C13	C14	C18	120.3(9)	F28	C49	C46	105(2)
C15	C14	C13	121.1(9)	F29	C49	F28	117(3)
C15	C14	C18	118.6(8)	F29	C49	F30	105.1(17)
C14	C15	C16	120.1(8)	F29	C49	C46	120.9(14)
C15	C16	C17	118.5(8)	F30	C49	C46	109.8(10)
C15	C16	C19	120.9(8)	F29A	C49	C46	108.1(11)
C17	C16	C19	120.6(8)	F28A	C49	C46	117.2(19)
C12	C17	C16	121.1(8)	F28A	C49	F29A	99(3)
F7	C18	F9	106.4(10)	F30A	C49	C46	113.6(10)
F7	C18	C14	113.1(8)	F30A	C49	F29A	102.6(12)
F8	C18	F7	107.7(9)	F30A	C49	F28A	113.6(19)
F8	C18	F9	106.1(9)	C51	C50	C41	118.7(7)
F8	C18	C14	112.4(10)	C55	C50	C41	122.0(7)
F9	C18	C14	110.7(9)	C55	C50	C51	119.2(7)
F10	C19	F11	98.4(10)	C52	C51	C50	120.7(8)
F10	C19	C16	116.1(9)	C51	C52	C53	120.4(8)
F11	C19	C16	110.6(9)	C51	C52	C56	120.3(8)
F12	C19	F10	110.6(12)	C53	C52	C56	119.3(8)
F12	C19	F11	104.0(11)	C54	C53	C52	118.6(8)

F12	C19	C16	115.2(12)	C53	C54	C55	121.7(8)
F11A	C19	C16	112.7(10)	C53	C54	C57	119.0(8)
F11A	C19	F12A	98.5(10)	C55	C54	C57	119.3(8)
F12A	C19	C16	112.3(9)	C50	C55	C54	119.4(8)
F10A	C19	C16	117.7(10)	F31	C56	F32	106.2(9)
F10A	C19	F11A	106.0(11)	F31	C56	F33	108.3(10)
F10A	C19	F12A	107.8(11)	F31	C56	C52	113.2(9)
N3	C20	C21	109.2(7)	F32	C56	F33	102.7(10)
N3	C20	C23	122.2(7)	F32	C56	C52	113.7(8)
C21	C20	C23	128.5(7)	F33	C56	C52	112.1(8)
C22	C21	C20	104.1(7)	F34	C57	C54	112.8(8)
N4	C22	C21	110.4(7)	F35	C57	F34	106.5(9)
N4	C22	C31	122.6(7)	F35	C57	F36	107.2(10)
C21	C22	C31	127.0(7)	F35	C57	C54	112.8(8)
C24	C23	C20	120.6(7)	F36	C57	F34	102.9(9)
C28	C23	C20	120.7(7)	F36	C57	C54	113.8(7)
C28	C23	C24	118.7(8)	C59	C58	C64	118.6(11)
C25	C24	C23	120.0(8)	C63	C58	C59	115.6(10)
C24	C25	C29	119.0(9)	C63	C58	C64	125.8(12)
C26	C25	C24	120.7(8)	C60	C59	C58	122.8(12)
C26	C25	C29	120.3(8)	C59	C60	C61	120.2(13)
C27	C26	C25	119.4(8)	C62	C61	C60	121.9(13)
C26	C27	C28	120.2(8)	C61	C62	C63	118.0(12)
C26	C27	C30	118.8(8)	C58	C63	C62	121.3(12)
C28	C27	C30	121.0(9)	C1C	C1B	C1A	120.6(14)
C23	C28	C27	121.1(8)	C1G	C1B	C1A	120.4(15)
F13	C29	F15	104.4(9)	C1G	C1B	C1C	119.0(13)
F13	C29	C25	113.6(8)	C1D	C1C	C1B	120.4(14)
F14	C29	F13	105.8(10)	C1C	C1D	C1E	120.3(14)
F14	C29	F15	107.4(10)	C1D	C1E	C1F	119.1(14)
F14	C29	C25	112.8(9)	C1G	C1F	C1E	120.6(14)
F15	C29	C25	112.2(9)	C1F	C1G	C1B	120.5(14)

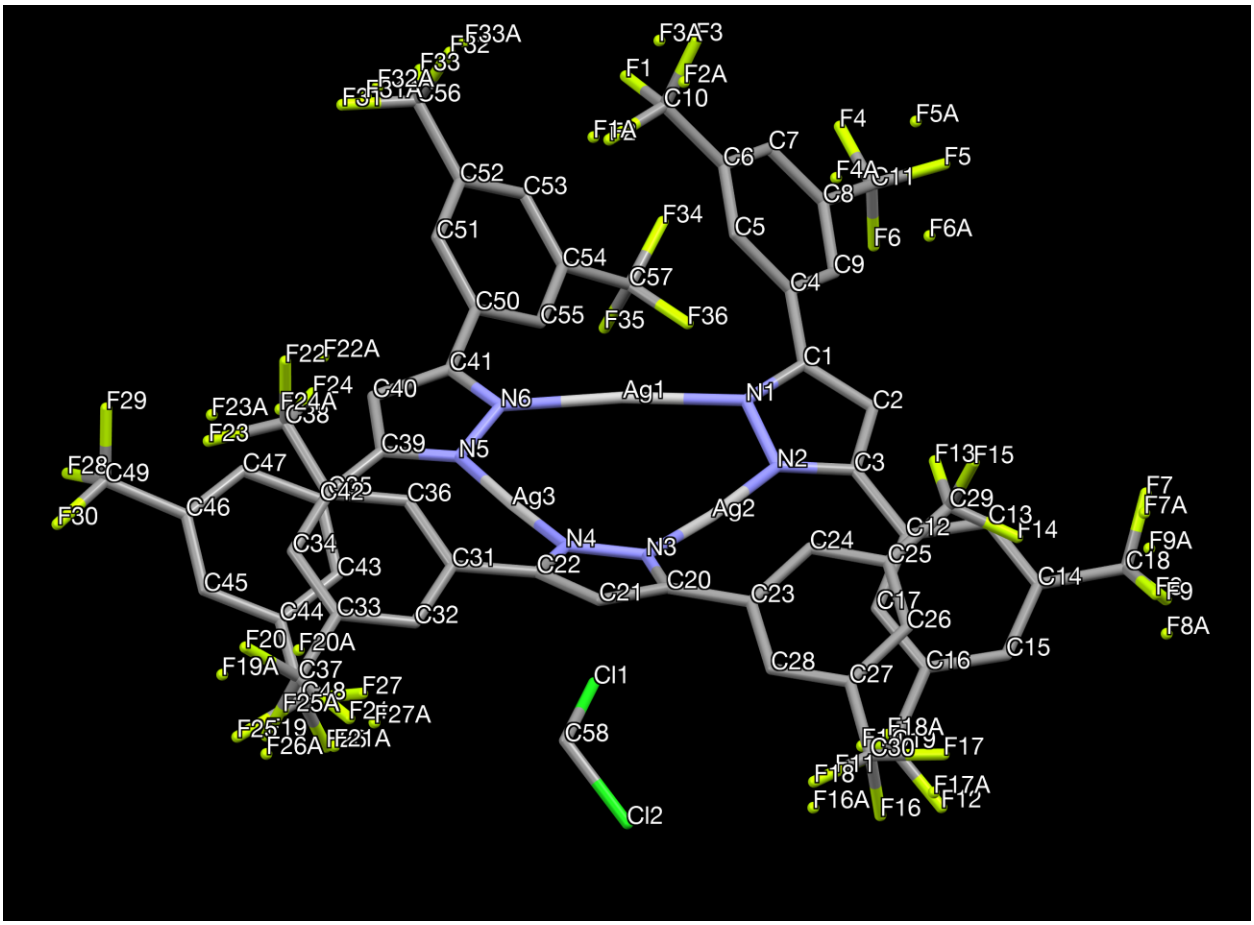


Figure S27. Molecular structure and atom labeling scheme of {[3,5-(3,5-$(CF_3)_2Ph)_2Pz]Ag\}_3 \bullet CH_2Cl_2$

Table S9. Crystal data and structure refinement for {[3,5-(3,5-$(CF_3)_2Ph)_2Pz]Ag\}_3 \bullet CH_2Cl_2$.

Identification code	Rad378
Empirical formula	$C_{58}H_{23}Ag_3Cl_2F_{36}N_6$
Formula weight	1882.33
Temperature/K	299.06
Crystal system	triclinic
Space group	P-1
a/Å	8.6941(5)
b/Å	15.8573(8)
c/Å	26.1433(13)
α/°	89.287(2)
β/°	85.728(2)
γ/°	87.428(2)
Volume/$Å^3$	3590.5(3)
Z	2

ρ_{calc}g/cm^3	1.741
μ/mm^{-1}	1.019
F(000)	1824.0
Crystal size/mm^3	0.19 × 0.15 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.768 to 52.998
Index ranges	$-10 \le h \le 10$, $-19 \le k \le 19$, $-32 \le l \le 32$
Reflections collected	37199
Independent reflections	14836 [R_{int} = 0.0332, R_{sigma} = 0.0407]
Data/restraints/parameters	14836/1905/1170
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0615, wR_2 = 0.1723
Final R indexes [all data]	R_1 = 0.0923, wR_2 = 0.1945
Largest diff. peak/hole / e Å^{-3}	1.06/-0.75

Table S10. Bond Lengths for {[3,5-(3,5-(CF$_3$)$_2$Ph)$_2$Pz]Ag}$_3$•CH$_2$Cl$_2$

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	N1	2.082(4)	N2	C3	1.343(7)
Ag1	N6	2.072(4)	N3	N4	1.355(6)
Ag2	Ag3	3.3676(6)	N3	C20	1.356(8)
Ag2	N2	2.076(5)	N4	C22	1.333(7)
Ag2	N3	2.087(5)	N5	N6	1.356(6)
Ag3	N4	2.088(5)	N5	C39	1.346(7)
Ag3	N5	2.076(5)	N6	C41	1.327(7)
F10	C19	1.298(5)	C1	C2	1.386(8)
F11	C19	1.309(5)	C1	C4	1.465(9)
F12	C19	1.310(5)	C2	C3	1.372(8)
F13	C29	1.309(5)	C3	C12	1.477(9)
F14	C29	1.311(5)	C4	C5	1.394(9)
F15	C29	1.299(5)	C4	C9	1.389(8)
F28	C49	1.313(5)	C5	C6	1.359(10)
F29	C49	1.307(5)	C6	C7	1.393(10)
F30	C49	1.304(5)	C6	C10	1.512(11)
F34	C57	1.306(5)	C7	C8	1.355(10)
F35	C57	1.306(5)	C8	C9	1.384(9)
F36	C57	1.304(5)	C8	C11	1.490(9)
F1	C10	1.318(6)	C12	C13	1.400(8)
F2	C10	1.311(6)	C12	C17	1.385(9)
F3	C10	1.304(6)	C13	C14	1.404(10)
F4	C11	1.317(6)	C14	C15	1.359(11)
F5	C11	1.302(6)	C14	C18	1.503(11)

F6	C11	1.308(6)	C15	C16	1.368(11)
F7	C18	1.308(6)	C16	C17	1.373(10)
F8	C18	1.317(6)	C16	C19	1.500(11)
F9	C18	1.295(6)	C20	C21	1.367(8)
F16	C30	1.325(6)	C20	C23	1.469(8)
F17	C30	1.303(6)	C21	C22	1.383(8)
F18	C30	1.301(6)	C22	C31	1.473(8)
F19	C37	1.313(6)	C23	C24	1.388(9)
F20	C37	1.307(5)	C23	C28	1.382(9)
F21	C37	1.316(6)	C24	C25	1.373(9)
F22	C38	1.338(6)	C25	C26	1.355(11)
F23	C38	1.352(6)	C25	C29	1.449(10)
F24	C38	1.350(6)	C26	C27	1.384(11)
F25	C48	1.304(6)	C27	C28	1.386(9)
F26	C48	1.302(6)	C27	C30	1.491(11)
F27	C48	1.312(6)	C31	C32	1.390(8)
F31	C56	1.305(6)	C31	C36	1.385(9)
F32	C56	1.313(6)	C32	C33	1.361(8)
F33	C56	1.310(6)	C33	C34	1.364(10)
F1A	C10	1.309(5)	C33	C37	1.520(10)
F2A	C10	1.317(6)	C34	C35	1.375(11)
F3A	C10	1.310(6)	C35	C36	1.385(9)
F4A	C11	1.302(6)	C35	C38	1.457(11)
F5A	C11	1.311(6)	C39	C40	1.370(8)
F6A	C11	1.315(6)	C39	C42	1.478(7)
F7A	C18	1.297(6)	C40	C41	1.389(7)
F8A	C18	1.300(6)	C41	C50	1.488(7)
F9A	C18	1.325(6)	C42	C43	1.384(9)
F16A	C30	1.310(6)	C42	C47	1.396(8)
F17A	C30	1.295(6)	C43	C44	1.391(8)
F18A	C30	1.325(6)	C44	C45	1.376(10)
F19A	C37	1.310(6)	C44	C48	1.490(10)
F20A	C37	1.317(6)	C45	C46	1.384(11)
F21A	C37	1.305(6)	C46	C47	1.376(8)
F22A	C38	1.378(7)	C46	C49	1.486(10)
F23A	C38	1.351(7)	C50	C51	1.372(8)
F24A	C38	1.325(7)	C50	C55	1.394(8)
F25A	C48	1.300(5)	C51	C52	1.382(9)
F26A	C48	1.313(6)	C52	C53	1.361(10)
F27A	C48	1.306(6)	C52	C56	1.526(10)
F31A	C56	1.309(6)	C53	C54	1.380(9)

F32A	C56	1.313(6)	C54	C55	1.377(8)
F33A	C56	1.305(6)	C54	C57	1.500(9)
N1	N2	1.369(7)	Cl1	C58	1.761(2)
N1	C1	1.347(7)	Cl2	C58	1.759(2)

Table S11. Bond Angles for {[3,5-(3,5-$(CF_3)_2$Ph)$_2$Pz]Ag}$_3$•CH_2Cl_2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N6	Ag1	N1	174.7(2)	F15	C29	F13	109.7(8)
N2	Ag2	Ag3	118.75(14)	F15	C29	F14	100.8(7)
N2	Ag2	N3	174.2(2)	F15	C29	C25	113.6(6)
N3	Ag2	Ag3	61.12(14)	F16	C30	C27	109.8(8)
N4	Ag3	Ag2	61.18(12)	F17	C30	F16	95.3(10)
N5	Ag3	Ag2	118.87(12)	F17	C30	C27	112.0(8)
N5	Ag3	N4	177.1(2)	F18	C30	F16	102.0(10)
N2	N1	Ag1	116.8(3)	F18	C30	F17	120.2(11)
C1	N1	Ag1	131.0(4)	F18	C30	C27	114.7(8)
C1	N1	N2	108.2(5)	F16A	C30	F18A	103.9(11)
N1	N2	Ag2	116.5(3)	F16A	C30	C27	116.0(9)
C3	N2	Ag2	132.7(4)	F17A	C30	F16A	107.9(13)
C3	N2	N1	107.9(5)	F17A	C30	F18A	103.0(12)
N4	N3	Ag2	118.8(4)	F17A	C30	C27	116.3(10)
N4	N3	C20	108.4(4)	F18A	C30	C27	108.2(8)
C20	N3	Ag2	132.7(4)	C32	C31	C22	120.8(5)
N3	N4	Ag3	118.6(3)	C36	C31	C22	121.5(6)
C22	N4	Ag3	132.9(4)	C36	C31	C32	117.6(5)
C22	N4	N3	108.3(5)	C33	C32	C31	120.6(6)
N6	N5	Ag3	119.1(3)	C32	C33	C34	121.8(7)
C39	N5	Ag3	130.9(4)	C32	C33	C37	119.3(6)
C39	N5	N6	108.0(4)	C34	C33	C37	118.9(6)
N5	N6	Ag1	119.7(3)	C33	C34	C35	118.9(6)
C41	N6	Ag1	132.4(4)	C34	C35	C36	119.9(7)
C41	N6	N5	107.9(4)	C34	C35	C38	121.6(6)
N1	C1	C2	108.5(5)	C36	C35	C38	118.4(7)
N1	C1	C4	122.3(5)	C31	C36	C35	121.1(7)
C2	C1	C4	129.1(5)	F19	C37	F21	99.3(9)
C3	C2	C1	106.0(5)	F19	C37	C33	113.4(7)
N2	C3	C2	109.3(5)	F20	C37	F19	108.9(10)
N2	C3	C12	122.0(5)	F20	C37	F21	107.7(10)
C2	C3	C12	128.7(5)	F20	C37	C33	112.4(8)

C5	C4	C1	121.3(5)	F21	C37	C33	114.2(7)
C9	C4	C1	120.6(6)	F19A	C37	F20A	99.4(13)
C9	C4	C5	118.1(6)	F19A	C37	C33	106.8(9)
C6	C5	C4	121.2(6)	F20A	C37	C33	107.5(10)
C5	C6	C7	119.6(7)	F21A	C37	F19A	119.3(16)
C5	C6	C10	118.6(6)	F21A	C37	F20A	104.6(17)
C7	C6	C10	121.7(7)	F21A	C37	C33	117.1(12)
C8	C7	C6	120.3(7)	F22	C38	F23	107.0(6)
C7	C8	C9	120.1(6)	F22	C38	F24	106.0(7)
C7	C8	C11	120.8(7)	F22	C38	C35	116.7(8)
C9	C8	C11	119.0(7)	F23	C38	C35	109.5(9)
C8	C9	C4	120.6(6)	F24	C38	F23	104.6(6)
F1	C10	C6	106.7(12)	F24	C38	C35	112.2(8)
F2	C10	F1	105(2)	F22A	C38	C35	108.8(8)
F2	C10	C6	112.5(16)	F23A	C38	F22A	101.5(6)
F3	C10	F1	98.0(16)	F23A	C38	C35	114.8(8)
F3	C10	F2	118(2)	F24A	C38	F22A	105.7(7)
F3	C10	C6	114.0(12)	F24A	C38	F23A	108.0(7)
F1A	C10	F2A	105.9(9)	F24A	C38	C35	116.6(8)
F1A	C10	F3A	109.0(10)	N5	C39	C40	109.6(4)
F1A	C10	C6	111.5(7)	N5	C39	C42	121.0(5)
F2A	C10	C6	111.6(7)	C40	C39	C42	129.4(5)
F3A	C10	F2A	105.1(10)	C39	C40	C41	104.5(5)
F3A	C10	C6	113.2(8)	N6	C41	C40	110.0(5)
F4	C11	C8	110.4(7)	N6	C41	C50	122.2(5)
F5	C11	F4	107.1(9)	C40	C41	C50	127.9(5)
F5	C11	F6	108.4(10)	C43	C42	C39	121.0(5)
F5	C11	C8	113.3(7)	C43	C42	C47	118.6(5)
F6	C11	F4	105.4(10)	C47	C42	C39	120.3(5)
F6	C11	C8	111.8(7)	C42	C43	C44	120.8(6)
F4A	C11	F5A	108.8(13)	C43	C44	C48	119.1(6)
F4A	C11	F6A	105.5(13)	C45	C44	C43	119.9(7)
F4A	C11	C8	118.9(9)	C45	C44	C48	121.0(6)
F5A	C11	F6A	97.7(12)	C44	C45	C46	119.7(6)
F5A	C11	C8	110.1(9)	C45	C46	C49	121.5(6)
F6A	C11	C8	113.7(8)	C47	C46	C45	120.6(6)
C13	C12	C3	119.3(6)	C47	C46	C49	117.8(7)
C17	C12	C3	122.1(5)	C46	C47	C42	120.3(6)
C17	C12	C13	118.5(6)	F25	C48	F27	120.7(12)
C12	C13	C14	119.3(7)	F25	C48	C44	109.3(9)
C13	C14	C18	117.2(7)	F26	C48	F25	98.8(12)

C15	C14	C13	120.2(7)	F26	C48	F27	104.6(11)
C15	C14	C18	122.6(7)	F26	C48	C44	111.4(8)
C14	C15	C16	120.7(7)	F27	C48	C44	111.1(8)
C15	C16	C17	120.1(7)	F25A	C48	F26A	108.0(9)
C15	C16	C19	120.1(7)	F25A	C48	F27A	110.6(10)
C17	C16	C19	119.8(7)	F25A	C48	C44	115.4(7)
C16	C17	C12	121.1(6)	F26A	C48	C44	108.3(8)
F7	C18	F8	100.3(12)	F27A	C48	F26A	96.6(10)
F7	C18	C14	115.2(8)	F27A	C48	C44	115.9(7)
F8	C18	C14	109.3(9)	F28	C49	C46	113.7(6)
F9	C18	F7	107.2(11)	F29	C49	F28	103.6(6)
F9	C18	F8	108.8(12)	F29	C49	C46	112.6(6)
F9	C18	C14	115.0(9)	F30	C49	F28	103.3(7)
F7A	C18	F8A	116.1(12)	F30	C49	F29	109.3(6)
F7A	C18	F9A	110.5(13)	F30	C49	C46	113.4(6)
F7A	C18	C14	112.0(9)	C51	C50	C41	119.8(5)
F8A	C18	F9A	97.1(12)	C51	C50	C55	118.9(5)
F8A	C18	C14	111.6(9)	C55	C50	C41	121.3(5)
F9A	C18	C14	108.5(10)	C50	C51	C52	120.7(6)
F10	C19	F11	106.1(8)	C51	C52	C56	118.0(6)
F10	C19	F12	106.8(8)	C53	C52	C51	120.3(6)
F10	C19	C16	111.4(7)	C53	C52	C56	121.5(6)
F11	C19	F12	101.6(8)	C52	C53	C54	119.8(6)
F11	C19	C16	114.1(6)	C53	C54	C57	121.5(5)
F12	C19	C16	116.0(7)	C55	C54	C53	120.3(6)
N3	C20	C21	108.1(5)	C55	C54	C57	118.2(6)
N3	C20	C23	121.3(5)	C54	C55	C50	120.0(6)
C21	C20	C23	130.6(6)	F31	C56	F32	105.3(10)
C20	C21	C22	106.4(5)	F31	C56	F33	107.4(12)
N4	C22	C21	108.8(5)	F31	C56	C52	114.7(7)
N4	C22	C31	121.6(5)	F32	C56	C52	110.1(8)
C21	C22	C31	129.5(5)	F33	C56	F32	110.2(12)
C24	C23	C20	121.6(6)	F33	C56	C52	109.1(9)
C28	C23	C20	119.5(5)	F31A	C56	F32A	107.0(12)
C28	C23	C24	118.9(6)	F31A	C56	C52	110.9(8)
C25	C24	C23	120.6(7)	F32A	C56	C52	114.0(9)
C24	C25	C29	121.0(7)	F33A	C56	F31A	102.5(11)
C26	C25	C24	120.3(7)	F33A	C56	F32A	109.9(12)
C26	C25	C29	118.7(6)	F33A	C56	C52	111.9(8)
C25	C26	C27	120.5(6)	F34	C57	F35	106.4(5)
C26	C27	C28	119.5(7)	F34	C57	C54	113.2(6)

C26	C27	C30	121.4(6)	F35	C57	C54	111.2(5)
C28	C27	C30	119.1(6)	F36	C57	F34	104.9(6)
C23	C28	C27	120.2(6)	F36	C57	F35	107.2(6)
F13	C29	F14	99.2(7)	F36	C57	C54	113.3(5)
F13	C29	C25	115.5(6)	Cl2	C58	Cl1	111.8(3)
F14	C29	C25	116.2(7)				

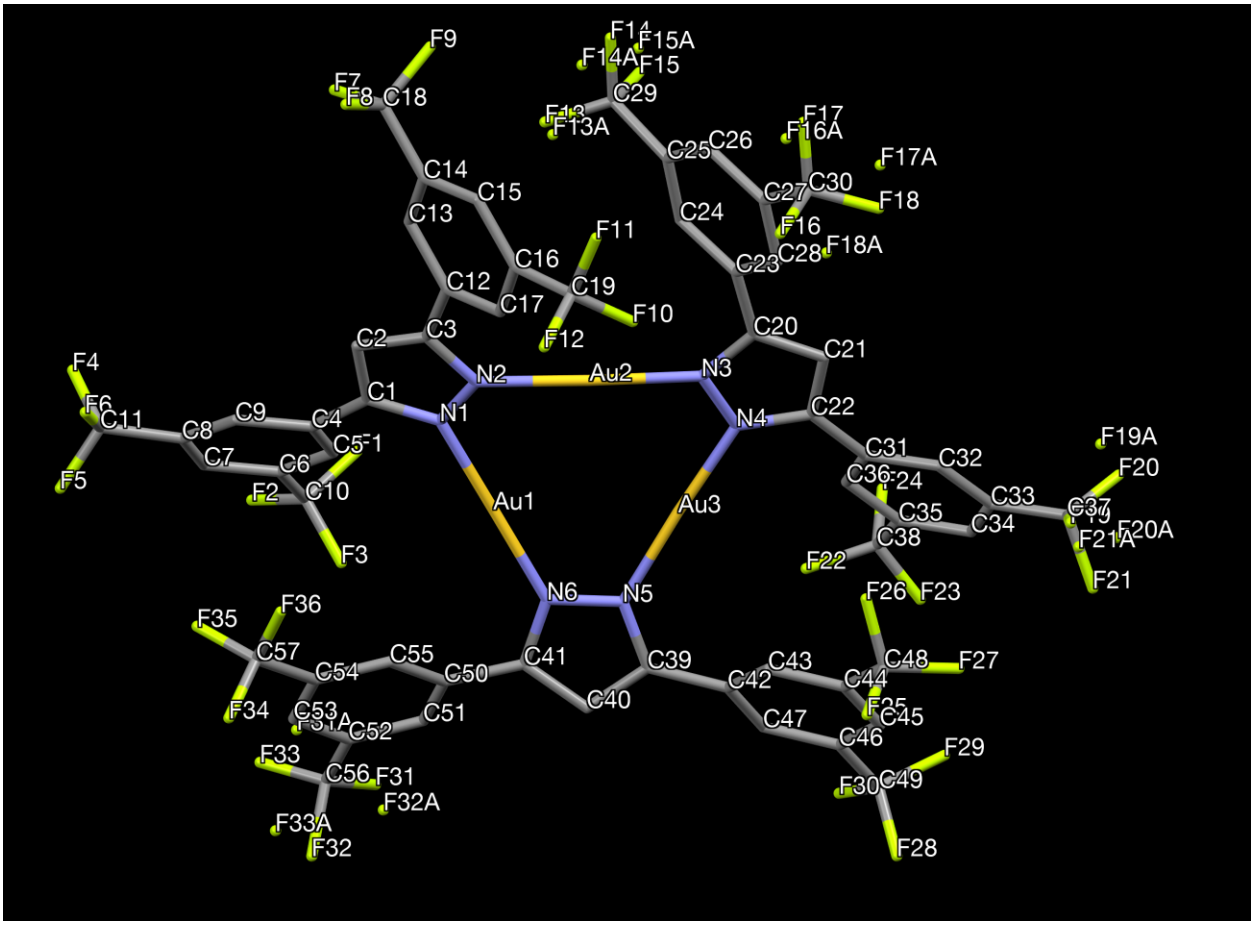


Figure S28. Molecular structure and atom labeling scheme of $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Au\}_3$

Table S12. Crystal data and structure refinement for $\{[3,5\text{-}(3,5\text{-}(CF_3)_2Ph)_2Pz]Au\}_3$

Identification code	Rad533
Empirical formula	$C_{57}H_{21}Au_3F_{36}N_6$
Formula weight	2064.70
Temperature/K	100.0

Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.3667(5)
b/Å	31.7232(19)
c/Å	25.7197(15)
α/°	90
β/°	91.507(2)
γ/°	90
Volume/Å^3	6824.1(7)
Z	4
ρ_{calc}g/cm^3	2.010
μ/mm^{-1}	6.573
F(000)	3864.0
Crystal size/mm^3	0.28 × 0.15 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.694 to 60.054
Index ranges	$-11 \le h \le 11$, $-44 \le k \le 44$, $-36 \le l \le 36$
Reflections collected	89629
Independent reflections	19862 [R_{int} = 0.0345, R_{sigma} = 0.0273]
Data/restraints/parameters	19862/366/1031
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0317, wR_2 = 0.0664
Final R indexes [all data]	R_1 = 0.0412, wR_2 = 0.0702
Largest diff. peak/hole / e Å^{-3}	1.84/-1.66

Table S13. Bond Lengths for {[3,5-(3,5-(CF$_3$)$_2$Ph)$_2$Pz]Au}.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au1	Au2	3.3693(3)	C7	C8	1.395(6)
Au1	Au3	3.2971(3)	C8	C9	1.392(5)
Au1	N1	2.010(3)	C8	C11	1.494(5)
Au1	N6	2.005(3)	C12	C13	1.393(5)
Au2	Au3	3.2876(2)	C12	C17	1.395(5)
Au2	N2	2.013(3)	C13	C14	1.385(6)
Au2	N3	2.005(3)	C14	C15	1.392(6)
Au3	N4	1.996(3)	C14	C18	1.502(6)
Au3	N5	1.996(3)	C15	C16	1.381(6)
F1	C10	1.365(6)	C16	C17	1.395(6)
F2	C10	1.317(6)	C16	C19	1.499(6)
F3	C10	1.307(6)	C20	C21	1.387(5)
F4	C11	1.342(5)	C20	C23	1.463(6)
F5	C11	1.339(5)	C21	C22	1.388(6)

F6	C11	1.334(5)	C22	C31	1.466(6)
F7	C18	1.319(6)	C23	C24	1.395(6)
F8	C18	1.303(6)	C23	C28	1.399(6)
F9	C18	1.330(6)	C24	C25	1.391(7)
F10	C19	1.329(6)	C25	C26	1.389(8)
F11	C19	1.349(6)	C25	C29	1.471(6)
F12	C19	1.305(7)	C26	C27	1.394(7)
F13	C29	1.314(11)	C27	C28	1.391(6)
F14	C29	1.315(9)	C27	C30	1.452(6)
F15	C29	1.468(10)	C29	F13A	1.345(10)
F16	C30	1.396(9)	C29	F15A	1.275(9)
F17	C30	1.321(9)	C29	F14A	1.432(10)
F18	C30	1.300(9)	C30	F16A	1.312(11)
F19	C37	1.279(9)	C30	F18A	1.310(9)
F20	C37	1.280(7)	C30	F17A	1.397(9)
F21	C37	1.433(9)	C31	C32	1.393(5)
F22	C38	1.333(7)	C31	C36	1.396(6)
F23	C38	1.328(6)	C32	C33	1.398(7)
F24	C38	1.336(6)	C33	C34	1.389(8)
F25	C48	1.339(6)	C33	C37	1.464(6)
F26	C48	1.331(5)	C34	C35	1.389(7)
F27	C48	1.335(6)	C35	C36	1.392(6)
F28	C49	1.320(8)	C35	C38	1.489(8)
F29	C49	1.332(7)	C37	F19A	1.419(11)
F30	C49	1.293(6)	C37	F21A	1.259(11)
F31	C56	1.304(8)	C37	F20A	1.286(9)
F32	C56	1.397(7)	C39	C40	1.387(6)
F33	C56	1.312(7)	C39	C42	1.473(5)
F34	C57	1.318(5)	C40	C41	1.393(5)
F35	C57	1.329(5)	C41	C50	1.469(5)
F36	C57	1.326(5)	C42	C43	1.388(6)
N1	N2	1.363(4)	C42	C47	1.392(6)
N1	C1	1.348(4)	C43	C44	1.389(6)
N2	C3	1.340(5)	C44	C45	1.374(6)
N3	N4	1.365(5)	C44	C48	1.501(6)
N3	C20	1.346(5)	C45	C46	1.383(6)
N4	C22	1.351(5)	C46	C47	1.393(6)
N5	N6	1.364(4)	C46	C49	1.509(6)
N5	C39	1.350(5)	C50	C51	1.392(6)
N6	C41	1.351(5)	C50	C55	1.395(5)
C1	C2	1.388(5)	C51	C52	1.389(6)

C1	C4	1.474(5)	C52	C53	1.390(6)
C2	C3	1.384(5)	C52	C56	1.466(6)
C3	C12	1.477(5)	C53	C54	1.387(6)
C4	C5	1.384(5)	C54	C55	1.385(5)
C4	C9	1.397(5)	C54	C57	1.499(5)
C5	C6	1.391(6)	C56	F33A	1.270(10)
C6	C7	1.382(5)	C56	F32A	1.337(11)
C6	C10	1.509(6)	C56	F31A	1.379(11)

Table S14. Bond Angles for {[3,5-(3,5-$(CF_3)_2$Ph)$_2$Pz]Au}.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Au3	Au1	Au2	59.085(4)	F14	C29	F15	100.6(7)
N1	Au1	Au2	59.53(9)	F14	C29	C25	117.2(7)
N1	Au1	Au3	118.10(9)	F15	C29	C25	107.2(6)
N6	Au1	Au2	119.51(9)	F13A	C29	C25	109.5(9)
N6	Au1	Au3	61.41(9)	F13A	C29	F14A	102.2(9)
N6	Au1	N1	177.13(14)	F15A	C29	C25	116.8(7)
Au3	Au2	Au1	59.362(6)	F15A	C29	F13A	112.3(12)
N2	Au2	Au1	59.14(9)	F15A	C29	F14A	106.1(7)
N2	Au2	Au3	118.43(9)	F14A	C29	C25	108.8(7)
N3	Au2	Au1	120.10(10)	F16	C30	C27	110.6(5)
N3	Au2	Au3	61.10(10)	F17	C30	F16	100.2(8)
N3	Au2	N2	176.66(14)	F17	C30	C27	114.6(8)
Au2	Au3	Au1	61.552(5)	F18	C30	F16	104.4(8)
N4	Au3	Au1	121.50(9)	F18	C30	F17	108.8(9)
N4	Au3	Au2	61.14(9)	F18	C30	C27	116.5(6)
N4	Au3	N5	177.28(14)	F16A	C30	C27	117.3(11)
N5	Au3	Au1	60.69(9)	F16A	C30	F17A	102.6(10)
N5	Au3	Au2	120.61(9)	F18A	C30	C27	113.6(6)
N2	N1	Au1	117.7(2)	F18A	C30	F16A	112.2(11)
C1	N1	Au1	132.3(3)	F18A	C30	F17A	99.2(9)
C1	N1	N2	108.2(3)	F17A	C30	C27	109.7(7)
N1	N2	Au2	118.5(2)	C32	C31	C22	119.7(4)
C3	N2	Au2	131.3(3)	C32	C31	C36	118.9(4)
C3	N2	N1	108.1(3)	C36	C31	C22	121.4(4)
N4	N3	Au2	118.1(2)	C31	C32	C33	120.1(5)
C20	N3	Au2	133.4(3)	C32	C33	C37	119.9(5)
C20	N3	N4	108.5(3)	C34	C33	C32	120.8(4)
N3	N4	Au3	118.6(2)	C34	C33	C37	119.3(5)

C22	N4	Au3	131.1(3)	C35	C34	C33	119.0(4)
C22	N4	N3	108.3(3)	C34	C35	C36	120.5(5)
N6	N5	Au3	120.0(2)	C34	C35	C38	120.6(4)
C39	N5	Au3	131.2(3)	C36	C35	C38	118.8(4)
C39	N5	N6	108.6(3)	C35	C36	C31	120.7(4)
N5	N6	Au1	117.6(2)	F19	C37	F20	116.6(9)
C41	N6	Au1	134.0(3)	F19	C37	F21	99.8(8)
C41	N6	N5	108.4(3)	F19	C37	C33	113.0(6)
N1	C1	C2	109.0(3)	F20	C37	F21	99.5(7)
N1	C1	C4	123.5(3)	F20	C37	C33	116.2(5)
C2	C1	C4	127.4(3)	F21	C37	C33	109.0(6)
C3	C2	C1	105.1(3)	F19A	C37	C33	108.6(6)
N2	C3	C2	109.6(3)	F21A	C37	C33	120.6(9)
N2	C3	C12	122.1(3)	F21A	C37	F19A	101.0(11)
C2	C3	C12	128.3(3)	F21A	C37	F20A	109.1(10)
C5	C4	C1	121.6(3)	F20A	C37	C33	117.7(7)
C5	C4	C9	119.1(3)	F20A	C37	F19A	95.4(10)
C9	C4	C1	119.1(3)	F22	C38	F24	106.2(5)
C4	C5	C6	120.7(4)	F22	C38	C35	112.3(4)
C5	C6	C10	118.9(4)	F23	C38	F22	107.8(5)
C7	C6	C5	120.7(4)	F23	C38	F24	105.8(4)
C7	C6	C10	120.4(4)	F23	C38	C35	112.9(5)
C6	C7	C8	118.9(4)	F24	C38	C35	111.4(5)
C7	C8	C11	118.3(3)	N5	C39	C40	108.6(3)
C9	C8	C7	120.6(3)	N5	C39	C42	120.5(4)
C9	C8	C11	121.0(4)	C40	C39	C42	130.9(4)
C8	C9	C4	120.0(4)	C39	C40	C41	106.0(4)
F1	C10	C6	111.3(4)	N6	C41	C40	108.5(3)
F2	C10	F1	103.1(4)	N6	C41	C50	122.4(3)
F2	C10	C6	113.6(4)	C40	C41	C50	129.1(4)
F3	C10	F1	103.6(4)	C43	C42	C39	119.9(4)
F3	C10	F2	112.8(4)	C43	C42	C47	119.0(4)
F3	C10	C6	111.7(4)	C47	C42	C39	121.1(4)
F4	C11	C8	111.4(3)	C42	C43	C44	120.4(4)
F5	C11	F4	106.7(3)	C43	C44	C48	117.7(4)
F5	C11	C8	111.9(3)	C45	C44	C43	121.0(4)
F6	C11	F4	106.4(3)	C45	C44	C48	121.2(4)
F6	C11	F5	106.8(3)	C44	C45	C46	118.5(4)
F6	C11	C8	113.2(3)	C45	C46	C47	121.6(4)
C13	C12	C3	119.5(3)	C45	C46	C49	118.0(4)
C13	C12	C17	119.0(4)	C47	C46	C49	120.4(4)

C17	C12	C3	121.4(3)	C42	C47	C46	119.5(4)
C14	C13	C12	120.7(4)	F25	C48	C44	111.3(4)
C13	C14	C15	120.5(4)	F26	C48	F25	106.1(4)
C13	C14	C18	120.6(4)	F26	C48	F27	107.2(4)
C15	C14	C18	118.9(4)	F26	C48	C44	112.3(4)
C16	C15	C14	118.8(4)	F27	C48	F25	106.6(4)
C15	C16	C17	121.3(4)	F27	C48	C44	112.7(4)
C15	C16	C19	120.4(4)	F28	C49	F29	104.2(4)
C17	C16	C19	118.2(4)	F28	C49	C46	111.5(5)
C16	C17	C12	119.7(4)	F29	C49	C46	110.8(5)
F7	C18	F9	105.3(4)	F30	C49	F28	107.3(5)
F7	C18	C14	112.8(4)	F30	C49	F29	109.7(6)
F8	C18	F7	106.9(5)	F30	C49	C46	113.0(4)
F8	C18	F9	107.9(5)	C51	C50	C41	119.9(3)
F8	C18	C14	112.1(4)	C51	C50	C55	118.9(4)
F9	C18	C14	111.4(4)	C55	C50	C41	121.1(4)
F10	C19	F11	105.6(5)	C52	C51	C50	120.5(4)
F10	C19	C16	112.0(4)	C51	C52	C53	120.7(4)
F11	C19	C16	111.8(5)	C51	C52	C56	120.9(4)
F12	C19	F10	107.0(5)	C53	C52	C56	118.4(4)
F12	C19	F11	108.1(5)	C54	C53	C52	118.6(4)
F12	C19	C16	111.9(5)	C53	C54	C57	118.4(4)
N3	C20	C21	108.6(4)	C55	C54	C53	121.3(4)
N3	C20	C23	123.3(3)	C55	C54	C57	120.3(4)
C21	C20	C23	128.0(4)	C54	C55	C50	120.1(4)
C20	C21	C22	106.1(3)	F31	C56	F32	103.5(7)
N4	C22	C21	108.5(4)	F31	C56	F33	110.3(7)
N4	C22	C31	122.5(4)	F31	C56	C52	115.4(7)
C21	C22	C31	128.9(4)	F32	C56	C52	110.6(5)
C24	C23	C20	121.3(4)	F33	C56	F32	99.8(5)
C24	C23	C28	119.0(4)	F33	C56	C52	115.4(5)
C28	C23	C20	119.7(4)	F33A	C56	C52	116.2(8)
C25	C24	C23	120.2(4)	F33A	C56	F32A	109.8(12)
C24	C25	C29	118.5(5)	F33A	C56	F31A	106.7(11)
C26	C25	C24	120.8(4)	F32A	C56	C52	113.3(11)
C26	C25	C29	120.6(5)	F32A	C56	F31A	102.1(10)
C25	C26	C27	119.4(5)	F31A	C56	C52	107.6(7)
C26	C27	C30	120.2(5)	F34	C57	F35	104.9(4)
C28	C27	C26	120.0(5)	F34	C57	F36	106.7(4)
C28	C27	C30	119.7(5)	F34	C57	C54	113.2(4)
C27	C28	C23	120.7(4)	F35	C57	C54	112.9(4)

F13	C29	F14	109.8(9)	F36	C57	F35	105.4(4)
F13	C29	F15	100.1(12)	F36	C57	C54	113.0(3)
F13	C29	C25	118.7(11)				