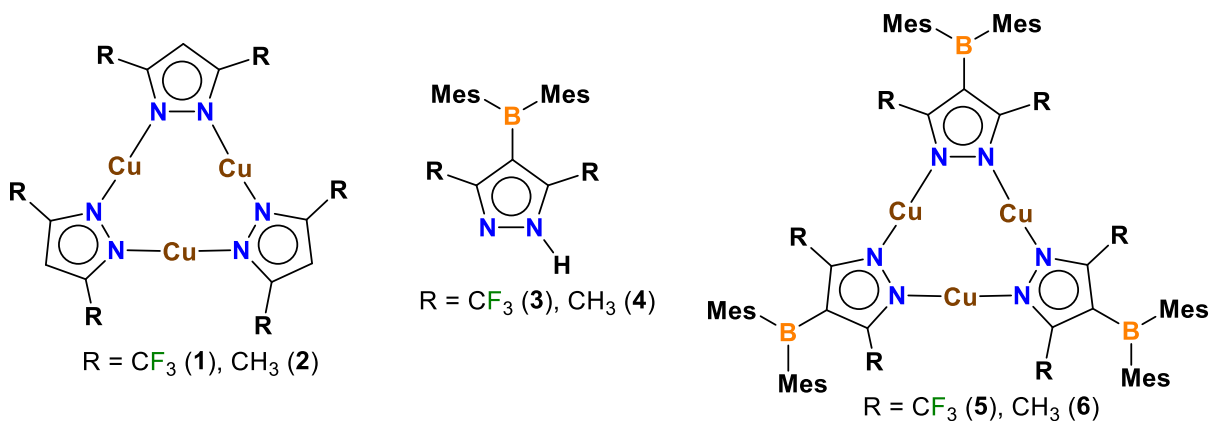


Filling the gap with a bulky diaryl boron: fluorinated and non-fluorinated copper pyrazolates fitted with a dimesityl boron moiety on the backbone

Mukundam Vanga,[†] Benjamin T. Diroll,^{‡*} Álvaro R. Muñoz-Castro,^{±*} H. V. Rasika Dias^{†*}

[†]Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas 76019, USA; [‡]Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA; [±]Facultad de Ingeniería, Arquitectura y Diseño, Universidad San Sebastián, Bellavista 7, Santiago, 8420524, Chile

Supporting information



Molecules of focus

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1. Spectral data

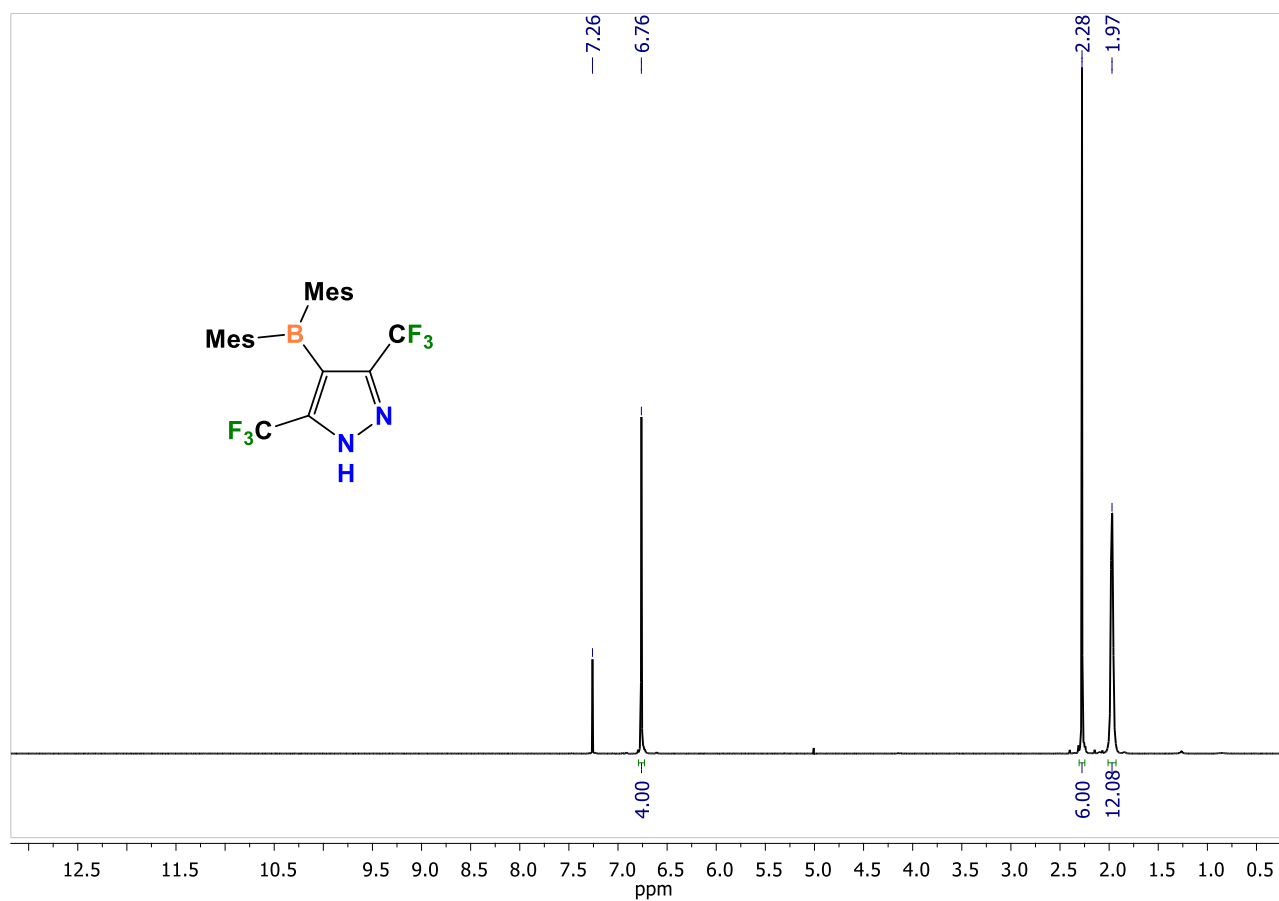


Figure S1. ¹H NMR spectrum of 4-BMes₂-3,5-(CF₃)₂PzH (**3**) in CDCl₃

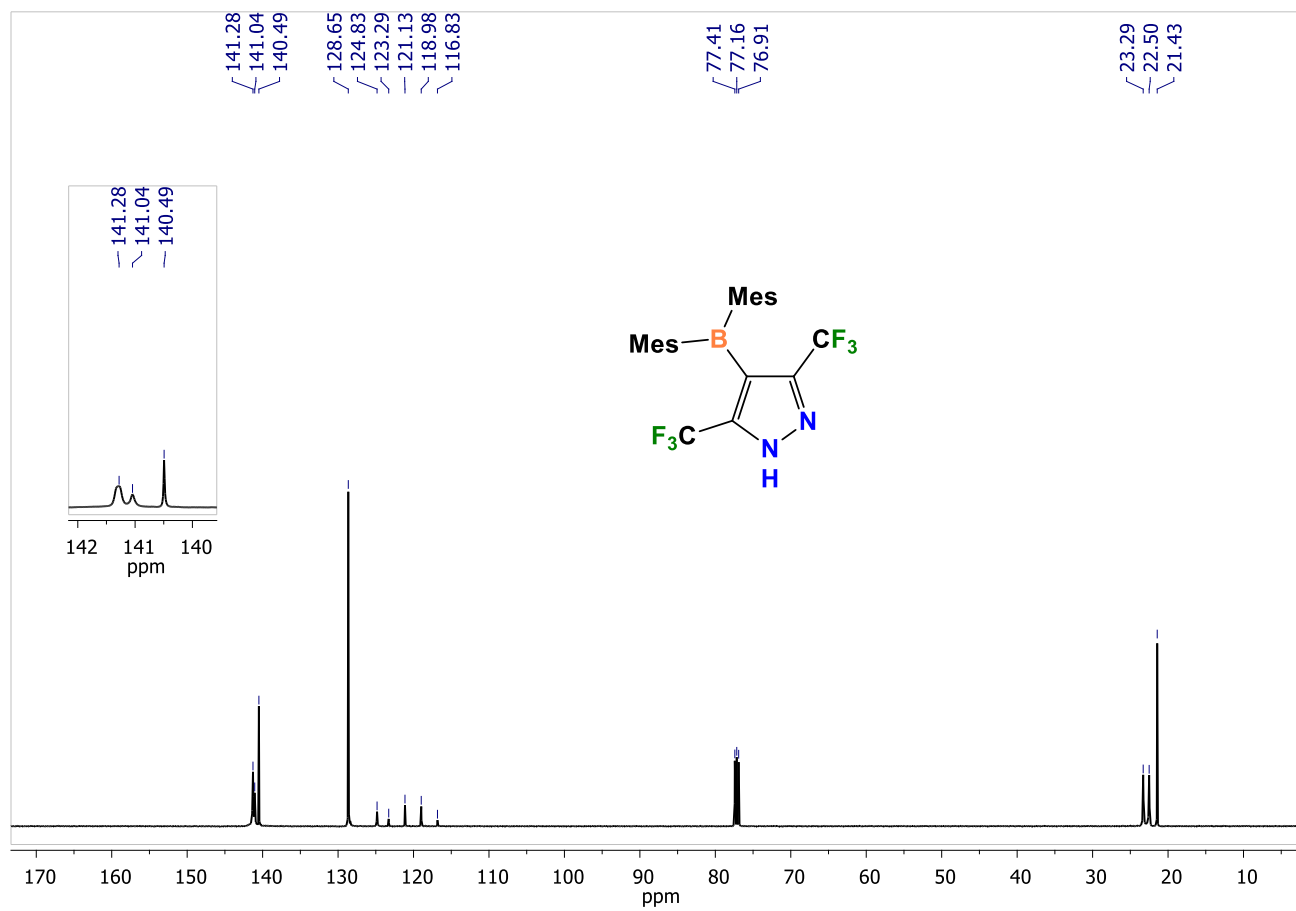


Figure S2. ^{13}C NMR spectrum of 4-BMes₂-3,5-(CF₃)₂PzH (**3**) in CDCl₃

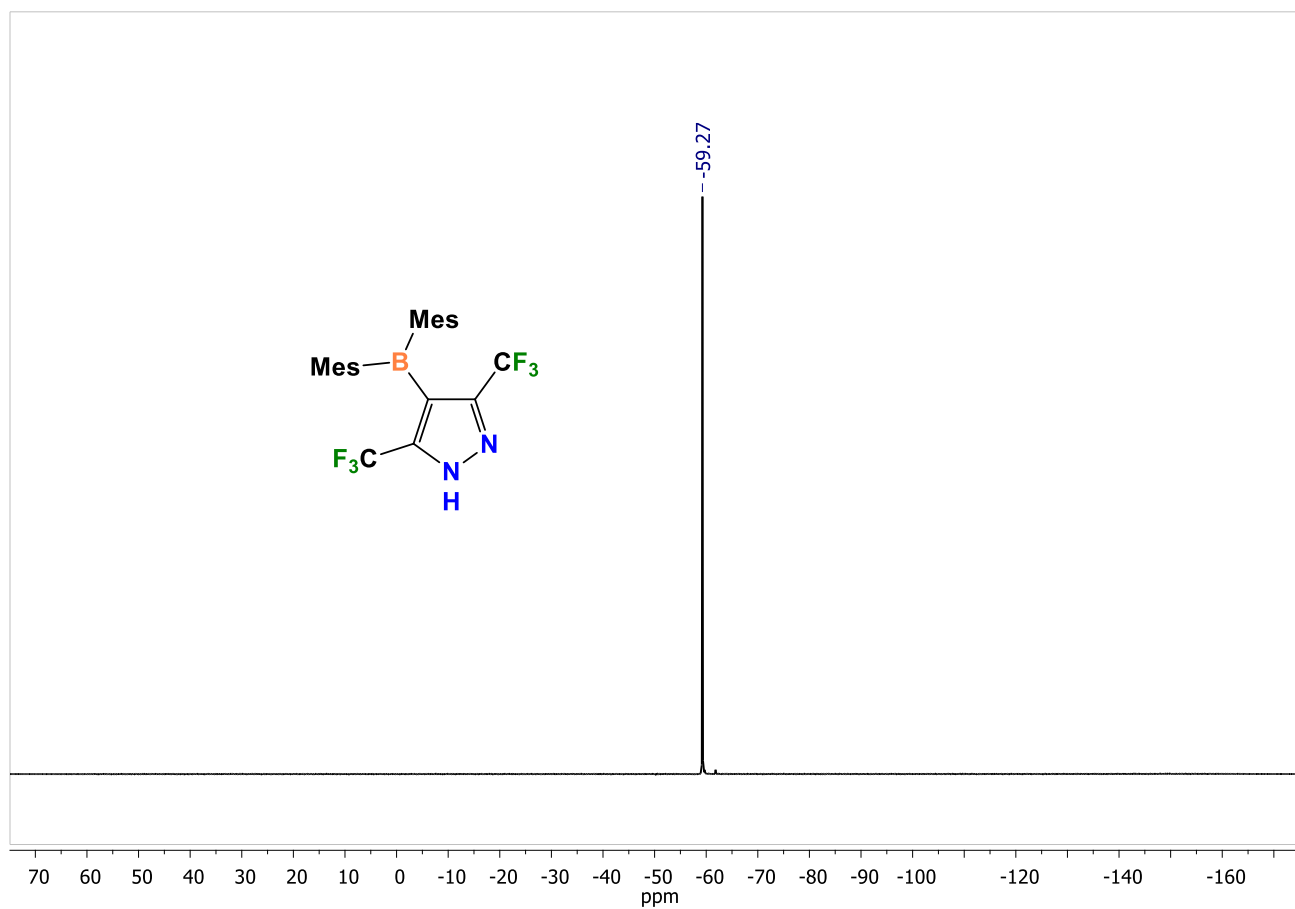


Figure S3. ^{19}F NMR spectrum of 4-BMes₂-3,5-(CF₃)₂PzH (**3**) in CDCl₃

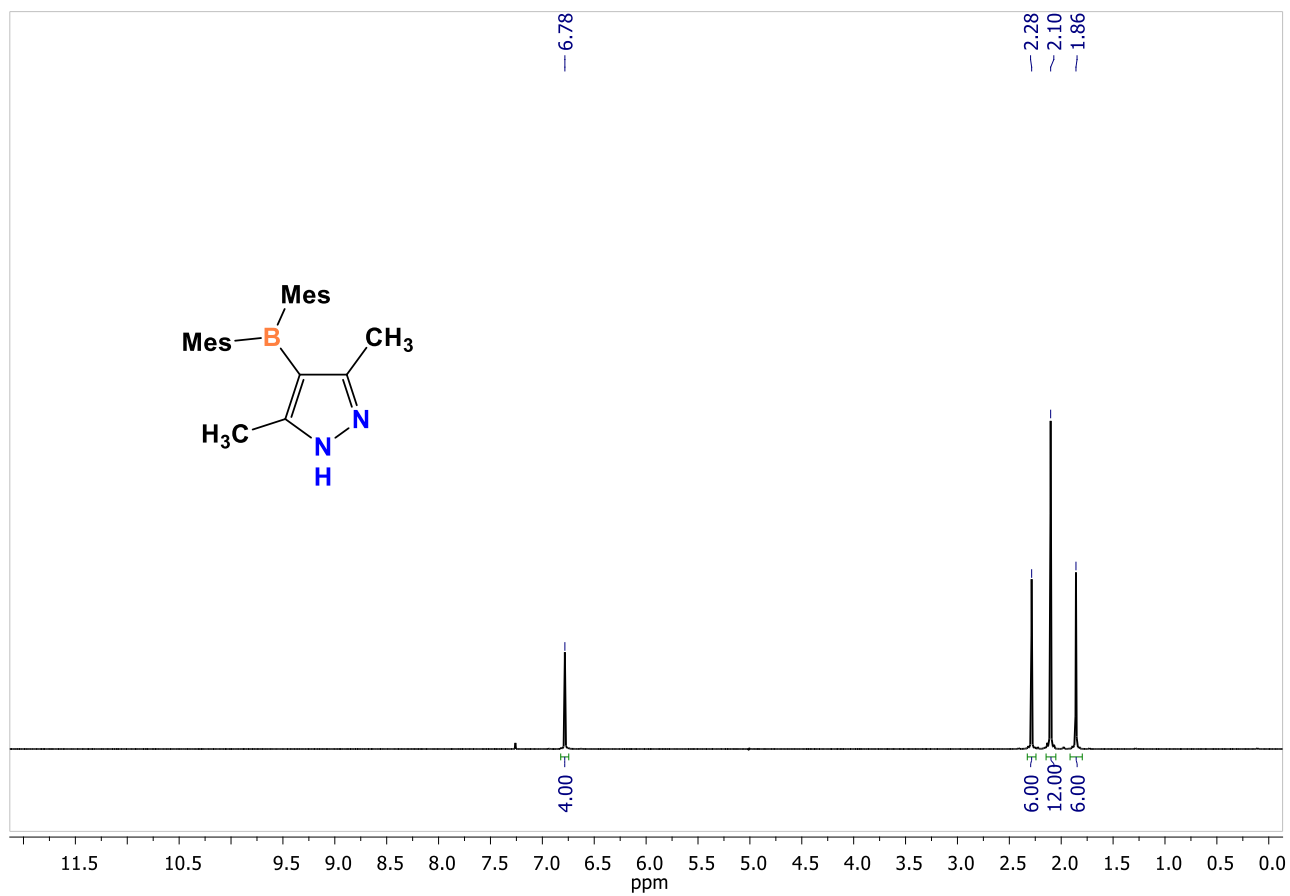


Figure S4. ¹H NMR spectrum of 4-BMes₂-3,5-(CH₃)₂PzH (**4**) in CDCl₃

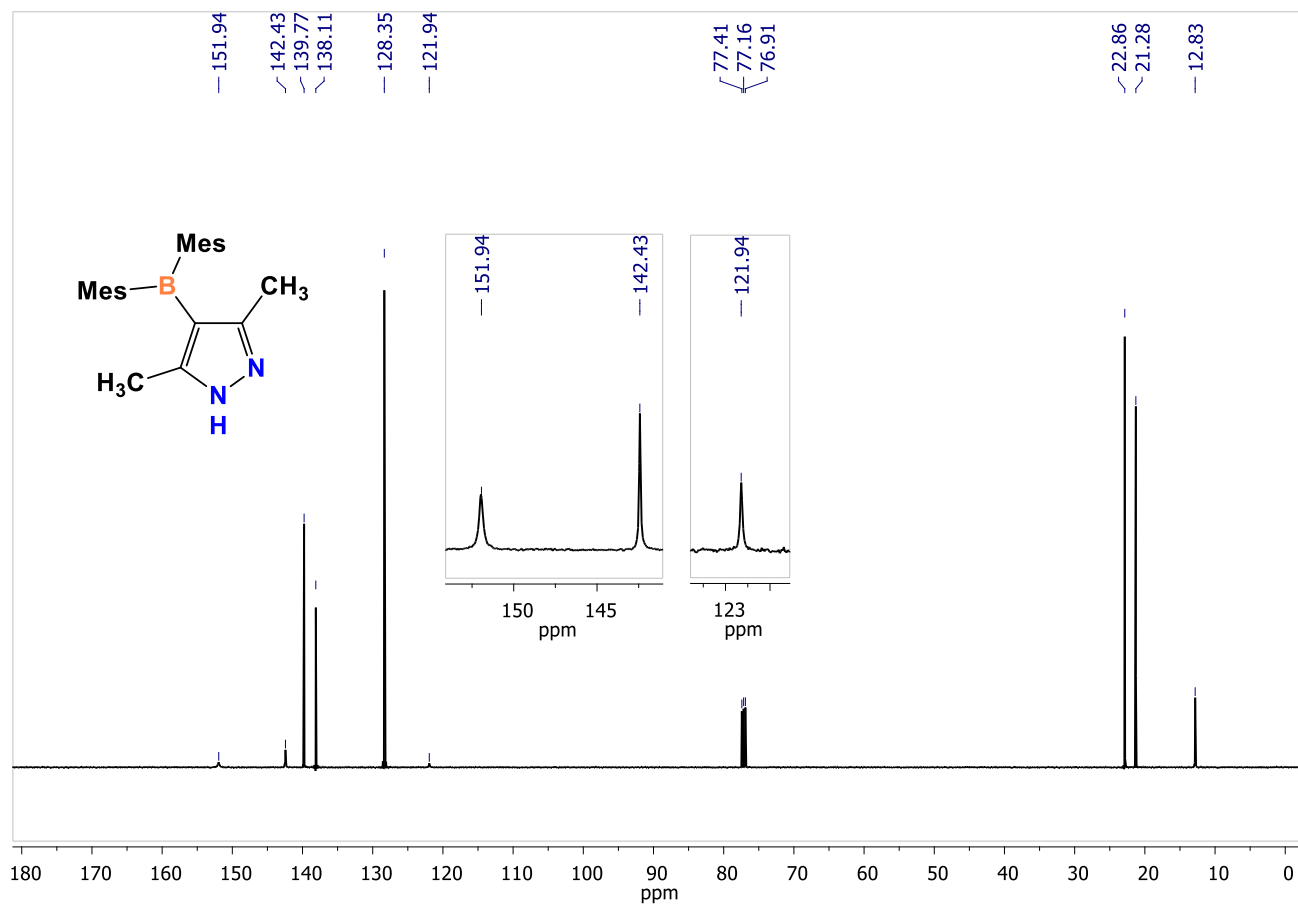


Figure S5. ¹³C NMR spectrum of 4-BMes₂-3,5-(CH₃)₂PzH (**4**) in CDCl₃

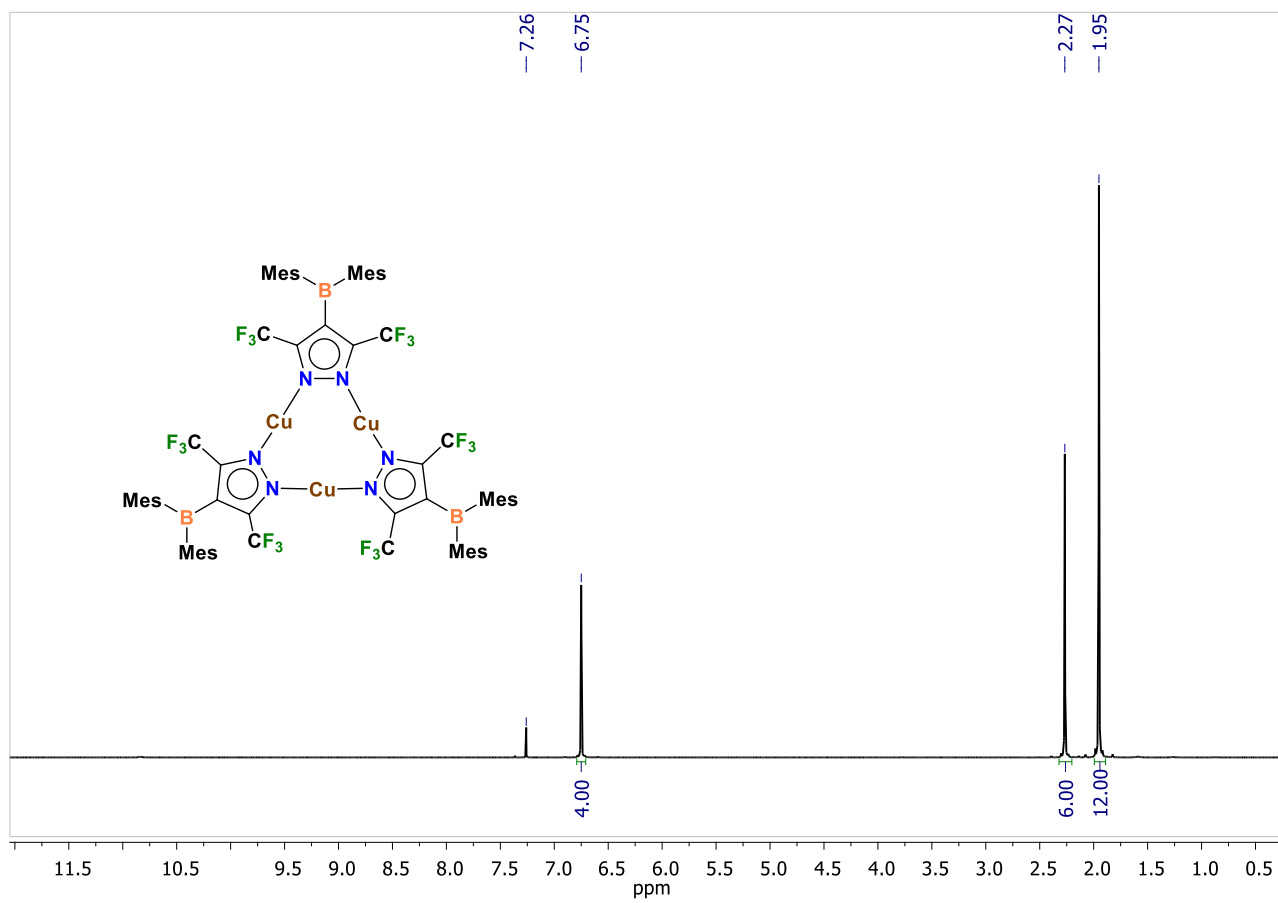


Figure S6. ¹H NMR spectrum of $\{[4\text{-BMes}_2\text{-}3,5\text{-(CF}_3)_2\text{Pz}]\text{Cu}\}_3$ (**5**) in CDCl₃

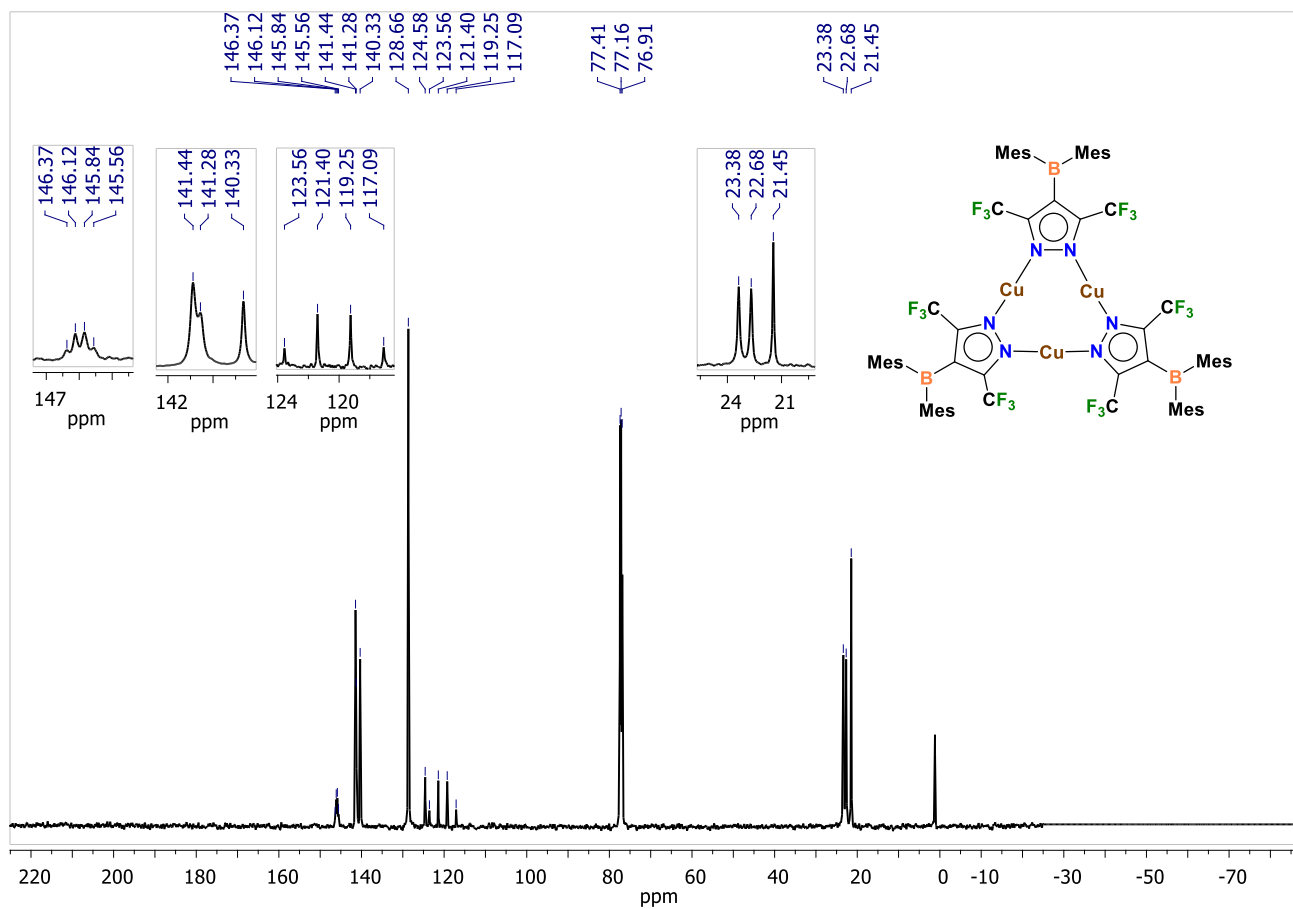


Figure S7. ^{13}C NMR spectrum of $\{[4\text{-BMes}_2\text{-}3,5\text{-(CF}_3)_2\text{Pz]Cu}\}_3$ (**5**) in CDCl_3

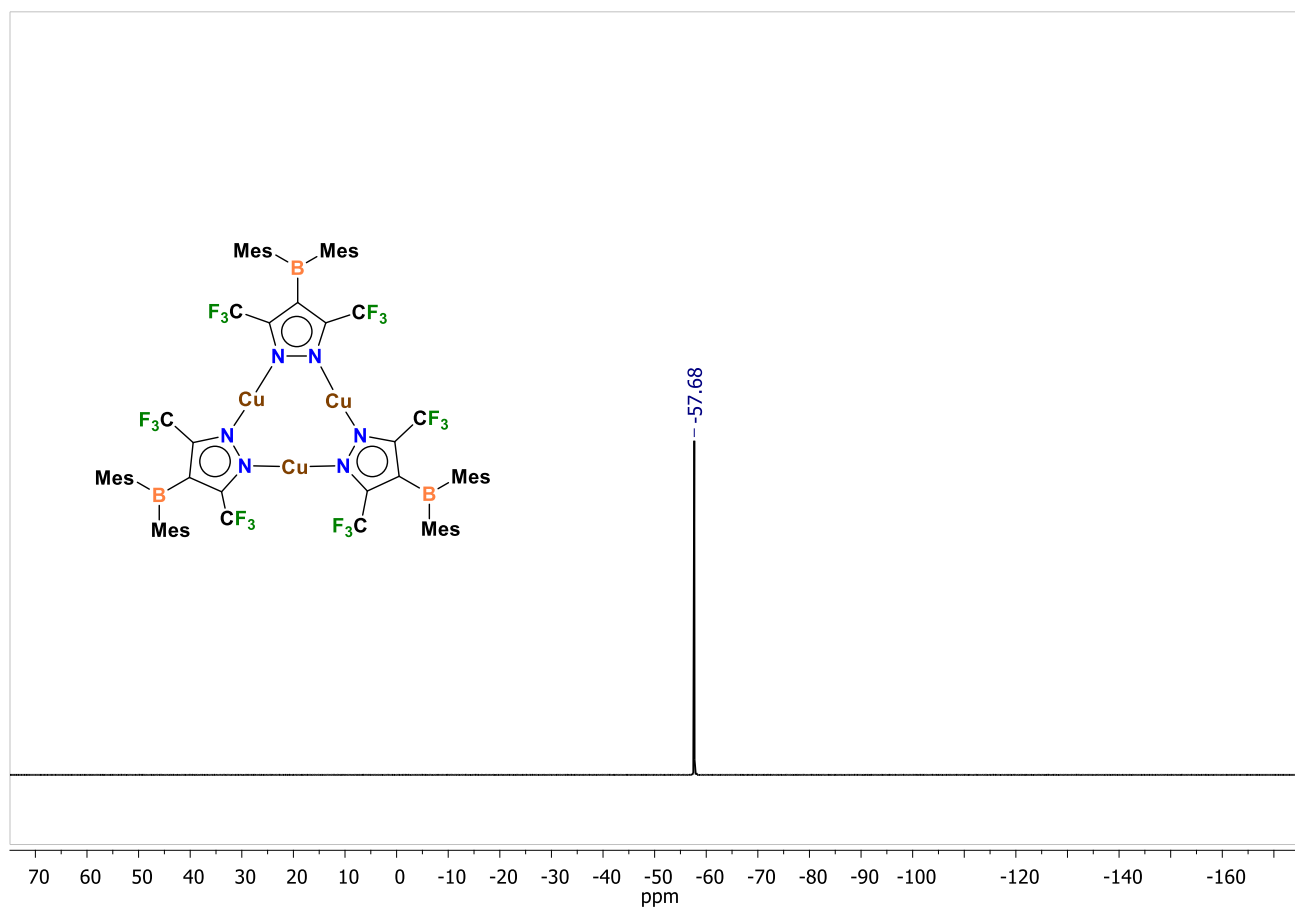


Figure S8. ^{19}F NMR spectrum of $\{[4\text{-BMes}_2\text{-}3,5\text{-(CF}_3)_2\text{PzCu}]_3\}$ (**5**) in CDCl_3

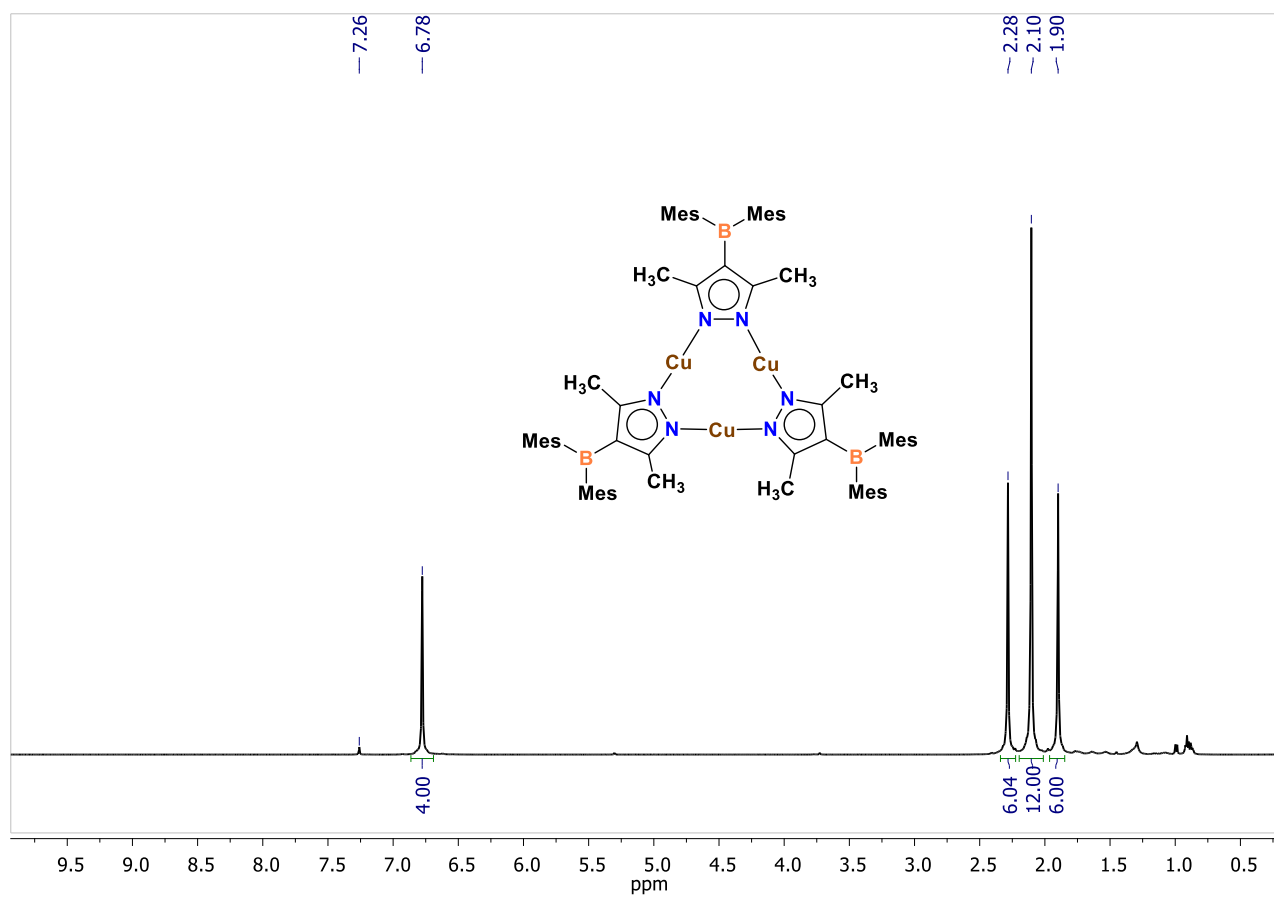


Figure S9. ¹H NMR spectrum of $\{[4\text{-BMes}_2\text{-}3,5\text{-(CH}_3)_2\text{Pz}]\text{Cu}\}_3$ (**6**) in CDCl₃

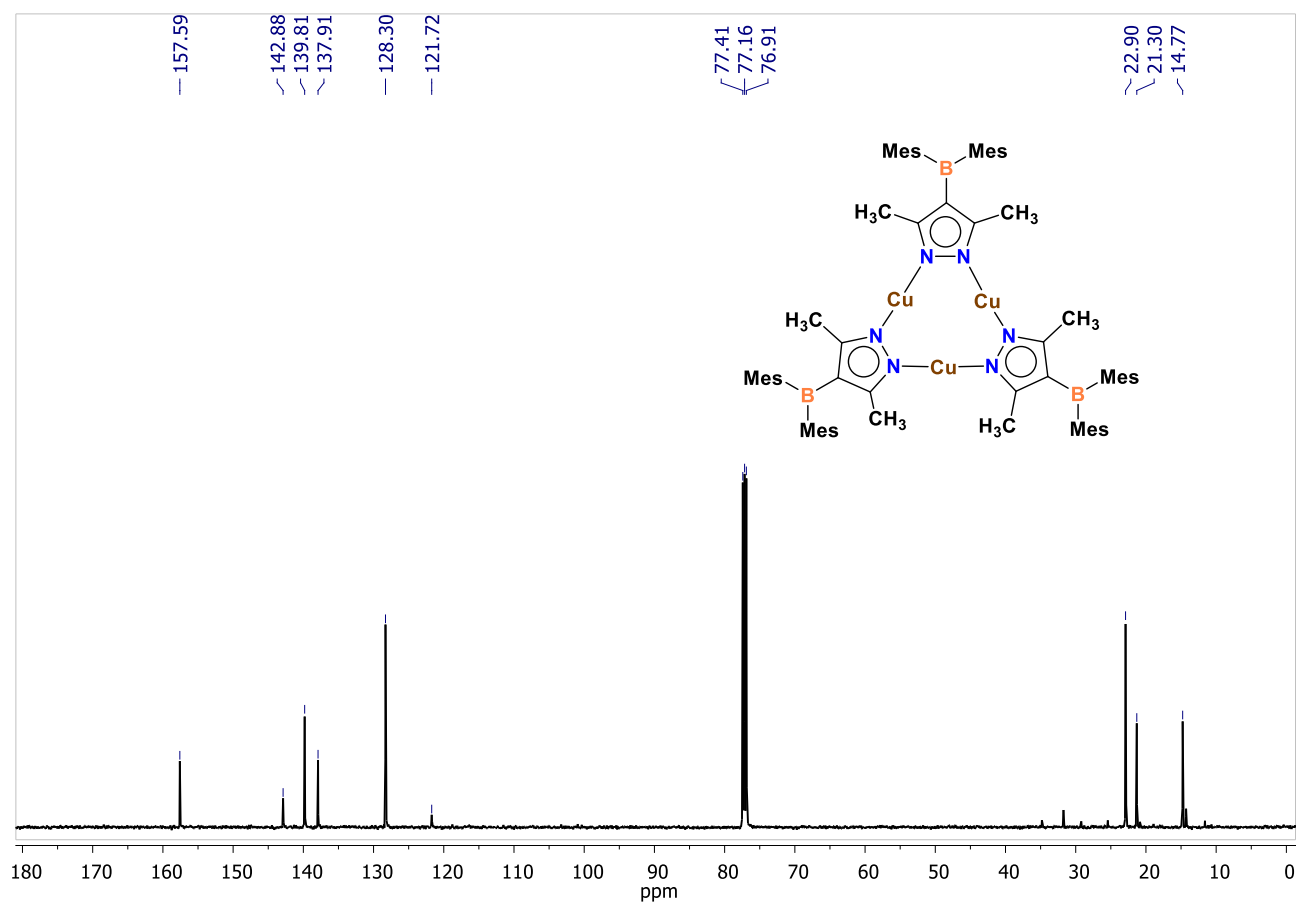


Figure S10. ^{13}C NMR spectrum of $\{[4\text{-BMes}_2\text{-}3,5\text{-(CH}_3)_2\text{Pz}]\text{Cu}\}_3$ (6) in CDCl_3

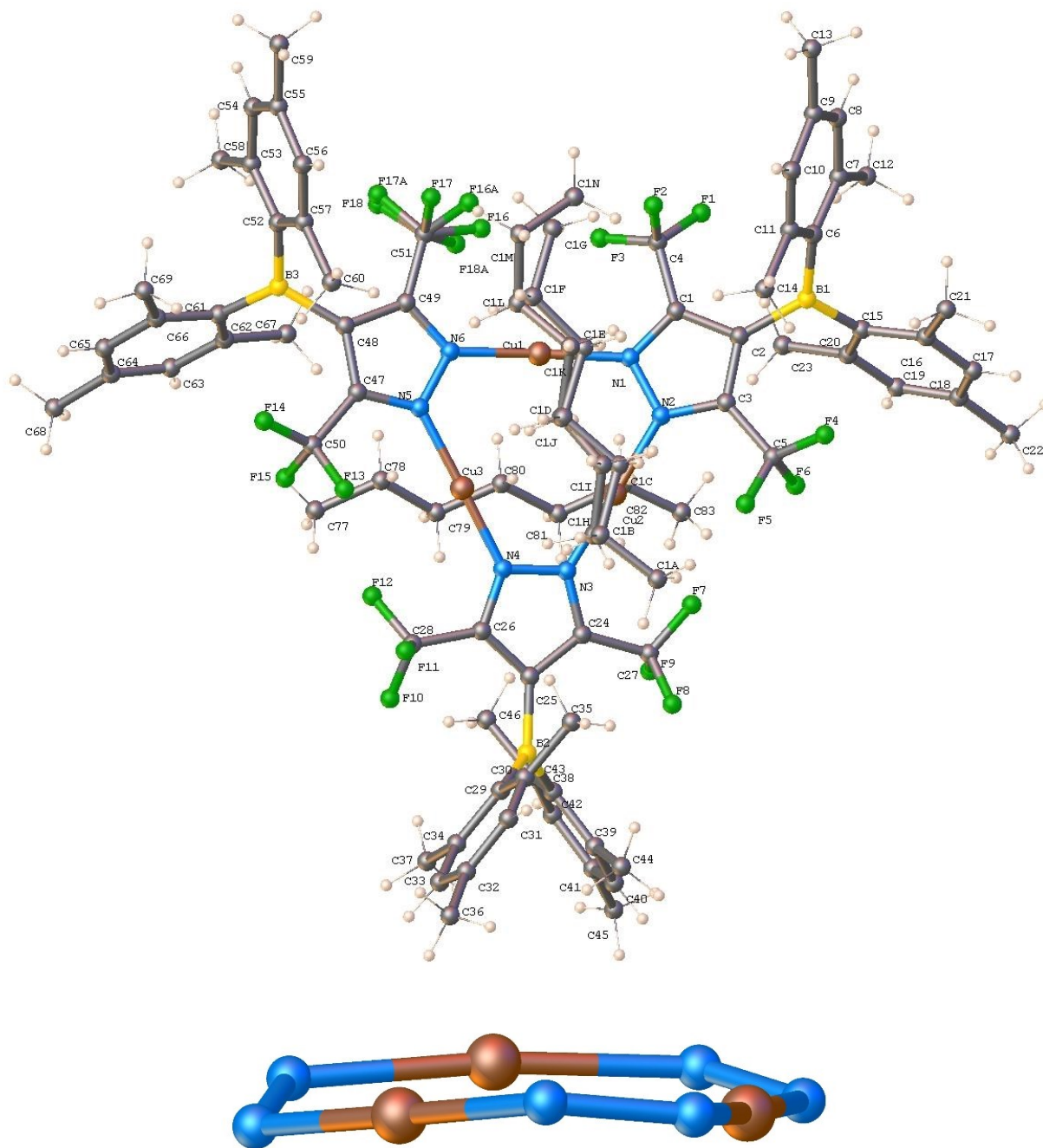


Figure S12. Labelling scheme of $\{[4\text{-}(\text{BMe}_2)\text{-}3,5\text{-}(\text{CF}_3)_2\text{Pz}]\text{Cu}\}_3 \cdot 1.5(\text{heptane})$ (top-figure) and Cu_3N_6 core (bottom figure)

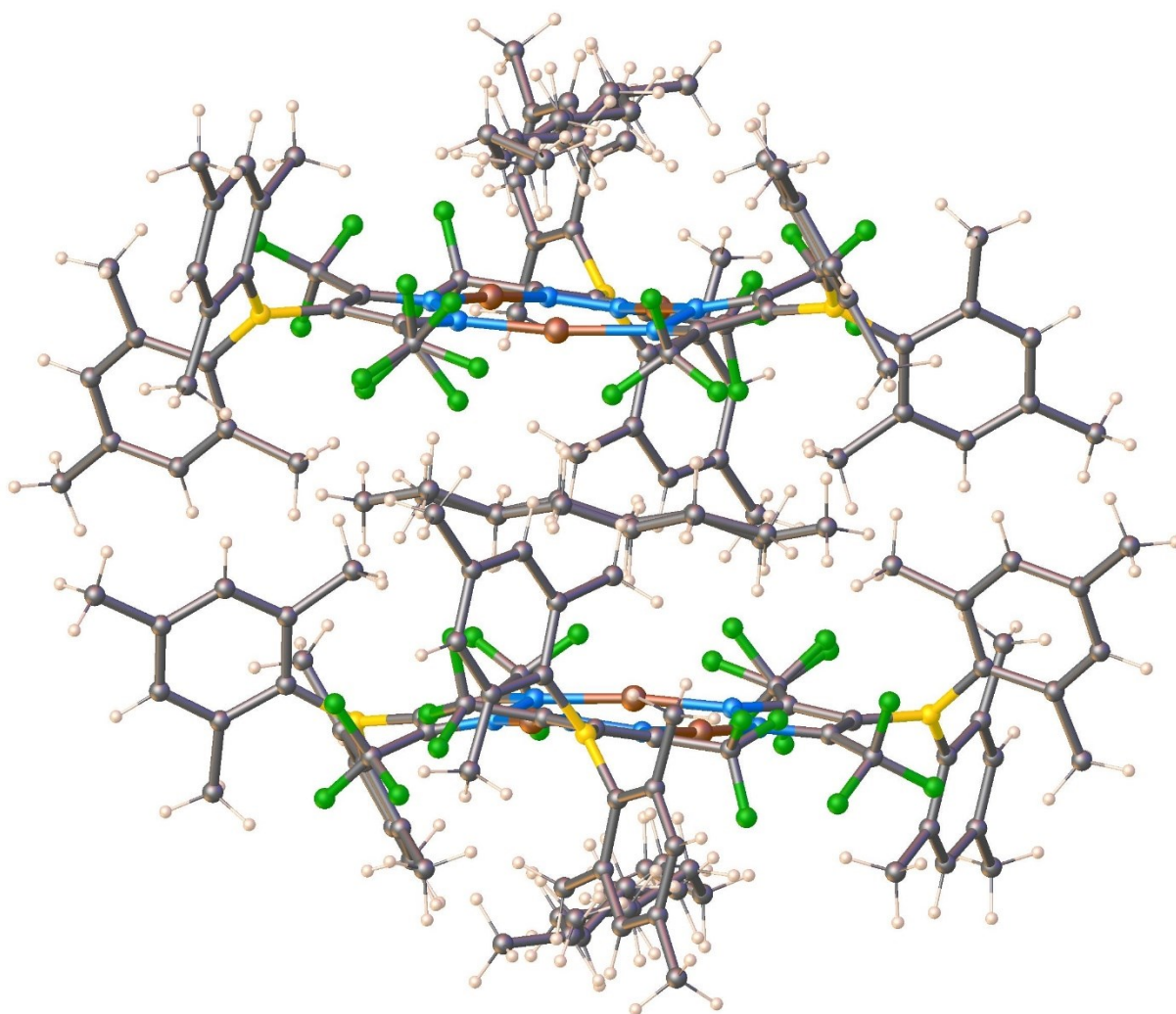


Figure S13. Packing diagram of **5** showing the pockets created by Mes₂B⁻ units and heptane molecules

Table S1. Crystal data and structure refinement for $\{[4-(\text{BMes}_2)\text{-}3,5\text{-(CF}_3)_2\text{Pz}]\text{Cu}\}_3 \cdot 1.5(\text{heptane})$ (**5**).

Identification code	HRD85
Empirical formula	$\text{C}_{79.5}\text{H}_{90}\text{B}_3\text{Cu}_3\text{F}_{18}\text{N}_6$
Formula weight	1694.62
Temperature/K	100.00
Crystal system	triclinic
Space group	P-1
$a/\text{\AA}$	16.9215(7)
$b/\text{\AA}$	16.9436(7)
$c/\text{\AA}$	17.6659(8)
$\alpha/^\circ$	72.604(2)
$\beta/^\circ$	69.820(2)
$\gamma/^\circ$	60.055(2)
Volume/ \AA^3	4069.1(3)
Z	2
$\rho_{\text{calc}}/\text{g/cm}^3$	1.383
μ/mm^{-1}	0.864
F(000)	1746.0
Crystal size/ mm^3	$0.2 \times 0.19 \times 0.03$
Radiation	Mo $\text{K}\alpha$ ($\lambda = 0.71073$)
2Θ range for data collection/ $^\circ$	5.118 to 61.064
Index ranges	$-24 \leq h \leq 24, -24 \leq k \leq 24, -25 \leq l \leq 25$
Reflections collected	68277
Independent reflections	24572 [$R_{\text{int}} = 0.0269, R_{\text{sigma}} = 0.0364$]
Data/restraints/parameters	24572/441/1134

Goodness-of-fit on F^2 1.014
 Final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0436$, $wR_2 = 0.1014$
 Final R indexes [all data] $R_1 = 0.0617$, $wR_2 = 0.1093$
 Largest diff. peak/hole / $e \text{ \AA}^{-3}$ 0.87/-0.71

Table S2. Bond Lengths for $\{[4\text{-(BMes}_2\text{)-3,5-(CF}_3\text{)}_2\text{Pz]Cu}\}_3 \cdot 1.5(\text{heptane})$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	N1	1.8752(14)	C29	B2	1.566(3)
Cu1	N6	1.8748(15)	C30	C31	1.391(3)
Cu2	N2	1.8601(15)	C30	C35	1.516(3)
Cu2	N3	1.8613(16)	C31	C32	1.389(3)
Cu3	N4	1.8663(15)	C32	C33	1.389(3)
Cu3	N5	1.8645(14)	C32	C36	1.512(3)
F1	C4	1.339(2)	C33	C34	1.394(3)
F2	C4	1.333(2)	C34	C37	1.510(3)
F3	C4	1.334(2)	C38	C39	1.420(2)
F4	C5	1.338(2)	C38	C43	1.411(3)
F5	C5	1.341(2)	C38	B2	1.564(3)
F6	C5	1.334(2)	C39	C40	1.391(2)
F7	C27	1.330(2)	C39	C44	1.514(3)
F8	C27	1.338(3)	C40	C41	1.388(3)
F9	C27	1.331(3)	C41	C42	1.389(3)
F10	C28	1.332(2)	C41	C45	1.507(3)
F11	C28	1.320(3)	C42	C43	1.390(3)
F12	C28	1.336(2)	C43	C46	1.523(3)
F13	C50	1.343(2)	C47	C48	1.393(2)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F14	C50	1.336(2)	C47	C50	1.490(2)
F15	C50	1.335(3)	C48	C49	1.401(2)
F16	C51	1.323(2)	C48	B3	1.581(2)
F17	C51	1.364(2)	C49	C51	1.492(3)
F18	C51	1.333(2)	C51	F16A	1.308(6)
N1	N2	1.368(2)	C51	F18A	1.381(6)
N1	C1	1.345(2)	C51	F17A	1.343(6)
N2	C3	1.350(2)	C52	C53	1.422(2)
N3	N4	1.360(2)	C52	C57	1.408(3)
N3	C24	1.351(2)	C52	B3	1.571(3)
N4	C26	1.344(2)	C53	C54	1.393(3)
N5	N6	1.362(2)	C53	C58	1.509(3)
N5	C47	1.352(2)	C54	C55	1.383(3)
N6	C49	1.348(2)	C55	C56	1.391(3)
C1	C2	1.400(2)	C55	C59	1.515(3)
C1	C4	1.491(2)	C56	C57	1.390(3)
C2	C3	1.399(2)	C57	C60	1.516(3)
C2	B1	1.577(3)	C61	C62	1.418(3)
C3	C5	1.496(2)	C61	C66	1.425(2)
C6	C7	1.419(3)	C61	B3	1.560(3)
C6	C11	1.413(2)	C62	C63	1.394(3)
C6	B1	1.569(3)	C62	C67	1.516(3)
C7	C8	1.393(3)	C63	C64	1.385(3)
C7	C12	1.510(3)	C64	C65	1.386(3)
C8	C9	1.383(3)	C64	C68	1.508(3)
C9	C10	1.389(3)	C65	C66	1.393(3)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C9	C13	1.512(3)	C66	C69	1.515(3)
C10	C11	1.393(3)	C77	C78	1.481(9)
C11	C14	1.516(3)	C78	C79	1.460(9)
C15	C16	1.420(2)	C79	C80	1.453(9)
C15	C20	1.414(2)	C80	C81	1.465(7)
C15	B1	1.567(2)	C81	C82	1.453(9)
C16	C17	1.392(2)	C82	C83	1.441(9)
C16	C21	1.508(3)	C1A	C1B	1.473(10)
C17	C18	1.386(3)	C1B	C1C	1.508(9)
C18	C19	1.387(3)	C1C	C1D	1.500(8)
C18	C22	1.508(3)	C1D	C1E	1.512(8)
C19	C20	1.398(2)	C1E	C1F	1.482(8)
C20	C23	1.514(3)	C1F	C1G	1.513(8)
C24	C25	1.399(3)	C1H	C1I	1.504(11)
C24	C27	1.502(3)	C1I	C1J	1.492(11)
C25	C26	1.401(2)	C1J	C1K	1.530(10)
C25	B2	1.573(3)	C1K	C1L	1.494(10)
C26	C28	1.491(3)	C1L	C1M	1.522(10)
C29	C30	1.415(3)	C1M	C1N	1.460(10)
C29	C34	1.417(3)			

Table S3. Bond Angles for {[4-(BMes₂)-3,5-(CF₃)₂Pz]Cu}₃ (**5**)•1.5(heptane).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N6	Cu1	N1	174.18(7)	C31	C32	C36	120.7(2)
N2	Cu2	N3	178.99(7)	C33	C32	C36	121.4(2)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N5	Cu3	N4	176.97(8)	C32	C33	C34	121.87(19)
N2	N1	Cu1	118.52(11)	C29	C34	C37	122.54(17)
C1	N1	Cu1	132.19(12)	C33	C34	C29	120.13(18)
C1	N1	N2	107.23(13)	C33	C34	C37	117.33(17)
N1	N2	Cu2	120.44(11)	C39	C38	B2	120.19(16)
C3	N2	Cu2	132.16(12)	C43	C38	C39	118.03(16)
C3	N2	N1	107.04(14)	C43	C38	B2	121.70(16)
N4	N3	Cu2	118.85(12)	C38	C39	C44	122.91(16)
C24	N3	Cu2	134.05(13)	C40	C39	C38	119.62(17)
C24	N3	N4	106.83(15)	C40	C39	C44	117.45(15)
N3	N4	Cu3	119.33(12)	C41	C40	C39	122.32(16)
C26	N4	Cu3	133.09(12)	C40	C41	C42	117.82(17)
C26	N4	N3	107.52(14)	C40	C41	C45	121.00(17)
N6	N5	Cu3	120.78(11)	C42	C41	C45	121.17(18)
C47	N5	Cu3	131.46(12)	C41	C42	C43	121.87(18)
C47	N5	N6	107.42(13)	C38	C43	C46	122.47(17)
N5	N6	Cu1	119.15(11)	C42	C43	C38	120.29(17)
C49	N6	Cu1	133.52(13)	C42	C43	C46	117.16(18)
C49	N6	N5	107.10(14)	N5	C47	C48	111.88(15)
N1	C1	C2	112.35(15)	N5	C47	C50	119.15(15)
N1	C1	C4	120.27(14)	C48	C47	C50	128.94(15)
C2	C1	C4	127.34(15)	C47	C48	C49	101.51(14)
C1	C2	B1	128.72(15)	C47	C48	B3	130.05(16)
C3	C2	C1	101.13(14)	C49	C48	B3	128.16(16)
C3	C2	B1	130.13(15)	N6	C49	C48	112.05(15)
N2	C3	C2	112.23(15)	N6	C49	C51	120.75(15)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	C3	C5	119.44(16)	C48	C49	C51	127.19(15)
C2	C3	C5	128.28(16)	F13	C50	C47	111.46(15)
F1	C4	C1	111.51(14)	F14	C50	F13	106.94(17)
F2	C4	F1	106.86(14)	F14	C50	C47	111.60(15)
F2	C4	F3	106.96(15)	F15	C50	F13	106.63(16)
F2	C4	C1	112.75(15)	F15	C50	F14	107.18(15)
F3	C4	F1	106.56(15)	F15	C50	C47	112.70(17)
F3	C4	C1	111.82(15)	F16	C51	F17	105.02(18)
F4	C5	F5	106.89(17)	F16	C51	F18	109.9(2)
F4	C5	C3	111.12(15)	F16	C51	C49	113.37(15)
F5	C5	C3	111.71(15)	F17	C51	C49	111.21(17)
F6	C5	F4	107.41(15)	F18	C51	F17	105.58(17)
F6	C5	F5	106.57(15)	F18	C51	C49	111.3(2)
F6	C5	C3	112.80(17)	F16A	C51	C49	121.6(6)
C7	C6	B1	120.33(16)	F16A	C51	F18A	101.8(9)
C11	C6	C7	117.92(16)	F16A	C51	F17A	113.3(13)
C11	C6	B1	121.65(16)	F18A	C51	C49	99.3(6)
C6	C7	C12	122.35(17)	F17A	C51	C49	118.1(15)
C8	C7	C6	120.07(18)	F17A	C51	F18A	95.3(13)
C8	C7	C12	117.56(17)	C53	C52	B3	120.21(17)
C9	C8	C7	121.73(19)	C57	C52	C53	118.06(17)
C8	C9	C10	118.30(18)	C57	C52	B3	121.72(16)
C8	C9	C13	120.3(2)	C52	C53	C58	122.30(17)
C10	C9	C13	121.4(2)	C54	C53	C52	119.58(18)
C9	C10	C11	121.85(19)	C54	C53	C58	118.12(16)
C6	C11	C14	122.67(17)	C55	C54	C53	122.16(18)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	C11	C6	120.00(18)	C54	C55	C56	118.08(18)
C10	C11	C14	117.30(17)	C54	C55	C59	121.1(2)
C16	C15	B1	120.30(15)	C56	C55	C59	120.8(2)
C20	C15	C16	117.93(15)	C57	C56	C55	121.7(2)
C20	C15	B1	121.65(15)	C52	C57	C60	122.66(17)
C15	C16	C21	121.98(15)	C56	C57	C52	120.36(17)
C17	C16	C15	120.06(16)	C56	C57	C60	116.95(18)
C17	C16	C21	117.95(16)	C62	C61	C66	117.51(17)
C18	C17	C16	121.91(16)	C62	C61	B3	122.09(15)
C17	C18	C19	118.15(16)	C66	C61	B3	120.35(16)
C17	C18	C22	120.49(17)	C61	C62	C67	123.07(17)
C19	C18	C22	121.36(18)	C63	C62	C61	120.35(17)
C18	C19	C20	121.92(17)	C63	C62	C67	116.53(18)
C15	C20	C23	122.93(16)	C64	C63	C62	121.82(19)
C19	C20	C15	119.90(16)	C63	C64	C65	118.23(19)
C19	C20	C23	117.14(16)	C63	C64	C68	121.1(2)
N3	C24	C25	112.50(16)	C65	C64	C68	120.64(19)
N3	C24	C27	119.99(16)	C64	C65	C66	122.04(18)
C25	C24	C27	127.51(16)	C61	C66	C69	122.01(17)
C24	C25	C26	100.75(15)	C65	C66	C61	119.96(18)
C24	C25	B2	129.56(15)	C65	C66	C69	118.03(17)
C26	C25	B2	129.64(16)	C6	B1	C2	117.30(15)
N4	C26	C25	112.36(16)	C15	B1	C2	117.06(15)
N4	C26	C28	119.66(15)	C15	B1	C6	125.64(15)
C25	C26	C28	127.96(16)	C29	B2	C25	120.02(16)
F7	C27	F8	107.37(19)	C38	B2	C25	119.62(16)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
F7	C27	F9	107.0(2)	C38	B2	C29	120.34(15)
F7	C27	C24	112.11(16)	C52	B3	C48	118.13(16)
F8	C27	C24	111.07(18)	C61	B3	C48	116.66(15)
F9	C27	F8	106.66(16)	C61	B3	C52	125.21(15)
F9	C27	C24	112.35(19)	C79	C78	C77	119.5(9)
F10	C28	F12	106.30(17)	C80	C79	C78	120.6(10)
F10	C28	C26	111.50(16)	C79	C80	C81	123.0(10)
F11	C28	F10	106.98(18)	C82	C81	C80	120.9(8)
F11	C28	F12	106.94(18)	C83	C82	C81	124.4(11)
F11	C28	C26	112.63(18)	C1A	C1B	C1C	111.9(9)
F12	C28	C26	112.10(17)	C1D	C1C	C1B	115.1(7)
C30	C29	C34	117.77(17)	C1C	C1D	C1E	113.5(6)
C30	C29	B2	121.56(17)	C1F	C1E	C1D	116.5(6)
C34	C29	B2	120.29(16)	C1E	C1F	C1G	115.3(6)
C29	C30	C35	122.24(18)	C1J	C1I	C1H	114.8(11)
C31	C30	C29	120.16(19)	C1I	C1J	C1K	112.9(10)
C31	C30	C35	117.52(19)	C1L	C1K	C1J	111.4(9)
C32	C31	C30	122.0(2)	C1K	C1L	C1M	114.1(9)
C31	C32	C33	117.9(2)	C1N	C1M	C1L	111.0(9)

Crystal Data for $C_{79.5}H_{90}B_3Cu_3F_{18}N_6$ ($M=1694.62$ g/mol): triclinic, space group P-1 (no. 2), $a = 16.9215(7)$ Å, $b = 16.9436(7)$ Å, $c = 17.6659(8)$ Å, $\alpha = 72.604(2)^\circ$, $\beta = 69.820(2)^\circ$, $\gamma = 60.055(2)^\circ$, $V = 4069.1(3)$ Å³, $Z = 2$, $T = 100.00$ K, $\mu(\text{Mo K}\alpha) = 0.864$ mm⁻¹, $D_{\text{calc}} = 1.383$ g/cm³, 68277 reflections measured ($5.118^\circ \leq 2\theta \leq 61.064^\circ$), 24572 unique ($R_{\text{int}} = 0.0269$, $R_{\text{sigma}} = 0.0364$) which were used in all calculations. The final R_1 was 0.0436 ($I > 2\sigma(I)$) and wR_2 was 0.1093 (all data).

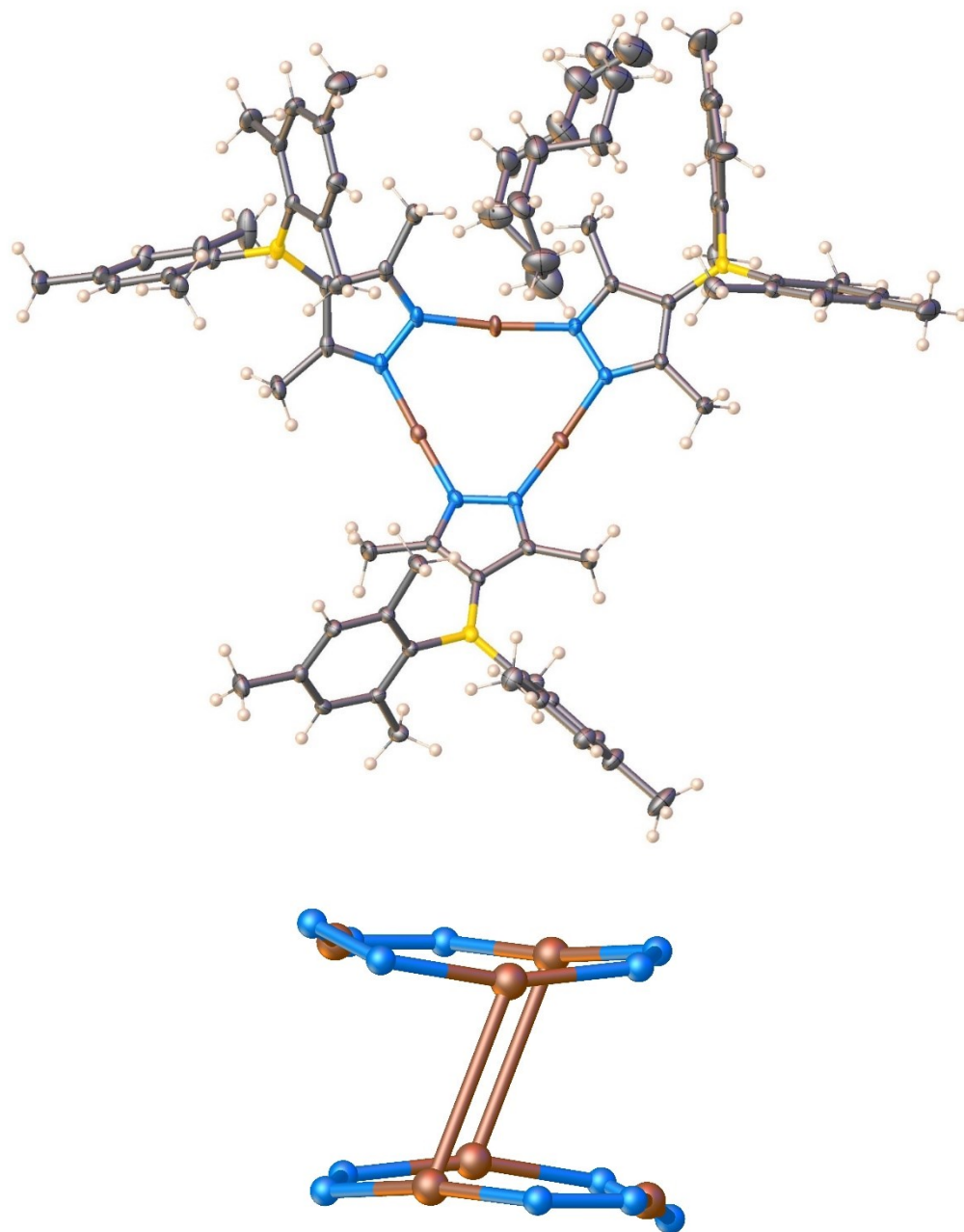


Figure S14. Asymmetric unit of $\{[4\text{-}(\text{BMe}_2)\text{-}3,5\text{-}(\text{CH}_3)_2\text{Pz}]\text{Cu}\}_3$ (**6**)•heptane (top figure) and a view of Cu_3N_6 dimer with $\text{Cu}\cdots\text{Cu}$ contacts (bottom figure)

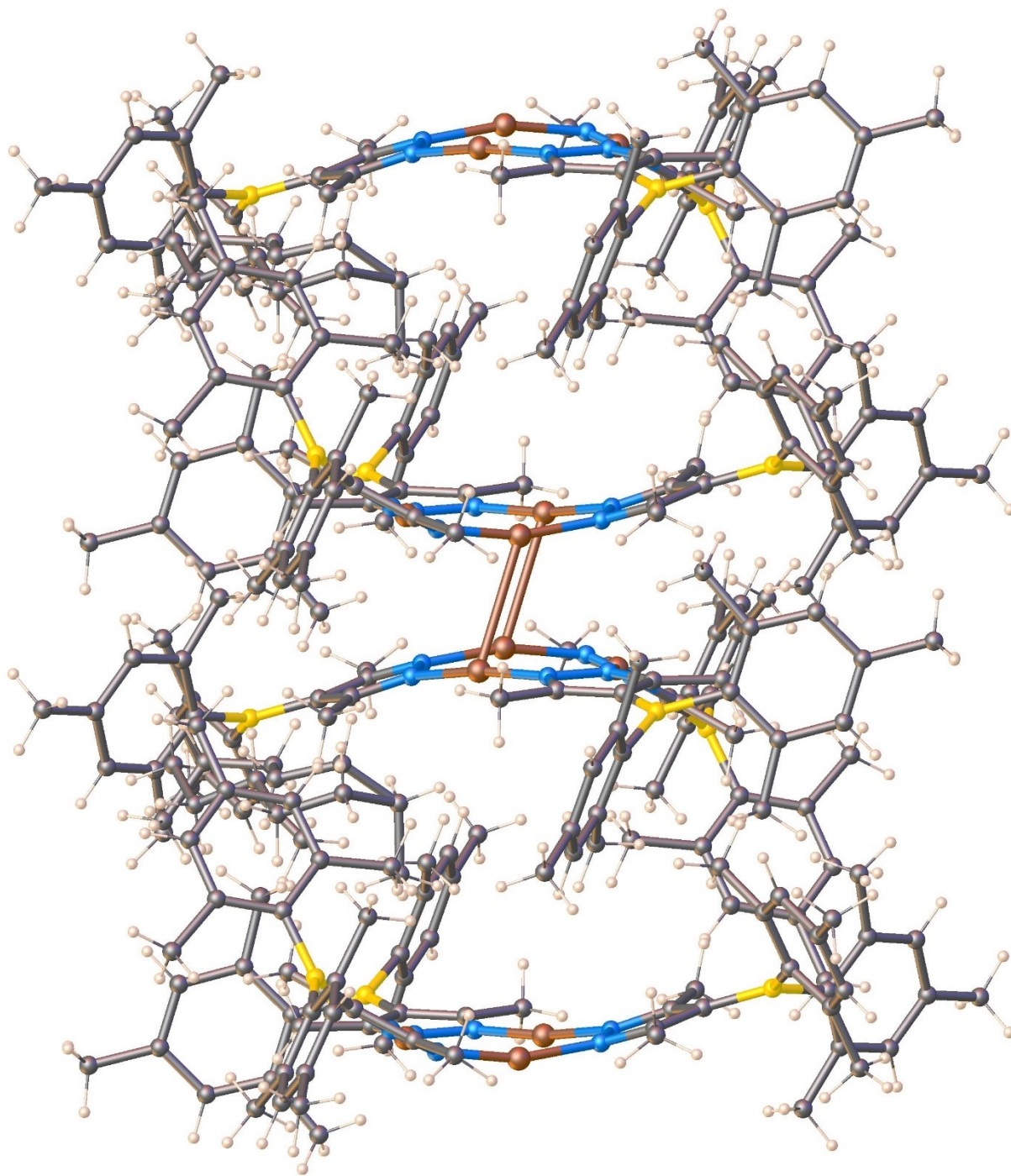


Figure S15. Packing diagram showing the pockets created by Mes₂B- units and heptane molecules

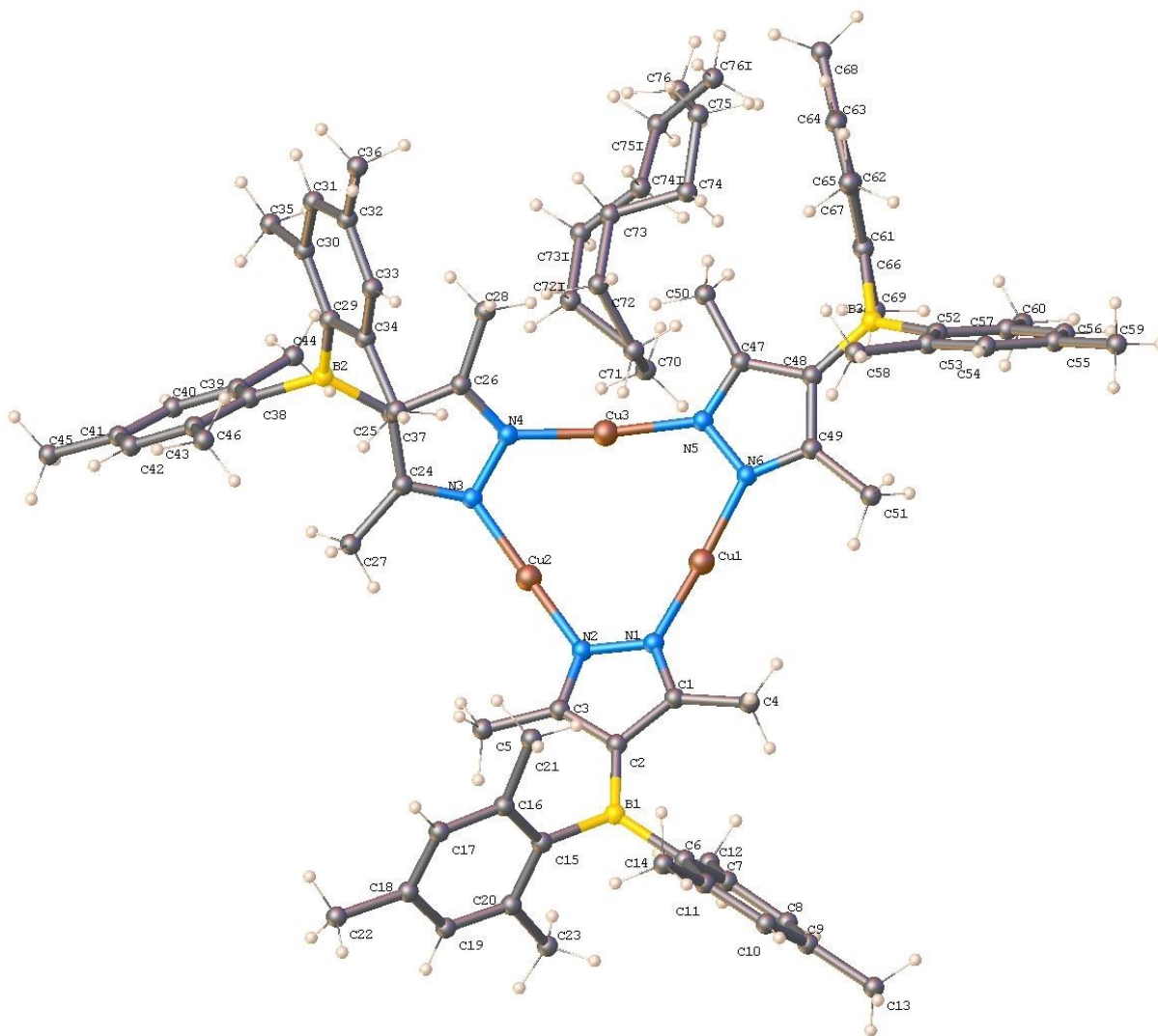


Figure S16. Labelling scheme of $\{[4-(\text{BMe}_2)\text{-}3,5\text{-(CH}_3)_2\text{Pz]Cu}_3\}_3$ (**6**) • heptane

Table S4. Crystal data and structure refinement for {[4-(BMes₂)-3,5-(CH₃)₂Pz]Cu}₃ (6) •heptane.

Identification code	HRD84
Empirical formula	C ₇₆ H ₉₉ B ₃ Cu ₃ N ₆
Formula weight	1319.66
Temperature/K	100.00
Crystal system	triclinic
Space group	P-1
a/Å	13.9999(5)
b/Å	16.1430(5)
c/Å	17.2755(6)
α/°	109.624(2)
β/°	93.285(2)
γ/°	105.508(2)
Volume/Å ³	3496.8(2)
Z	2
ρ _{calc} /cm ³	1.253
μ/mm ⁻¹	0.950
F(000)	1398.0
Crystal size/mm ³	0.35 × 0.1 × 0.03
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.82 to 61.11
Index ranges	-20 ≤ h ≤ 20, -23 ≤ k ≤ 22, -24 ≤ l ≤ 24
Reflections collected	56142
Independent reflections	21160 [R _{int} = 0.0306, R _{sigma} = 0.0390]
Data/restraints/parameters	21160/66/865

Goodness-of-fit on F^2 1.009
 Final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0441$, $wR_2 = 0.1078$
 Final R indexes [all data] $R_1 = 0.0619$, $wR_2 = 0.1161$
 Largest diff. peak/hole / $e \text{ \AA}^{-3}$ 1.09/-0.82

Table S5. Bond Lengths for {[4-(BMes₂)-3,5-(CH₃)₂Pz]Cu}₃ (6) •heptane.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	Cu2 ¹	3.0066(3)	C31	C32	1.380(3)
Cu1	N1	1.8662(16)	C32	C33	1.397(3)
Cu1	N6	1.8639(16)	C32	C36	1.510(3)
Cu2	N2	1.8632(17)	C33	C34	1.386(3)
Cu2	N3	1.8665(17)	C34	C37	1.517(3)
Cu3	N4	1.8520(15)	C38	C39	1.408(3)
Cu3	N5	1.8575(15)	C38	C43	1.412(3)
N1	N2	1.387(2)	C38	B2	1.586(3)
N1	C1	1.333(2)	C39	C40	1.394(3)
N2	C3	1.346(2)	C39	C44	1.520(3)
N3	N4	1.385(2)	C40	C41	1.387(3)
N3	C24	1.342(2)	C41	C42	1.384(3)
N4	C26	1.338(3)	C41	C45	1.507(3)
N5	N6	1.388(2)	C42	C43	1.397(3)
N5	C47	1.333(2)	C43	C46	1.503(3)
N6	C49	1.335(2)	C47	C48	1.413(2)
C1	C2	1.423(2)	C47	C50	1.496(3)
C1	C4	1.495(3)	C48	C49	1.417(2)
C2	C3	1.418(3)	C48	B3	1.539(3)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C2	B1	1.532(3)	C49	C51	1.496(3)
C3	C5	1.498(3)	C52	C53	1.411(3)
C6	C7	1.415(3)	C52	C57	1.414(3)
C6	C11	1.414(3)	C52	B3	1.582(3)
C6	B1	1.594(3)	C53	C54	1.397(3)
C7	C8	1.396(3)	C53	C58	1.521(3)
C7	C12	1.511(3)	C54	C55	1.391(3)
C8	C9	1.388(3)	C55	C56	1.387(3)
C9	C10	1.388(3)	C55	C59	1.510(3)
C9	C13	1.506(3)	C56	C57	1.395(3)
C10	C11	1.392(3)	C57	C60	1.513(3)
C11	C14	1.515(3)	C61	C62	1.413(3)
C15	C16	1.409(2)	C61	C66	1.406(3)
C15	C20	1.414(3)	C61	B3	1.595(3)
C15	B1	1.583(3)	C62	C63	1.398(3)
C16	C17	1.397(2)	C62	C67	1.506(3)
C16	C21	1.515(3)	C63	C64	1.379(4)
C17	C18	1.385(3)	C64	C65	1.379(4)
C18	C19	1.392(3)	C64	C68	1.520(3)
C18	C22	1.507(3)	C65	C66	1.405(3)
C19	C20	1.387(2)	C66	C69	1.508(3)
C20	C23	1.509(3)	C70	C71	1.485(4)
C24	C25	1.409(3)	C71	C72	1.496(4)
C24	C27	1.499(3)	C71	C72I	1.525(4)
C25	C26	1.415(2)	C72	C73	1.509(5)
C25	B2	1.540(3)	C73	C74	1.527(4)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C26	C28	1.494(3)	C74	C75	1.513(5)
C29	C30	1.412(3)	C75	C76	1.514(5)
C29	C34	1.419(3)	C72I	C73I	1.519(4)
C29	B2	1.580(3)	C73I	C74I	1.511(5)
C30	C31	1.393(3)	C74I	C75I	1.505(5)
C30	C35	1.508(3)	C75I	C76I	1.510(5)

¹1-X,1-Y,1-Z

Table S6. Bond Angles for {[4-(BMes₂)-3,5-(CH₃)₂Pz]Cu}₃ (**6**) •heptane.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Cu1	Cu2 ¹	97.48(5)	C31	C32	C33	117.2(2)
N6	Cu1	Cu2 ¹	88.59(5)	C31	C32	C36	122.2(2)
N6	Cu1	N1	172.63(7)	C33	C32	C36	120.6(2)
N2	Cu2	Cu1 ¹	119.95(5)	C34	C33	C32	122.63(19)
N2	Cu2	N3	165.45(7)	C29	C34	C37	122.52(18)
N3	Cu2	Cu1 ¹	74.35(5)	C33	C34	C29	119.91(18)
N4	Cu3	N5	171.62(8)	C33	C34	C37	117.58(17)
N2	N1	Cu1	120.44(12)	C39	C38	C43	117.93(17)
C1	N1	Cu1	130.94(13)	C39	C38	B2	120.31(17)
C1	N1	N2	108.37(15)	C43	C38	B2	121.76(17)
N1	N2	Cu2	122.02(12)	C38	C39	C44	121.70(19)
C3	N2	Cu2	128.73(13)	C40	C39	C38	120.06(19)
C3	N2	N1	107.81(16)	C40	C39	C44	118.20(19)
N4	N3	Cu2	113.54(11)	C41	C40	C39	122.1(2)
C24	N3	Cu2	133.96(14)	C40	C41	C45	121.1(2)
C24	N3	N4	107.54(16)	C42	C41	C40	117.84(18)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	N4	Cu3	119.71(13)	C42	C41	C45	121.0(2)
C26	N4	Cu3	131.80(14)	C41	C42	C43	121.78(18)
C26	N4	N3	108.40(15)	C38	C43	C46	121.09(17)
N6	N5	Cu3	120.70(12)	C42	C43	C38	120.24(18)
C47	N5	Cu3	129.84(13)	C42	C43	C46	118.64(17)
C47	N5	N6	108.55(14)	N5	C47	C48	110.06(16)
N5	N6	Cu1	115.14(11)	N5	C47	C50	118.79(16)
C49	N6	Cu1	136.75(13)	C48	C47	C50	131.06(17)
C49	N6	N5	107.77(15)	C47	C48	C49	103.29(15)
N1	C1	C2	110.58(17)	C47	C48	B3	126.71(17)
N1	C1	C4	119.89(17)	C49	C48	B3	129.85(17)
C2	C1	C4	129.44(18)	N6	C49	C48	110.30(16)
C1	C2	B1	129.62(17)	N6	C49	C51	120.16(16)
C3	C2	C1	102.74(16)	C48	C49	C51	129.52(16)
C3	C2	B1	127.64(16)	C53	C52	C57	117.55(17)
N2	C3	C2	110.47(16)	C53	C52	B3	121.33(16)
N2	C3	C5	118.99(17)	C57	C52	B3	121.02(17)
C2	C3	C5	130.54(17)	C52	C53	C58	123.18(18)
C7	C6	B1	121.22(17)	C54	C53	C52	120.27(19)
C11	C6	C7	117.43(17)	C54	C53	C58	116.54(19)
C11	C6	B1	121.32(16)	C55	C54	C53	121.8(2)
C6	C7	C12	122.95(17)	C54	C55	C59	120.4(2)
C8	C7	C6	120.38(18)	C56	C55	C54	118.11(19)
C8	C7	C12	116.65(17)	C56	C55	C59	121.5(2)
C9	C8	C7	121.93(19)	C55	C56	C57	121.48(19)
C8	C9	C13	121.1(2)	C52	C57	C60	121.26(17)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	C9	C8	117.72(19)	C56	C57	C52	120.71(19)
C10	C9	C13	121.2(2)	C56	C57	C60	117.98(18)
C9	C10	C11	122.0(2)	C62	C61	B3	119.97(18)
C6	C11	C14	121.96(17)	C66	C61	C62	117.61(19)
C10	C11	C6	120.48(18)	C66	C61	B3	122.25(18)
C10	C11	C14	117.54(19)	C61	C62	C67	121.33(18)
C16	C15	C20	117.71(16)	C63	C62	C61	120.4(2)
C16	C15	B1	121.67(16)	C63	C62	C67	118.2(2)
C20	C15	B1	120.61(16)	C64	C63	C62	121.8(2)
C15	C16	C21	122.67(16)	C63	C64	C68	121.1(3)
C17	C16	C15	120.11(17)	C65	C64	C63	118.0(2)
C17	C16	C21	117.22(16)	C65	C64	C68	120.9(3)
C18	C17	C16	122.15(17)	C64	C65	C66	122.0(2)
C17	C18	C19	117.54(17)	C61	C66	C69	122.68(19)
C17	C18	C22	121.24(17)	C65	C66	C61	120.0(2)
C19	C18	C22	121.21(17)	C65	C66	C69	117.3(2)
C20	C19	C18	121.99(17)	C2	B1	C6	121.35(16)
C15	C20	C23	120.99(16)	C2	B1	C15	119.30(16)
C19	C20	C15	120.46(16)	C15	B1	C6	119.31(16)
C19	C20	C23	118.49(16)	C25	B2	C29	117.11(16)
N3	C24	C25	110.70(17)	C25	B2	C38	120.13(18)
N3	C24	C27	120.11(19)	C29	B2	C38	122.72(17)
C25	C24	C27	128.94(17)	C48	B3	C52	122.09(17)
C24	C25	C26	103.19(16)	C48	B3	C61	117.29(16)
C24	C25	B2	128.79(17)	C52	B3	C61	120.47(16)
C26	C25	B2	127.21(19)	C70	C71	C72	126.4(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N4	C26	C25	110.08(17)	C70	C71	C72I	103.3(4)
N4	C26	C28	120.22(16)	C71	C72	C73	121.0(5)
C25	C26	C28	129.70(18)	C72	C73	C74	109.1(5)
C30	C29	C34	117.41(19)	C75	C74	C73	111.9(5)
C30	C29	B2	122.92(17)	C74	C75	C76	117.0(5)
C34	C29	B2	119.63(17)	C73I	C72I	C71	116.4(4)
C29	C30	C35	121.5(2)	C74I	C73I	C72I	112.9(5)
C31	C30	C29	120.67(18)	C75I	C74I	C73I	114.4(5)
C31	C30	C35	117.73(19)	C74I	C75I	C76I	111.9(6)
C32	C31	C30	122.16(19)				

¹1-X,1-Y,1-Z

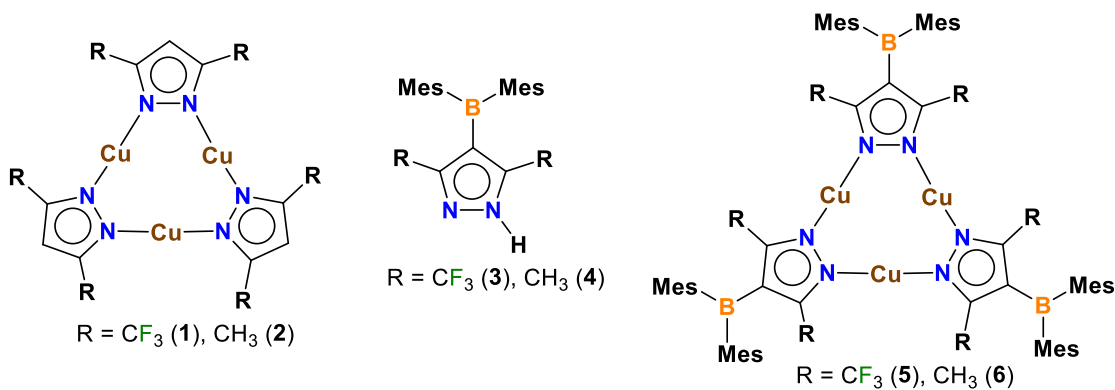
Crystal Data for C₇₆H₉₉B₃Cu₃N₆ (*M* = 1319.66 g/mol): triclinic, space group P-1 (no. 2), *a* = 13.9999(5) Å, *b* = 16.1430(5) Å, *c* = 17.2755(6) Å, α = 109.624(2)°, β = 93.285(2)°, γ = 105.508(2)°, *V* = 3496.8(2) Å³, *Z* = 2, *T* = 100.00 K, μ (Mo K α) = 0.950 mm⁻¹, *D*_{calc} = 1.253 g/cm³, 56142 reflections measured (4.82° ≤ 2 Θ ≤ 61.11°), 21160 unique (*R*_{int} = 0.0306, *R*_{sigma} = 0.0390) which were used in all calculations. The final *R*₁ was 0.0441 (*I* > 2 σ (*I*)) and *wR*₂ was 0.1161 (all data)

3. Optical Properties

Table S7. Comparison of photophysical properties in CHCl₃ solution and the solid state. The 80 K data in blue.

Compound	$\lambda_{\text{abs.}}$ CHCl ₃ /nm	$\lambda_{\text{Fl.}}$ CHCl ₃ RT [80 K] /nm [a]	Stokes, RT solution /cm ⁻¹	$\tau_{\text{Fl.}}$ CHCl ₃ RT [80 K] /ns [b]	λ_{PLE} solid /nm	$\lambda_{\text{Fl.}}$ solid RT [80 K] /nm [a]	Stokes, RT powder /cm ⁻¹	$\tau_{\text{Fl.}}$ solid RT [80 K] /ns [b]
3	332	390 [370, 424, 448]	4479	2.39 [1.92]	361	378 [393, 415]	1245	2.31 [2.45]
4	308	393 [354, 412, 431]	7022	3.62 [2.12]	335	360 [366, 379, 436]	2072	1.85 [2.10]
5	327	387 [371, 424, 448]	4741	2.09 [1.19]	359	384 [393, 415, 429]	1813	1.39 [2.20]
6	314	387 [374, 427, 434]	6007	0.91 [0.58]	351	704 [713]	14285	16106 [38907]

[a] Excited at 300 nm ; [b] excited with a 35 fs pulses centered at 325 nm and measured using a streak camera (**3**, **4**, **5** and **6**), Fitting error in all cases is less than 2%



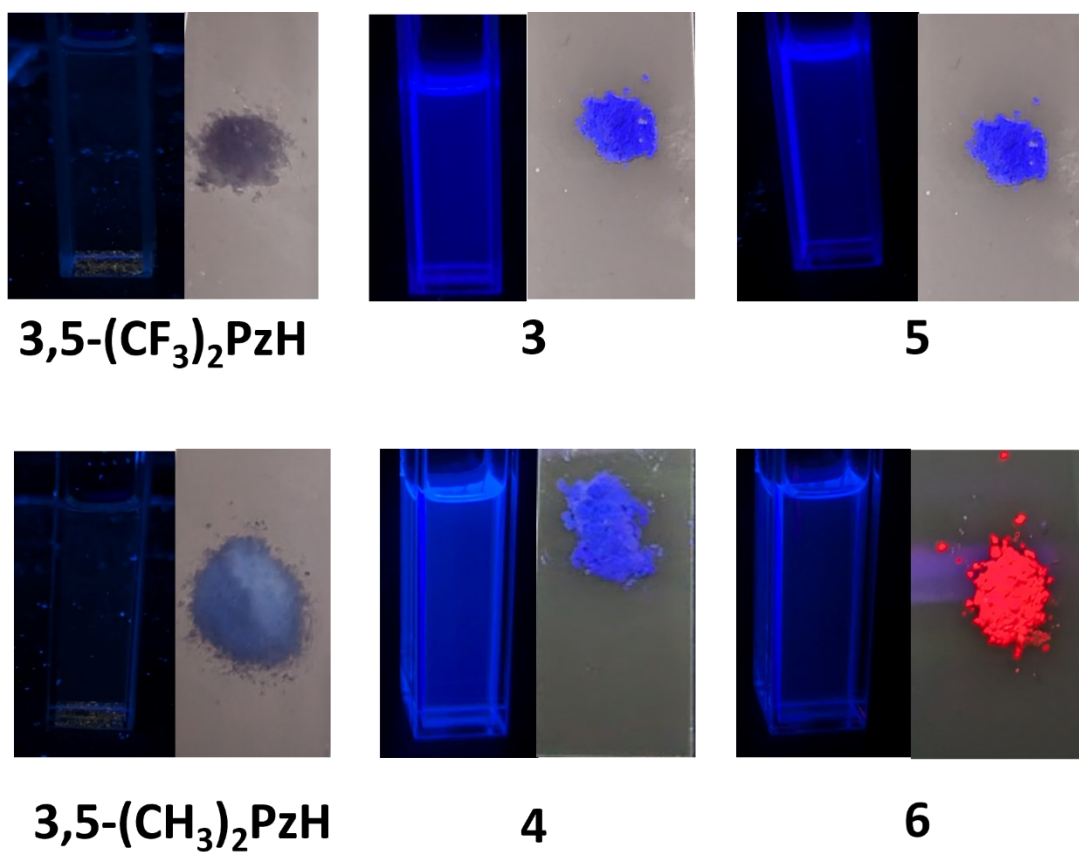


Figure S17. The emission photographs of pyrazoles with and without Mes₂B-substituent and copper complexes **5** and **6** in CHCl₃ solutions and in the solid state at room temperature. Irradiation was performed with a UV lamp (254 nm)

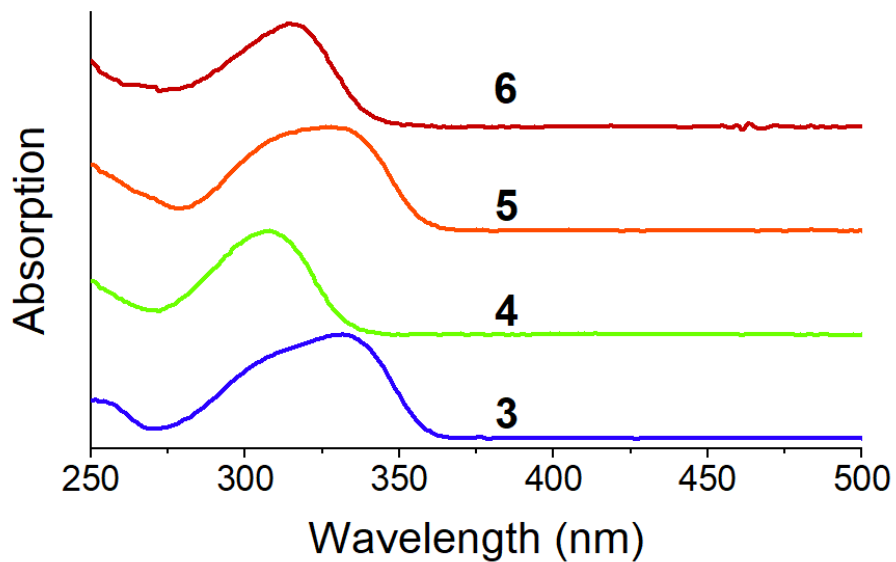


Figure S18. Absorption spectra of chloroform solutions at 295 K.

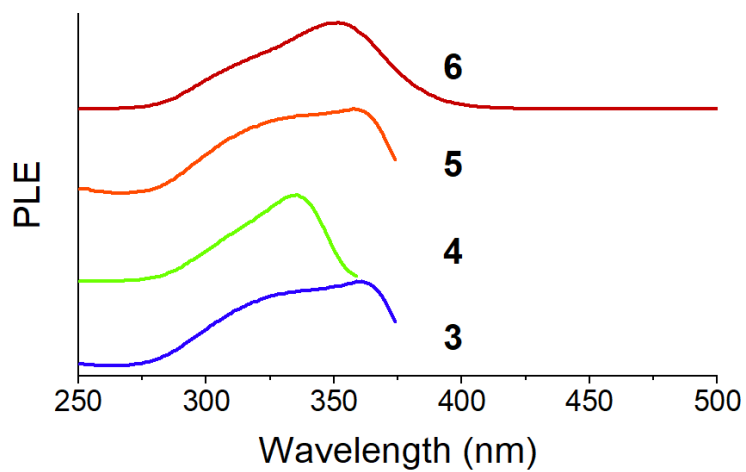


Figure S19. 295 K photoluminescence excitation (PLE) spectra of solid powder samples taken at the emission maximum.

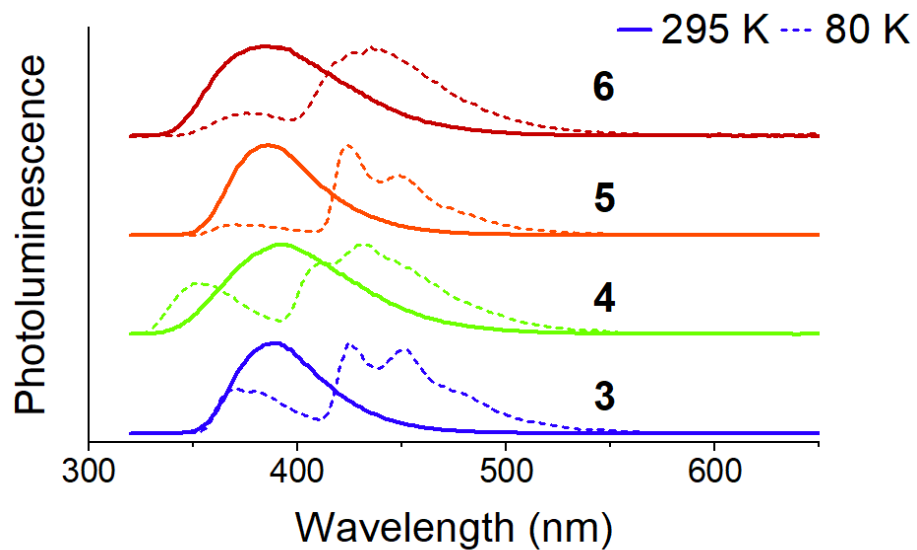


Figure S20. Photoluminescence of solutions at 295 K (solid lines) and 80 K (dashed). Excitation at 300 nm.

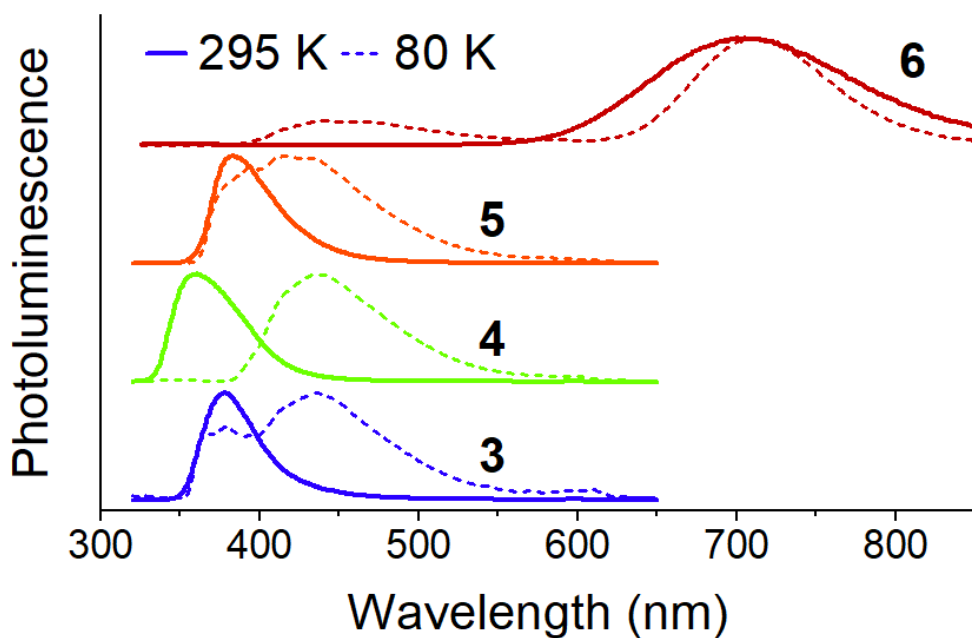


Figure S21. Photoluminescence of powders at 295 K (solid lines) and 80 K (dashed lines). Excitation at 300 nm.

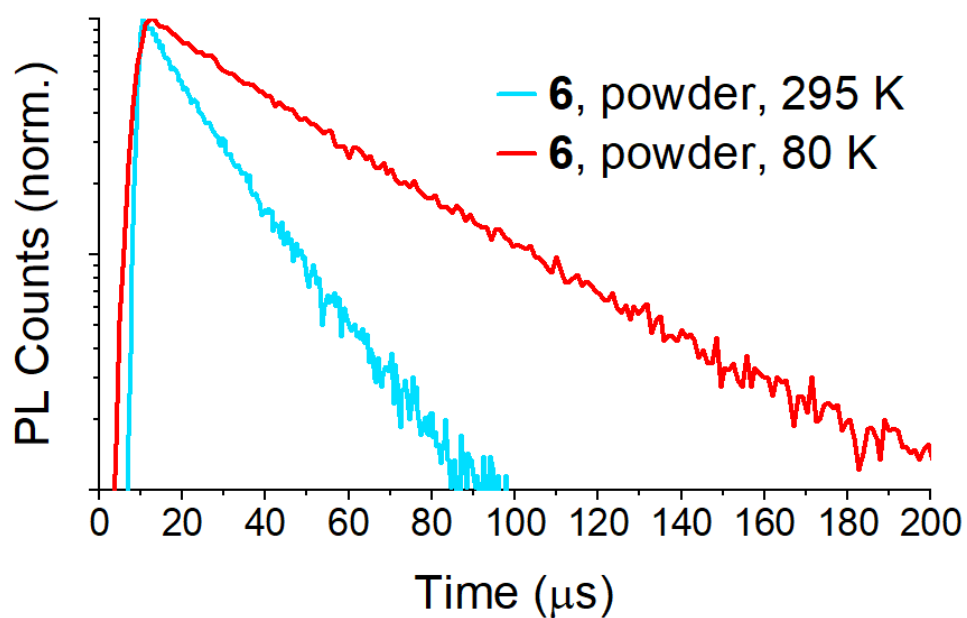


Figure S22. Photoluminescence lifetime of **6** powder sample at 295 K (blue) and 80 K (red).

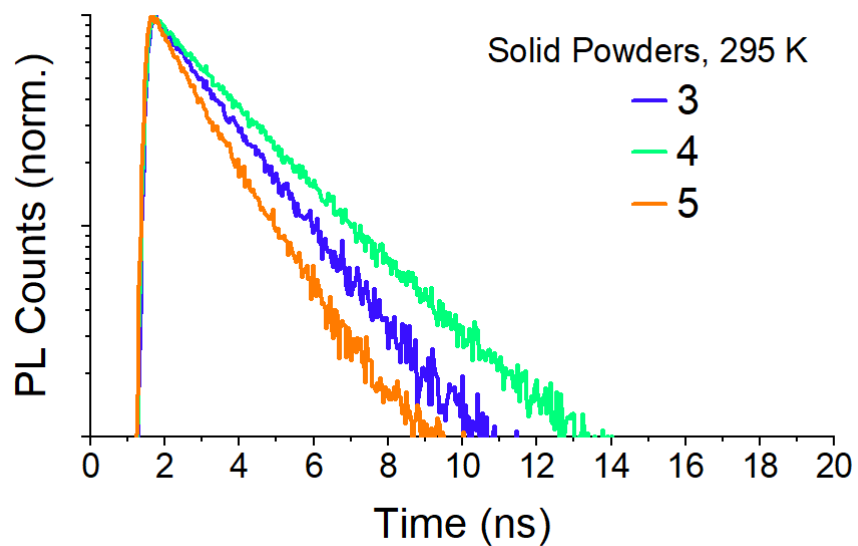


Figure S23. 295 K time-resolved photoluminescence of powder samples.

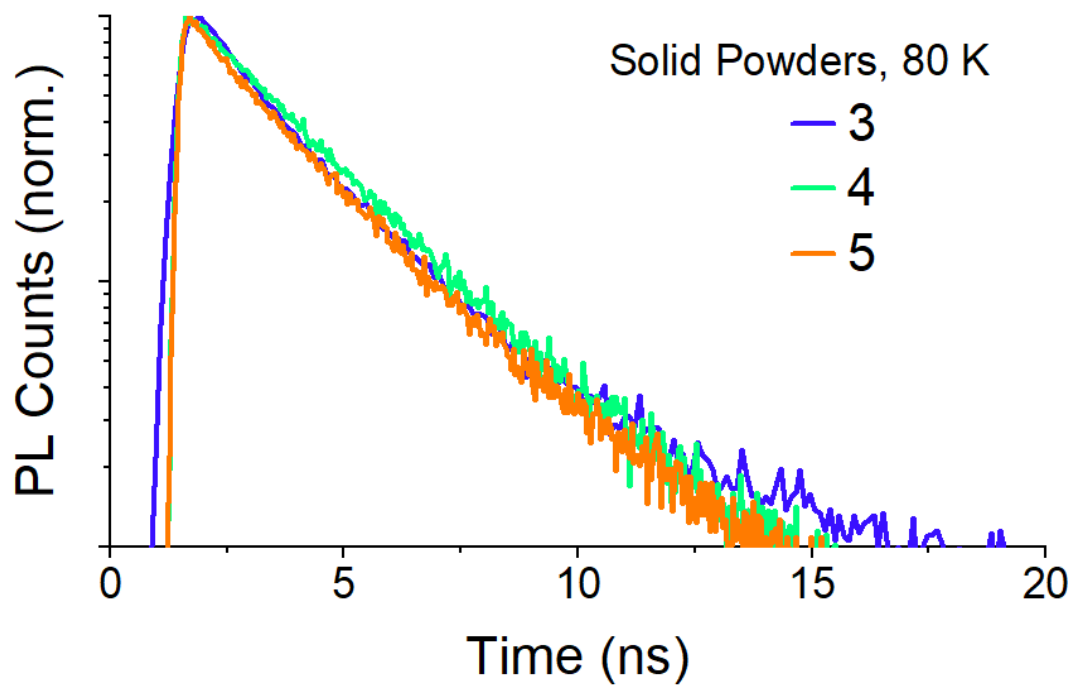


Figure S24. 80 K time-resolved photoluminescence of powder samples

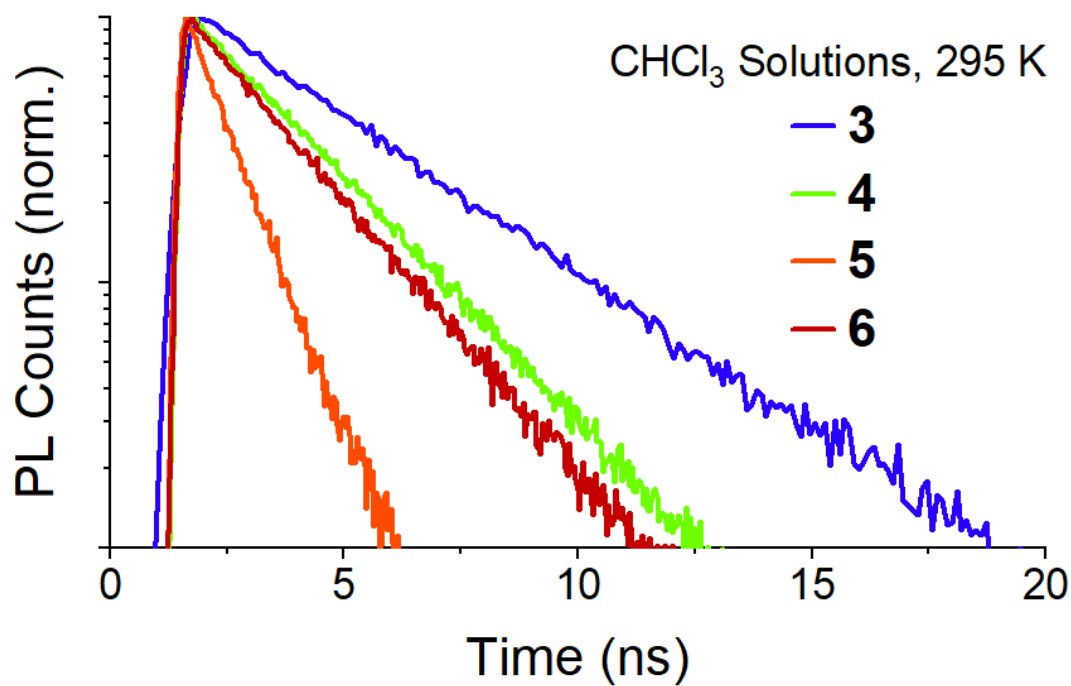


Figure S25. 295K time-resolved photoluminescence of solution samples

4. Computational Details

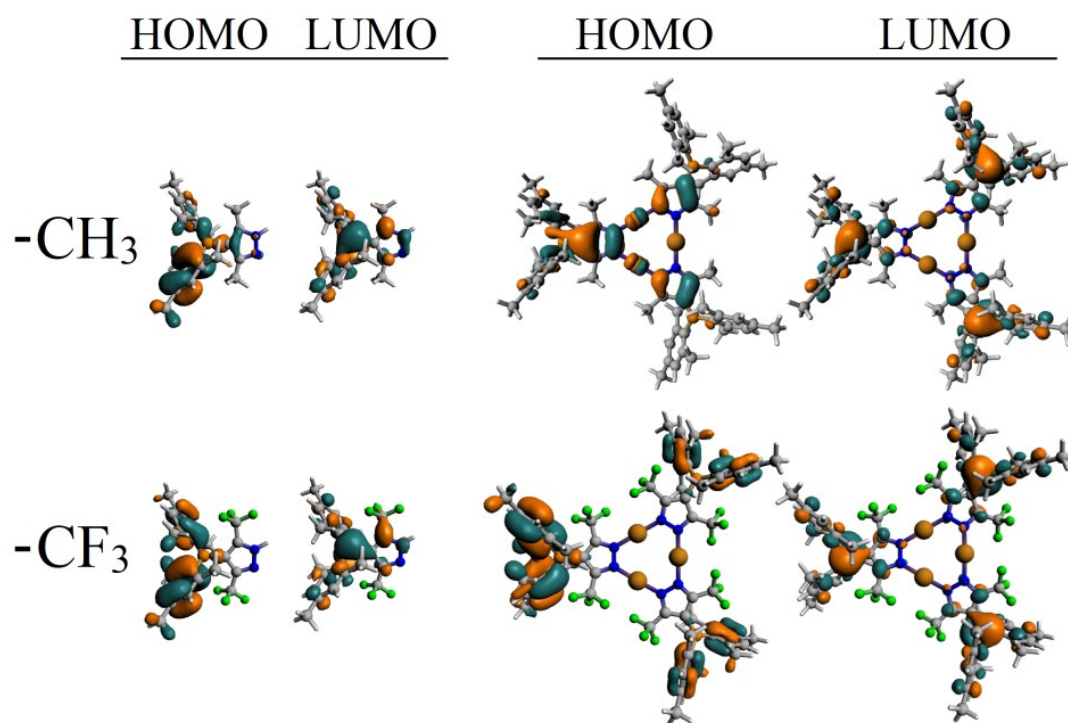


Figure S26. HOMO and LUMO isosurfaces, related to the radiative $T_1 \rightarrow S_0$ decay in both, isolated ligands **4** and **3** and trinuclear copper complexes **6** and **5**.

Table S8. HOMO-LUMO gap for the studied species. Values in eV.

4-BMes ₂ -3,5-(CH ₃) ₂ PzH (4)	3.172
4-BMes ₂ -3,5-(CF ₃) ₂ PzH (3)	2.762
{4-BMes ₂ -3,5-(CH ₃) ₂ Pz}Cu} ₃ (6)	2.876
{4-BMes ₂ -3,5-(CF ₃) ₂ Pz}Cu} ₃ (5)	2.815
[{4-BMes ₂ -3,5-(CH ₃) ₂ Pz}Cu} ₃] ₂	2.638
[{4-BMes ₂ -3,5-(CF ₃) ₂ Pz}Cu} ₃] ₂	2.708

Table S9. Energy decomposition analysis for the {4-BMes₂-3,5-(CH₃)₂Pz}Cu} ₃ (**6**) and {4-BMes₂-3,5-(CF₃)₂Pz}Cu} ₃ (**5**) interaction leading to the related dimer formation. Values in kcal/mol.

	Dimer of 6		Dimer of 5	
ΔE_{Pauli}	66.4		145.8	
ΔE_{elstat}	-49.0	29.6%	-82.3	37.0%
ΔE_{orb}	-33.1	20.0%	-42.2	19.0%
ΔE_{disp}	-83.5	50.4%	-97.6	43.9%
ΔE_{int}	-99.2		-76.3	

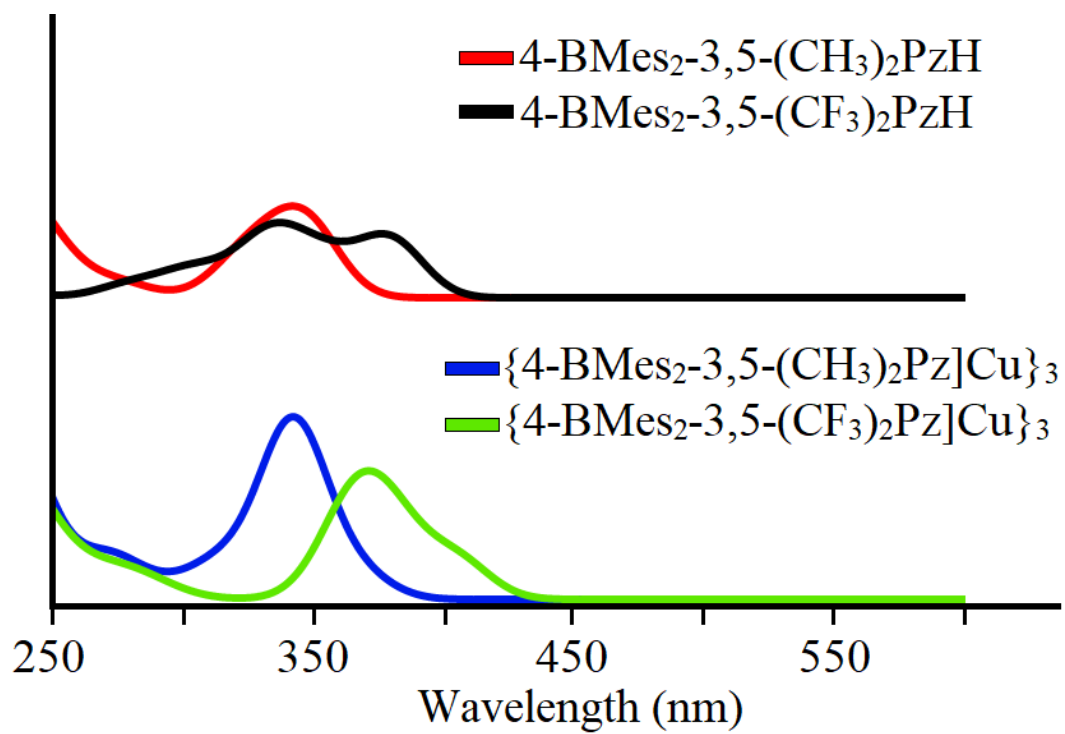


Figure S27. Calculated absorption spectrum for isolated ligands and related trinuclear copper complexes

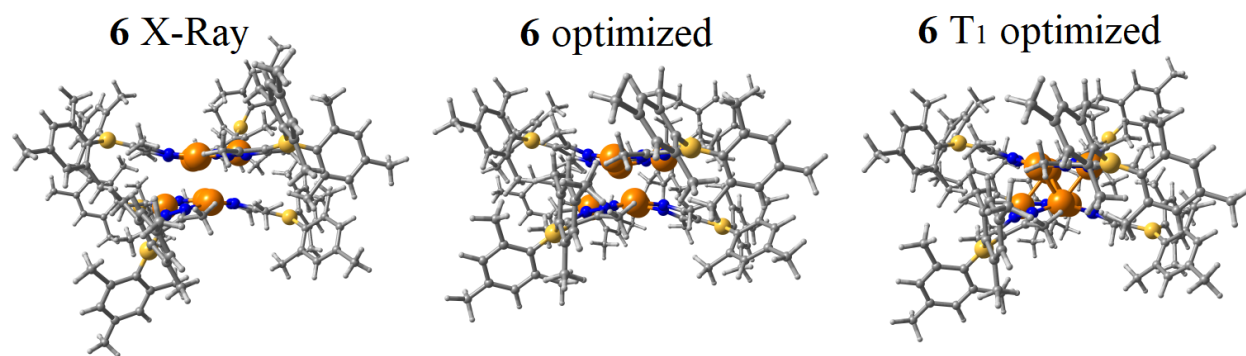


Figure S28. Comparison between X-Ray structure and optimized ground and T₁ state for **6**.

Table S10. Coordinates for optimized structures, in multiXYZ format. Values in Angstroms.

55			
CF3-Lig			
N	6.848005000	1.700480000	-7.881294000
N	7.723960000	0.857587000	-7.328941000
C	7.612816000	2.557615000	-8.564375000
C	9.012051000	2.264518000	-8.482063000
C	9.014085000	1.133529000	-7.663133000
C	6.929211000	3.646781000	-9.343464000
F	7.392274000	3.686837000	-10.627678000
F	5.591042000	3.467492000	-9.401341000
F	7.147034000	4.873543000	-8.805640000
C	10.120740000	0.288250000	-7.114723000
F	11.135372000	1.028777000	-6.611286000
F	9.646678000	-0.488509000	-6.082819000
F	10.644096000	-0.560786000	-8.024955000
C	10.290841000	4.579980000	-9.041395000
C	10.047086000	5.286443000	-7.833095000
C	10.101667000	6.679796000	-7.818580000
H	9.937807000	7.202852000	-6.872347000
C	10.346814000	7.424010000	-8.976302000
C	10.574971000	6.725997000	-10.162902000
H	10.766349000	7.286297000	-11.081875000
C	10.575314000	5.329332000	-10.213447000
C	9.751130000	4.584979000	-6.526460000
H	8.698438000	4.267293000	-6.478509000
H	10.367958000	3.689906000	-6.375587000
H	9.926796000	5.260691000	-5.679092000
C	10.348790000	8.929375000	-8.938158000
H	11.020289000	9.306935000	-8.153915000
H	10.665085000	9.356831000	-9.897752000
H	9.342918000	9.314500000	-8.713161000
C	10.845371000	4.666911000	-11.544527000
H	10.030297000	3.989553000	-11.834629000
H	10.952629000	5.419407000	-12.335210000
H	11.764300000	4.067185000	-11.514873000
C	11.433572000	2.167317000	-9.695353000
C	11.220501000	1.148739000	-10.659040000
C	12.297349000	0.388583000	-11.129533000
H	12.108665000	-0.384430000	-11.880880000
C	13.597763000	0.587069000	-10.671180000
C	13.806519000	1.596217000	-9.724147000
H	14.815676000	1.763320000	-9.338130000
C	12.768259000	2.395333000	-9.247669000
C	9.874417000	0.893175000	-11.293376000
H	9.690297000	-0.184309000	-11.401583000
H	9.044723000	1.328929000	-10.728892000
H	9.843246000	1.328262000	-12.304687000
C	14.747294000	-0.237166000	-11.188814000
H	15.463924000	-0.469447000	-10.389920000
H	14.398777000	-1.180687000	-11.627663000
H	15.298863000	0.308109000	-11.970364000
C	13.108421000	3.454559000	-8.224593000
H	14.170844000	3.400623000	-7.955382000
H	12.900363000	4.463796000	-8.603241000
H	12.523140000	3.335622000	-7.301680000
B	10.256606000	3.015425000	-9.096454000
H	7.395158000	0.118941000	-6.718155000
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CF3-Lig-T1			
N	6.721513000	1.832450000	-7.988616000
N	7.511832000	0.871582000	-7.500575000

C	7.565987000	2.683758000	-8.582187000
C	8.946648000	2.282815000	-8.501967000
C	8.837492000	1.084015000	-7.770951000
C	6.990181000	3.868016000	-9.294790000
F	7.476817000	3.967121000	-10.567585000
F	5.640698000	3.789083000	-9.391899000
F	7.268262000	5.050465000	-8.679537000
C	9.865947000	0.164306000	-7.224437000
F	10.926857000	0.814047000	-6.688036000
F	9.315834000	-0.611987000	-6.231256000
F	10.368884000	-0.707350000	-8.149052000
C	10.371525000	4.539633000	-9.042669000
C	10.157706000	5.258092000	-7.806988000
C	10.108403000	6.643426000	-7.818100000
H	9.889626000	7.173622000	-6.888192000
C	10.345135000	7.384339000	-8.988896000
C	10.657695000	6.680913000	-10.169747000
H	10.857264000	7.246933000	-11.081923000
C	10.716196000	5.293761000	-10.210861000
C	9.907322000	4.524021000	-6.521871000
H	8.892301000	4.097054000	-6.508622000
H	10.590468000	3.672352000	-6.400599000
H	10.002211000	5.192681000	-5.658089000
C	10.263380000	8.883040000	-8.974927000
H	10.724834000	9.304030000	-8.071254000
H	10.744478000	9.325212000	-9.855283000
H	9.210140000	9.208102000	-8.973939000
C	11.058122000	4.612541000	-11.507153000
H	10.381107000	3.762279000	-11.678118000
H	10.976154000	5.307178000	-12.351654000
H	12.078623000	4.201657000	-11.499462000
C	11.447805000	2.183630000	-9.642690000
C	11.232879000	1.161954000	-10.643941000
C	12.292377000	0.358675000	-11.057690000
H	12.100562000	-0.439230000	-11.779570000
C	13.599345000	0.572451000	-10.611442000
C	13.823441000	1.641602000	-9.712826000
H	14.840349000	1.824214000	-9.360090000
C	12.799668000	2.455844000	-9.254132000
C	9.868206000	0.907948000	-11.213093000
H	9.282607000	0.250070000	-10.548926000
H	9.285793000	1.835105000	-11.307513000
H	9.935236000	0.413715000	-12.190039000
C	14.748496000	-0.262876000	-11.095974000
H	15.346421000	-0.638079000	-10.252506000
H	14.406382000	-1.121227000	-11.684289000
H	15.431952000	0.330185000	-11.724470000
C	13.139355000	3.559028000	-8.289042000
H	14.143402000	3.420615000	-7.870244000
H	13.106041000	4.546751000	-8.769705000
H	12.417439000	3.584198000	-7.462524000
B	10.213981000	2.969621000	-9.051823000
H	7.105209000	0.108988000	-6.972500000

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CF3-Lig-S1

N	6.753803000	1.650042000	-8.023950000
N	7.595813000	0.721573000	-7.563038000
C	7.550488000	2.580731000	-8.564904000
C	8.953439000	2.267570000	-8.471426000
C	8.911823000	1.030173000	-7.790897000
C	6.893364000	3.726819000	-9.263886000
F	7.241358000	3.783130000	-10.583146000
F	5.536847000	3.659477000	-9.229526000

F	7.238523000	4.937511000	-8.736265000
C	9.976414000	0.136675000	-7.271154000
F	10.981480000	0.791731000	-6.633671000
F	9.462213000	-0.769559000	-6.357882000
F	10.570786000	-0.649784000	-8.220257000
C	10.265491000	4.584766000	-9.013138000
C	10.018315000	5.363573000	-7.823607000
C	10.187420000	6.738788000	-7.852707000
H	10.025800000	7.311882000	-6.936696000
C	10.571970000	7.432222000	-9.026413000
C	10.815373000	6.684531000	-10.188000000
H	11.105278000	7.204822000	-11.104429000
C	10.651276000	5.305034000	-10.210743000
C	9.648447000	4.693899000	-6.530532000
H	8.594988000	4.380110000	-6.527340000
H	10.238296000	3.778637000	-6.384847000
H	9.802778000	5.365674000	-5.677327000
C	10.696236000	8.928901000	-9.023236000
H	11.395004000	9.268628000	-8.243135000
H	11.041872000	9.311767000	-9.990997000
H	9.725066000	9.399246000	-8.800014000
C	10.865428000	4.549134000	-11.481924000
H	9.983571000	3.935412000	-11.720401000
H	11.083725000	5.218807000	-12.322289000
H	11.699134000	3.832150000	-11.373896000
C	11.382599000	2.151082000	-9.601336000
C	11.198675000	1.116244000	-10.572294000
C	12.302354000	0.449930000	-11.089795000
H	12.143986000	-0.308243000	-11.863391000
C	13.620555000	0.724976000	-10.670964000
C	13.811681000	1.735351000	-9.718049000
H	14.820647000	1.958806000	-9.368227000
C	12.738176000	2.421836000	-9.166467000
C	9.840969000	0.771714000	-11.129127000
H	9.469284000	-0.179353000	-10.715477000
H	9.103240000	1.547426000	-10.891381000
H	9.895382000	0.658658000	-12.222877000
C	14.781839000	-0.037473000	-11.238726000
H	15.563064000	-0.199379000	-10.481629000
H	14.467861000	-1.012222000	-11.637672000
H	15.248298000	0.523708000	-12.067332000
C	12.977403000	3.447260000	-8.107936000
H	14.039452000	3.525376000	-7.845143000
H	12.623451000	4.440885000	-8.444788000
H	12.390488000	3.225883000	-7.204264000
B	10.198887000	3.023856000	-9.037492000
H	7.236483000	-0.078026000	-7.058221000

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CH3-Lig

N	6.829245000	1.835854000	-7.865764000
N	7.657338000	0.783400000	-7.611815000
C	7.629076000	2.760119000	-8.395693000
C	8.992389000	2.295550000	-8.507575000
C	8.939743000	0.987637000	-7.981922000
C	7.030428000	4.053189000	-8.849621000
H	7.171215000	4.195277000	-9.931510000
H	5.955024000	4.051153000	-8.631735000
H	7.498767000	4.916423000	-8.358361000
C	9.976886000	-0.068854000	-7.775239000
H	10.922346000	0.368967000	-7.435670000
H	9.644572000	-0.806856000	-7.031584000
H	10.197501000	-0.601145000	-8.712109000
C	10.277055000	4.601476000	-9.081062000

C	10.095834000	5.357138000	-7.894561000
C	10.140995000	6.753155000	-7.937988000
H	10.025020000	7.313098000	-7.004688000
C	10.332959000	7.451108000	-9.133397000
C	10.503574000	6.703819000	-10.299989000
H	10.659017000	7.225282000	-11.249040000
C	10.495828000	5.305189000	-10.291730000
C	9.862734000	4.710475000	-6.545962000
H	8.785357000	4.598348000	-6.340607000
H	10.299797000	3.707310000	-6.476137000
H	10.287890000	5.331726000	-5.744576000
C	10.363651000	8.958491000	-9.153967000
H	11.138591000	9.347835000	-8.477279000
H	10.570080000	9.340675000	-10.162011000
H	9.403419000	9.379997000	-8.820593000
C	10.698373000	4.581151000	-11.603137000
H	9.842767000	3.933950000	-11.846091000
H	10.824517000	5.294230000	-12.428405000
H	11.585873000	3.934030000	-11.565807000
C	11.458764000	2.163720000	-9.583452000
C	11.298268000	1.198203000	-10.606062000
C	12.384557000	0.417042000	-11.017853000
H	12.234014000	-0.314102000	-11.817572000
C	13.647122000	0.542598000	-10.441339000
C	13.805954000	1.500967000	-9.436490000
H	14.785440000	1.621580000	-8.965190000
C	12.752800000	2.316312000	-9.015639000
C	9.990626000	0.992981000	-11.339302000
H	9.671214000	-0.058468000	-11.288391000
H	9.179524000	1.605808000	-10.935351000
H	10.109066000	1.236501000	-12.404453000
C	14.809738000	-0.294351000	-10.912568000
H	15.507166000	-0.509904000	-10.093094000
H	14.470401000	-1.247362000	-11.338325000
H	15.377689000	0.230928000	-11.695367000
C	13.025060000	3.322157000	-7.921890000
H	14.089507000	3.326002000	-7.654502000
H	12.739588000	4.336569000	-8.230182000
H	12.452515000	3.094693000	-7.010436000
B	10.233526000	3.021089000	-9.059050000
H	7.276190000	-0.039790000	-7.162130000

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CH3-Lig-T1

N	6.854418	1.782937	-7.738149
N	7.710533	0.736372	-7.500869
C	7.622431	2.707912	-8.318223
C	9.000259	2.291479	-8.436378
C	8.987023	0.973163	-7.886625
C	7.008648	3.975799	-8.806216
H	7.091238	4.061370	-9.891037
H	5.953273	4.018102	-8.539000
H	7.500936	4.856271	-8.393461
C	10.068333	-0.029078	-7.727203
H	10.991013	0.431460	-7.381889
H	9.787386	-0.815678	-7.028901
H	10.311441	-0.506673	-8.684706
C	10.318880	4.592103	-9.070370
C	10.016881	5.386647	-7.892055
C	9.993941	6.767281	-7.962157
H	9.758349	7.338028	-7.071036
C	10.330105	7.461112	-9.144968
C	10.691212	6.693199	-10.279493
H	10.940676	7.205663	-11.197801

C	10.729170	5.311815	-10.266378
C	9.707813	4.730905	-6.575380
H	8.627498	4.560007	-6.441770
H	10.191291	3.756302	-6.500269
H	10.042099	5.361964	-5.735012
C	10.324677	8.955606	-9.181621
H	10.968519	9.382706	-8.401281
H	10.672344	9.333569	-10.144331
H	9.322438	9.356867	-9.007006
C	11.080389	4.580508	-11.531052
H	10.263664	3.905958	-11.811017
H	11.240648	5.270784	-12.354538
H	11.964420	3.957509	-11.427079
C	11.414678	2.195842	-9.636844
C	11.224172	1.221194	-10.656751
C	12.287065	0.409264	-11.065922
H	12.120866	-0.324624	-11.852762
C	13.568822	0.549266	-10.523849
C	13.755911	1.531277	-9.532529
H	14.729317	1.639344	-9.071612
C	12.724051	2.359675	-9.097985
C	9.886957	1.018002	-11.323154
H	9.533710	-0.010046	-11.219212
H	9.130751	1.678882	-10.906895
H	9.952195	1.218357	-12.400494
C	14.713474	-0.303868	-10.989241
H	15.404764	-0.523514	-10.167490
H	14.362775	-1.254115	-11.398425
H	15.296842	0.193318	-11.774346
C	13.001941	3.343585	-7.985642
H	14.048264	3.333358	-7.686612
H	12.741906	4.362472	-8.264072
H	12.403709	3.100107	-7.099423
B	10.195293	3.034422	-9.045983
H	7.367180	-0.101800	-7.047747

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Cu3CF3

Cu	-0.954570000	1.653363000	0.000000000
N	1.886412000	1.910301000	-0.071189000
N	0.711163000	2.588831000	0.071189000
C	2.887862000	2.819586000	-0.101641000
C	2.382118000	4.125950000	0.000000000
C	0.997903000	3.910755000	0.101641000
C	4.430811000	5.626185000	0.886313000
C	4.427074000	5.238850000	2.248664000
C	5.559753000	5.452599000	3.031000000
H	5.537446000	5.168041000	4.084947000
C	6.723710000	6.012321000	2.503545000
C	6.728249000	6.373583000	1.157635000
H	7.635630000	6.798986000	0.721707000
C	5.605228000	6.209012000	0.348055000
C	3.211022000	4.644300000	2.913038000
H	3.038472000	3.607306000	2.583838000
H	2.293921000	5.211996000	2.690931000
H	3.340981000	4.633597000	4.004029000
C	7.926833000	6.239186000	3.370056000
H	7.798186000	7.150817000	3.970517000
H	8.836069000	6.359679000	2.766119000
H	8.077235000	5.401092000	4.064010000
C	5.705525000	6.644588000	-1.091587000
H	5.197029000	5.952543000	-1.774131000
H	6.759946000	6.705523000	-1.395494000
H	5.250785000	7.636186000	-1.242783000

C	2.657013000	6.650287000	-0.886313000
C	2.323440000	6.453383000	-2.248664000
C	1.942212000	7.541187000	-3.031000000
H	1.706932000	7.379589000	-4.084947000
C	1.844968000	8.829064000	-2.503545000
C	2.155560000	9.013627000	-1.157635000
H	2.070279000	10.012142000	-0.721707000
C	2.574548000	7.958776000	-0.348055000
C	2.416571000	5.102977000	-2.913038000
H	1.604783000	4.435047000	-2.583838000
H	3.366760000	4.592592000	-2.690931000
H	2.342322000	5.210173000	-4.004029000
C	1.439878000	9.984431000	-3.370056000
H	1.089610000	10.832100000	-2.766119000
H	0.638866000	9.695637000	-4.064010000
H	2.293696000	10.328836000	-3.970517000
C	2.901620000	8.263424000	1.091587000
H	2.427180000	9.207046000	1.395494000
H	3.987738000	8.365406000	1.242783000
H	2.556539000	7.477030000	1.774131000
B	3.160488000	5.474127000	0.000000000
Cu	-0.954570000	-1.653363000	0.000000000
N	-2.597575000	0.678530000	-0.071189000
N	-2.597575000	-0.678530000	0.071189000
C	-3.885764000	1.091168000	-0.101641000
C	-4.764236000	0.000000000	0.000000000
C	-3.885764000	-1.091168000	0.101641000
C	-7.087824000	1.024102000	0.886313000
C	-6.750514000	1.214534000	2.248664000
C	-7.501965000	2.088588000	3.031000000
H	-7.244377000	2.211548000	4.084947000
C	-8.568678000	2.816743000	2.503545000
C	-8.883810000	2.640043000	1.157635000
H	-9.705909000	3.213157000	0.721707000
C	-8.179776000	1.749764000	0.348055000
C	-5.627593000	0.458677000	2.913038000
H	-4.643255000	0.827741000	2.583838000
H	-5.660681000	-0.619404000	2.690931000
H	-5.683303000	0.576576000	4.004029000
C	-9.366710000	3.745245000	3.370056000
H	-10.091882000	3.178019000	3.970517000
H	-9.925678000	4.472420000	2.766119000
H	-8.716100000	4.294545000	4.064010000
C	-8.607145000	1.618836000	-1.091587000
H	-7.753567000	1.524487000	-1.774131000
H	-9.187126000	2.501523000	-1.395494000
H	-9.238523000	0.729220000	-1.242783000
C	-7.087824000	-1.024102000	-0.886313000
C	-6.750514000	-1.214534000	-2.248664000
C	-7.501965000	-2.088588000	-3.031000000
H	-7.244377000	-2.211548000	-4.084947000
C	-8.568678000	-2.816743000	-2.503545000
C	-8.883810000	-2.640043000	-1.157635000
H	-9.705909000	-3.213157000	-0.721707000
C	-8.179776000	-1.749764000	-0.348055000
C	-5.627593000	-0.458677000	-2.913038000
H	-4.643255000	-0.827741000	-2.583838000
H	-5.660681000	0.619404000	-2.690931000
H	-5.683303000	-0.576576000	-4.004029000
C	-9.366710000	-3.745245000	-3.370056000
H	-9.925678000	-4.472420000	-2.766119000
H	-8.716100000	-4.294545000	-4.064010000
H	-10.091882000	-3.178019000	-3.970517000

C	-8.607145000	-1.618836000	1.091587000
H	-9.187126000	-2.501523000	1.395494000
H	-9.238523000	-0.729220000	1.242783000
H	-7.753567000	-1.524487000	1.774131000
B	-6.320977000	0.000000000	0.000000000
Cu	1.909140000	0.000000000	0.000000000
N	0.711163000	-2.588831000	-0.071189000
N	1.886412000	-1.910301000	0.071189000
C	0.997903000	-3.910755000	-0.101641000
C	2.382118000	-4.125950000	0.000000000
C	2.887862000	-2.819586000	0.101641000
C	2.657013000	-6.650287000	0.886313000
C	2.323440000	-6.453383000	2.248664000
C	1.942212000	-7.541187000	3.031000000
H	1.706932000	-7.379589000	4.084947000
C	1.844968000	-8.829064000	2.503545000
C	2.155560000	-9.013627000	1.157635000
H	2.070279000	-10.012142000	0.721707000
C	2.574548000	-7.958776000	0.348055000
C	2.416571000	-5.102977000	2.913038000
H	1.604783000	-4.435047000	2.583838000
H	3.366760000	-4.592592000	2.690931000
H	2.342322000	-5.210173000	4.004029000
C	1.439878000	-9.984431000	3.370056000
H	2.293696000	-10.328836000	3.970517000
H	1.089610000	-10.832100000	2.766119000
H	0.638866000	-9.695637000	4.064010000
C	2.901620000	-8.263424000	-1.091587000
H	2.556539000	-7.477030000	-1.774131000
H	2.427180000	-9.207046000	-1.395494000
H	3.987738000	-8.365406000	-1.242783000
C	4.430811000	-5.626185000	-0.886313000
C	4.427074000	-5.238850000	-2.248664000
C	5.559753000	-5.452599000	-3.031000000
H	5.537446000	-5.168041000	-4.084947000
C	6.723710000	-6.012321000	-2.503545000
C	6.728249000	-6.373583000	-1.157635000
H	7.635630000	-6.798986000	-0.721707000
C	5.605228000	-6.209012000	-0.348055000
C	3.211022000	-4.644300000	-2.913038000
H	3.038472000	-3.607306000	-2.583838000
H	2.293921000	-5.211996000	-2.690931000
H	3.340981000	-4.633597000	-4.004029000
C	7.926833000	-6.239186000	-3.370056000
H	8.836069000	-6.359679000	-2.766119000
H	8.077235000	-5.401092000	-4.064010000
H	7.798186000	-7.150817000	-3.970517000
C	5.705525000	-6.644588000	1.091587000
H	6.759946000	-6.705523000	1.395494000
H	5.250785000	-7.636186000	1.242783000
H	5.197029000	-5.952543000	1.774131000
B	3.160488000	-5.474127000	0.000000000
C	4.308931000	-2.378325000	0.252345000
F	5.027335000	-3.258642000	0.992219000
F	4.936143000	-2.236207000	-0.946199000
F	4.383421000	-1.165959000	0.883706000
C	-0.094776000	-4.920806000	-0.252345000
F	-0.531459000	-5.392929000	0.946199000
F	-1.181960000	-4.379134000	-0.883706000
F	0.308399000	-5.983121000	-0.992219000
C	-4.214155000	-2.542481000	0.252345000
F	-5.335734000	-2.724479000	0.992219000
F	-4.404684000	-3.156722000	-0.946199000

F	-3.201461000	-3.213174000	0.883706000
C	-4.214155000	2.542481000	-0.252345000
F	-5.335734000	2.724479000	-0.992219000
F	-4.404684000	3.156722000	0.946199000
F	-3.201461000	3.213174000	-0.883706000
C	-0.094776000	4.920806000	0.252345000
F	-0.531459000	5.392929000	-0.946199000
F	-1.181960000	4.379134000	0.883706000
F	0.308399000	5.983121000	0.992219000
C	4.308931000	2.378325000	-0.252345000
F	4.383421000	1.165959000	-0.883706000
F	5.027335000	3.258642000	-0.992219000
F	4.936143000	2.236207000	0.946199000

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Cu3CF3-T1

Cu	-0.945634000	1.637886000	0.000000000
N	1.877914000	1.899678000	-0.076573000
N	0.706213000	2.576160000	0.076573000
C	2.880283000	2.807765000	-0.117103000
C	2.377326000	4.117649000	0.000000000
C	0.991455000	3.898281000	0.117103000
C	4.457187000	5.577855000	0.843026000
C	4.513968000	5.120533000	2.185199000
C	5.683005000	5.282672000	2.920480000
H	5.704607000	4.950700000	3.961137000
C	6.833139000	5.866548000	2.372348000
C	6.779017000	6.308561000	1.052799000
H	7.667514000	6.757053000	0.603392000
C	5.623822000	6.179375000	0.285209000
C	3.318892000	4.517086000	2.875056000
H	3.173996000	3.465412000	2.581004000
H	2.391145000	5.051885000	2.628550000
H	3.451381000	4.545980000	3.965669000
C	8.082445000	5.993112000	3.189466000
H	7.883476000	6.527559000	4.131045000
H	8.865149000	6.535559000	2.643606000
H	8.475247000	4.998091000	3.452640000
C	5.646017000	6.664662000	-1.133768000
H	5.258764000	5.903571000	-1.827324000
H	6.667754000	6.927944000	-1.441038000
H	5.008683000	7.557020000	-1.262857000
C	2.601971000	6.648965000	-0.843026000
C	2.177528000	6.469477000	-2.185199000
C	1.733425000	7.562963000	-2.920480000
H	1.435128000	7.415684000	-3.961137000
C	1.664010000	8.850946000	-2.372348000
C	2.073865000	9.025081000	-1.052799000
H	2.018023000	10.018788000	-0.603392000
C	2.539585000	7.960061000	-0.285209000
C	2.252465000	5.132787000	-2.875056000
H	1.414137000	4.481467000	-2.581004000
H	3.179488000	4.596735000	-2.628550000
H	2.211244000	5.261974000	-3.965669000
C	1.148964000	9.996159000	-3.189466000
H	1.227386000	10.945224000	-2.643606000
H	0.090850000	9.838825000	-3.452640000
H	1.711294000	10.091070000	-4.131045000
C	2.948758000	8.221926000	1.133768000
H	2.665898000	9.238416000	1.441038000
H	4.040230000	8.116156000	1.262857000
H	2.483261000	7.506009000	1.827324000
B	3.154334000	5.463466000	0.000000000
Cu	-0.945634000	-1.637886000	0.000000000

N	-2.584126000	0.676482000	-0.076573000
N	-2.584126000	-0.676482000	0.076573000
C	-3.871738000	1.090515000	-0.117103000
C	-4.754651000	0.000000000	0.000000000
C	-3.871738000	-1.090515000	0.117103000
C	-7.059158000	1.071109000	0.843026000
C	-6.691496000	1.348944000	2.185199000
C	-7.416430000	2.280291000	2.920480000
H	-7.139735000	2.464984000	3.961137000
C	-8.497149000	2.984398000	2.372348000
C	-8.852882000	2.716521000	1.052799000
H	-9.685536000	3.261735000	0.603392000
C	-8.163407000	1.780685000	0.285209000
C	-5.571357000	0.615702000	2.875056000
H	-4.588133000	1.016055000	2.581004000
H	-5.570633000	-0.455150000	2.628550000
H	-5.662625000	0.715993000	3.965669000
C	-9.231410000	4.003047000	3.189466000
H	-9.594770000	3.563511000	4.131045000
H	-10.092535000	4.409665000	2.643606000
H	-8.566098000	4.840734000	3.452640000
C	-8.594776000	1.557263000	-1.133768000
H	-7.742025000	1.602438000	-1.827324000
H	-9.333652000	2.310472000	-1.441038000
H	-9.048913000	0.559137000	-1.262857000
C	-7.059158000	-1.071109000	-0.843026000
C	-6.691496000	-1.348944000	-2.185199000
C	-7.416430000	-2.280291000	-2.920480000
H	-7.139735000	-2.464984000	-3.961137000
C	-8.497149000	-2.984398000	-2.372348000
C	-8.852882000	-2.716521000	-1.052799000
H	-9.685536000	-3.261735000	-0.603392000
C	-8.163407000	-1.780685000	-0.285209000
C	-5.571357000	-0.615702000	-2.875056000
H	-4.588133000	-1.016055000	-2.581004000
H	-5.570633000	0.455150000	-2.628550000
H	-5.662625000	-0.715993000	-3.965669000
C	-9.231410000	-4.003047000	-3.189466000
H	-10.092535000	-4.409665000	-2.643606000
H	-8.566098000	-4.840734000	-3.452640000
H	-9.594770000	-3.563511000	-4.131045000
C	-8.594776000	-1.557263000	1.133768000
H	-9.333652000	-2.310472000	1.441038000
H	-9.048913000	-0.559137000	1.262857000
H	-7.742025000	-1.602438000	1.827324000
B	-6.308667000	0.000000000	0.000000000
Cu	1.891268000	0.000000000	0.000000000
N	0.706213000	-2.576160000	-0.076573000
N	1.877914000	-1.899678000	0.076573000
C	0.991455000	-3.898281000	-0.117103000
C	2.377326000	-4.117649000	0.000000000
C	2.880283000	-2.807765000	0.117103000
C	2.601971000	-6.648965000	0.843026000
C	2.177528000	-6.469477000	2.185199000
C	1.733425000	-7.562963000	2.920480000
H	1.435128000	-7.415684000	3.961137000
C	1.664010000	-8.850946000	2.372348000
C	2.073865000	-9.025081000	1.052799000
H	2.018023000	-10.018788000	0.603392000
C	2.539585000	-7.960061000	0.285209000
C	2.252465000	-5.132787000	2.875056000
H	1.414137000	-4.481467000	2.581004000
H	3.179488000	-4.596735000	2.628550000

H	2.211244000	-5.261974000	3.965669000
C	1.148964000	-9.996159000	3.189466000
H	1.711294000	-10.091070000	4.131045000
H	1.227386000	-10.945224000	2.643606000
H	0.090850000	-9.838825000	3.452640000
C	2.948758000	-8.221926000	-1.133768000
H	2.483261000	-7.506009000	-1.827324000
H	2.665898000	-9.238416000	-1.441038000
H	4.040230000	-8.116156000	-1.262857000
C	4.457187000	-5.577855000	-0.843026000
C	4.513968000	-5.120533000	-2.185199000
C	5.683005000	-5.282672000	-2.920480000
H	5.704607000	-4.950700000	-3.961137000
C	6.833139000	-5.866548000	-2.372348000
C	6.779017000	-6.308561000	-1.052799000
H	7.667514000	-6.757053000	-0.603392000
C	5.623822000	-6.179375000	-0.285209000
C	3.318892000	-4.517086000	-2.875056000
H	3.173996000	-3.465412000	-2.581004000
H	2.391145000	-5.051885000	-2.628550000
H	3.451381000	-4.545980000	-3.965669000
C	8.082445000	-5.993112000	-3.189466000
H	8.865149000	-6.535559000	-2.643606000
H	8.475247000	-4.998091000	-3.452640000
H	7.883476000	-6.527559000	-4.131045000
C	5.646017000	-6.664662000	1.133768000
H	6.667754000	-6.927944000	1.441038000
H	5.008683000	-7.557020000	1.262857000
H	5.258764000	-5.903571000	1.827324000
B	3.154334000	-5.463466000	0.000000000
C	4.289450000	-2.351199000	0.299882000
F	5.015425000	-3.235446000	1.029878000
F	4.936510000	-2.169394000	-0.885644000
F	4.339801000	-1.150434000	0.957968000
C	-0.108527000	-4.890372000	-0.299882000
F	-0.589505000	-5.359840000	0.885644000
F	-1.173596000	-4.333595000	-0.957968000
F	0.294266000	-5.961208000	-1.029878000
C	-4.180923000	-2.539173000	0.299882000
F	-5.309690000	-2.725762000	1.029878000
F	-4.347005000	-3.190447000	-0.885644000
F	-3.166205000	-3.183161000	0.957968000
C	-4.180923000	2.539173000	-0.299882000
F	-5.309690000	2.725762000	-1.029878000
F	-4.347005000	3.190447000	0.885644000
F	-3.166205000	3.183161000	-0.957968000
C	-0.108527000	4.890372000	0.299882000
F	-0.589505000	5.359840000	-0.885644000
F	-1.173596000	4.333595000	0.957968000
F	0.294266000	5.961208000	1.029878000
C	4.289450000	2.351199000	-0.299882000
F	4.339801000	1.150434000	-0.957968000
F	5.015425000	3.235446000	-1.029878000
F	4.936510000	2.169394000	0.885644000

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Cu₃CH₃

Cu	-1.878310000	0.000000000	0.000000000
N	-0.688773000	-2.579510000	-0.003585000
N	-1.889535000	-1.886251000	0.003585000
C	-0.955497000	-3.893119000	-0.019864000
C	-2.361783000	-4.090727000	0.000000000
C	-2.893792000	-2.774044000	0.019864000
C	0.160830000	-4.875746000	0.054370000

H	0.448096000	-5.048008000	1.105543000
H	1.045651000	-4.494508000	-0.478584000
H	-0.122488000	-5.844951000	-0.375382000
C	-2.483213000	-6.688540000	-0.643293000
C	-1.978968000	-6.660166000	-1.964466000
C	-1.440508000	-7.816551000	-2.528656000
H	-1.072493000	-7.782413000	-3.557270000
C	-1.353713000	-9.012052000	-1.815233000
C	-1.844550000	-9.032158000	-0.510778000
H	-1.784097000	-9.957215000	0.066987000
C	-2.420513000	-7.903928000	0.075432000
C	-2.005619000	-5.412586000	-2.811721000
H	-1.113677000	-4.790321000	-2.631518000
H	-2.873269000	-4.775704000	-2.597130000
H	-2.021784000	-5.675111000	-3.879701000
C	-0.783260000	-10.248294000	-2.449173000
H	-1.543380000	-10.747206000	-3.072335000
H	-0.448181000	-10.966780000	-1.688672000
H	0.072630000	-10.005885000	-3.095811000
C	-2.946497000	-8.016101000	1.482936000
H	-2.560111000	-7.213055000	2.127878000
H	-2.654138000	-8.976142000	1.929644000
H	-4.044751000	-7.943709000	1.504637000
C	-4.550839000	-5.494795000	0.643293000
C	-4.778389000	-5.043920000	1.964466000
C	-6.049078000	-5.155792000	2.528656000
H	-6.203521000	-4.820013000	3.557270000
C	-7.127810000	-5.678376000	1.815233000
C	-6.899803000	-6.113506000	0.510778000
H	-7.731153000	-6.523681000	-0.066987000
C	-5.634746000	-6.048190000	-0.075432000
C	-3.684628000	-4.443210000	2.811721000
H	-3.591701000	-3.359633000	2.631518000
H	-2.699246000	-4.876176000	2.597130000
H	-3.903898000	-4.588472000	3.879701000
C	-8.483652000	-5.802470000	2.449173000
H	-9.273420000	-5.871526000	1.688672000
H	-8.701666000	-4.940043000	3.095811000
H	-8.535663000	-6.710209000	3.072335000
C	-5.468899000	-6.559792000	-1.482936000
H	-6.446498000	-6.786622000	-1.929644000
H	-4.857078000	-7.474711000	-1.504637000
H	-4.966634000	-5.823649000	-2.127878000
B	-3.123269000	-5.409660000	0.000000000
C	-4.302934000	-2.298590000	-0.054370000
H	-4.595751000	-2.135942000	-1.105543000
H	-5.000632000	-3.028553000	0.375382000
H	-4.415184000	-1.341693000	0.478584000
Cu	0.939155000	1.626664000	0.000000000
N	-1.889535000	1.886251000	-0.003585000
N	-0.688773000	2.579510000	0.003585000
C	-2.893792000	2.774044000	-0.019864000
C	-2.361783000	4.090727000	0.000000000
C	-0.955497000	3.893119000	0.019864000
C	-4.302934000	2.298590000	0.054370000
H	-4.595751000	2.135942000	1.105543000
H	-4.415184000	1.341693000	-0.478584000
H	-5.000632000	3.028553000	-0.375382000
C	-4.550839000	5.494795000	-0.643293000
C	-4.778389000	5.043920000	-1.964466000
C	-6.049078000	5.155792000	-2.528656000
H	-6.203521000	4.820013000	-3.557270000
C	-7.127810000	5.678376000	-1.815233000

C	-6.899803000	6.113506000	-0.510778000
H	-7.731153000	6.523681000	0.066987000
C	-5.634746000	6.048190000	0.075432000
C	-3.684628000	4.443210000	-2.811721000
H	-3.591701000	3.359633000	-2.631518000
H	-2.699246000	4.876176000	-2.597130000
H	-3.903898000	4.588472000	-3.879701000
C	-8.483652000	5.802470000	-2.449173000
H	-8.535663000	6.710209000	-3.072335000
H	-9.273420000	5.871526000	-1.688672000
H	-8.701666000	4.940043000	-3.095811000
C	-5.468899000	6.559792000	1.482936000
H	-4.966634000	5.823649000	2.127878000
H	-6.446498000	6.786622000	1.929644000
H	-4.857078000	7.474711000	1.504637000
C	-2.483213000	6.688540000	0.643293000
C	-1.978968000	6.660166000	1.964466000
C	-1.440508000	7.816551000	2.528656000
H	-1.072493000	7.782413000	3.557270000
C	-1.353713000	9.012052000	1.815233000
C	-1.844550000	9.032158000	0.510778000
H	-1.784097000	9.957215000	-0.066987000
C	-2.420513000	7.903928000	-0.075432000
C	-2.005619000	5.412586000	2.811721000
H	-1.113677000	4.790321000	2.631518000
H	-2.873269000	4.775704000	2.597130000
H	-2.021784000	5.675111000	3.879701000
C	-0.783260000	10.248294000	2.449173000
H	-0.448181000	10.966780000	1.688672000
H	0.072630000	10.005885000	3.095811000
H	-1.543380000	10.747206000	3.072335000
C	-2.946497000	8.016101000	-1.482936000
H	-2.654138000	8.976142000	-1.929644000
H	-4.044751000	7.943709000	-1.504637000
H	-2.560111000	7.213055000	-2.127878000
B	-3.123269000	5.409660000	0.000000000
C	0.160830000	4.875746000	-0.054370000
H	0.448096000	5.048008000	-1.105543000
H	-0.122488000	5.844951000	0.375382000
H	1.045651000	4.494508000	0.478584000
Cu	0.939155000	-1.626664000	0.000000000
N	2.578308000	0.693260000	-0.003585000
N	2.578308000	-0.693260000	0.003585000
C	3.849289000	1.119075000	-0.019864000
C	4.723565000	0.000000000	0.000000000
C	3.849289000	-1.119075000	0.019864000
C	4.142105000	2.577156000	0.054370000
H	4.147656000	2.912066000	1.105543000
H	3.369532000	3.152815000	-0.478584000
H	5.123120000	2.816398000	-0.375382000
C	7.034052000	1.193745000	-0.643293000
C	6.757357000	1.616246000	-1.964466000
C	7.489586000	2.660759000	-2.528656000
H	7.276014000	2.962401000	-3.557270000
C	8.481522000	3.333676000	-1.815233000
C	8.744353000	2.918651000	-0.510778000
H	9.515250000	3.433534000	0.066987000
C	8.055259000	1.855738000	0.075432000
C	5.690246000	0.969376000	-2.811721000
H	4.705378000	1.430688000	-2.631518000
H	5.572516000	-0.100472000	-2.597130000
H	5.925682000	1.086639000	-3.879701000
C	9.266913000	4.445823000	-2.449173000

H	10.079043000	4.036997000	-3.072335000
H	9.721601000	5.095254000	-1.688672000
H	8.629035000	5.065842000	-3.095811000
C	8.415396000	1.456310000	1.482936000
H	7.526745000	1.389406000	2.127878000
H	9.100636000	2.189520000	1.929644000
H	8.901829000	0.468997000	1.504637000
C	7.034052000	-1.193745000	0.643293000
C	6.757357000	-1.616246000	1.964466000
C	7.489586000	-2.660759000	2.528656000
H	7.276014000	-2.962401000	3.557270000
C	8.481522000	-3.333676000	1.815233000
C	8.744353000	-2.918651000	0.510778000
H	9.515250000	-3.433534000	-0.066987000
C	8.055259000	-1.855738000	-0.075432000
C	5.690246000	-0.969376000	2.811721000
H	4.705378000	-1.430688000	2.631518000
H	5.572516000	0.100472000	2.597130000
H	5.925682000	-1.086639000	3.879701000
C	9.266913000	-4.445823000	2.449173000
H	9.721601000	-5.095254000	1.688672000
H	8.629035000	-5.065842000	3.095811000
H	10.079043000	-4.036997000	3.072335000
C	8.415396000	-1.456310000	-1.482936000
H	9.100636000	-2.189520000	-1.929644000
H	8.901829000	-0.468997000	-1.504637000
H	7.526745000	-1.389406000	-2.127878000
B	6.246538000	0.000000000	0.000000000
C	4.142105000	-2.577156000	-0.054370000
H	4.147656000	-2.912066000	-1.105543000
H	5.123120000	-2.816398000	0.375382000
H	3.369532000	-3.152815000	0.478584000

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Cu3CH3-T1

Cu	-1.877767000	0.000000000	0.000000000
N	-0.683783000	-2.572694000	0.056331000
N	-1.886127000	-1.878521000	-0.056331000
C	-0.952867000	-3.885958000	0.081225000
C	-2.359987000	-4.087617000	0.000000000
C	-2.888905000	-2.768186000	-0.081225000
C	0.147212000	-4.877969000	0.187622000
H	-0.171495000	-5.759193000	0.761087000
H	1.024806000	-4.426947000	0.675968000
H	0.453307000	-5.239169000	-0.807652000
C	-2.403575000	-6.733936000	-0.437250000
C	-1.689662000	-6.842745000	-1.657981000
C	-1.004332000	-8.017961000	-1.969746000
H	-0.460846000	-8.079208000	-2.916187000
C	-1.007102000	-9.119460000	-1.117369000
C	-1.730946000	-9.020778000	0.074391000
H	-1.738881000	-9.869498000	0.762437000
C	-2.429623000	-7.866560000	0.418677000
C	-1.704829000	-5.752190000	-2.694734000
H	-0.754122000	-5.719925000	-3.248642000
H	-1.898315000	-4.760886000	-2.264418000
H	-2.503730000	-5.949012000	-3.431892000
C	-0.287864000	-10.386416000	-1.478245000
H	-0.974494000	-11.097922000	-1.965774000
H	0.120180000	-10.879771000	-0.584771000
H	0.539793000	-10.191383000	-2.173653000
C	-3.155785000	-7.832287000	1.737256000
H	-2.853929000	-6.956068000	2.330985000
H	-2.937762000	-8.734935000	2.325657000

H	-4.245826000	-7.764197000	1.595794000
C	-4.629973000	-5.448525000	0.437250000
C	-5.081160000	-4.884662000	1.657981000
C	-6.441592000	-4.878758000	1.969746000
H	-6.766376000	-4.438709000	2.916187000
C	-7.394133000	-5.431905000	1.117369000
C	-6.946750000	-6.009432000	-0.074391000
H	-7.677796000	-6.440665000	-0.762437000
C	-5.597830000	-6.037395000	-0.418677000
C	-4.129128000	-4.352520000	2.694734000
H	-4.576540000	-3.513051000	3.248642000
H	-3.173891000	-4.024432000	2.264418000
H	-3.900131000	-5.142800000	3.431892000
C	-8.850968000	-5.442506000	1.478245000
H	-9.482248000	-5.335806000	0.584771000
H	-9.095893000	-4.628217000	2.173653000
H	-9.123835000	-6.392897000	1.965774000
C	-5.205067000	-6.649133000	-1.737256000
H	-6.095794000	-6.911644000	-2.325657000
H	-4.601078000	-7.559092000	-1.595794000
H	-4.597167000	-5.949609000	-2.330985000
B	-3.126351000	-5.415000000	0.000000000
C	-4.298051000	-2.311495000	-0.187622000
H	-4.901860000	-3.028116000	-0.761087000
H	-4.763907000	-2.227009000	0.807652000
H	-4.346252000	-1.325966000	-0.675968000
Cu	0.938884000	1.626194000	0.000000000
N	-1.886127000	1.878521000	0.056331000
N	-0.683783000	2.572694000	-0.056331000
C	-2.888905000	2.768186000	0.081225000
C	-2.359987000	4.087617000	0.000008000
C	-0.952867000	3.885958000	-0.081225000
C	-4.298051000	2.311495000	0.187622000
H	-4.901860000	3.028116000	0.761087000
H	-4.346252000	1.325966000	0.675968000
H	-4.763907000	2.227009000	-0.807652000
C	-4.629973000	5.448525000	-0.437250000
C	-5.081160000	4.884662000	-1.657981000
C	-6.441592000	4.878758000	-1.969746000
H	-6.766376000	4.438709000	-2.916187000
C	-7.394133000	5.431905000	-1.117369000
C	-6.946750000	6.009432000	0.074391000
H	-7.677796000	6.440665000	0.762437000
C	-5.597830000	6.037395000	0.418677000
C	-4.129128000	4.352520000	-2.694734000
H	-4.576540000	3.513051000	-3.248642000
H	-3.173891000	4.024432000	-2.264418000
H	-3.900131000	5.142800000	-3.431892000
C	-8.850968000	5.442506000	-1.478245000
H	-9.123835000	6.392897000	-1.965774000
H	-9.482248000	5.335806000	-0.584771000
H	-9.095893000	4.628217000	-2.173653000
C	-5.205067000	6.649133000	1.737256000
H	-4.597167000	5.949609000	2.330985000
H	-6.095794000	6.911644000	2.325657000
H	-4.601078000	7.559092000	1.595794000
C	-2.403575000	6.733936000	0.437250000
C	-1.689662000	6.842745000	1.657981000
C	-1.004332000	8.017961000	1.969746000
H	-0.460846000	8.079208000	2.916187000
C	-1.007102000	9.119460000	1.117369000
C	-1.730946000	9.020778000	-0.074391000
H	-1.738881000	9.869498000	-0.762437000

C	-2.429623000	7.866560000	-0.418677000
C	-1.704829000	5.752190000	2.694734000
H	-0.754122000	5.719925000	3.248642000
H	-1.898315000	4.760886000	2.264418000
H	-2.503730000	5.949012000	3.431892000
C	-0.287864000	10.386416000	1.478245000
H	0.120180000	10.879771000	0.584771000
H	0.539793000	10.191383000	2.173653000
H	-0.974494000	11.097922000	1.965774000
C	-3.155785000	7.832287000	-1.737256000
H	-2.937762000	8.734935000	-2.325657000
H	-4.245826000	7.764197000	-1.595794000
H	-2.853929000	6.956068000	-2.330985000
B	-3.126351000	5.415000000	0.000000000
C	0.147212000	4.877969000	-0.187622000
H	-0.171495000	5.759193000	-0.761087000
H	0.453307000	5.239169000	0.807652000
H	1.024806000	4.426947000	-0.675968000
Cu	0.938884000	-1.626194000	0.000000000
N	2.569910000	0.694174000	0.056331000
N	2.569910000	-0.694174000	-0.056331000
C	3.841772000	1.117772000	0.081225000
C	4.719974000	0.000000000	0.000000000
C	3.841772000	-1.117772000	-0.081225000
C	4.150839000	2.566474000	0.187622000
H	5.073355000	2.731077000	0.761087000
H	3.321446000	3.100981000	0.675968000
H	4.310600000	3.012159000	-0.807652000
C	7.033547000	1.285411000	-0.437250000
C	6.770822000	1.958083000	-1.657981000
C	7.445924000	3.139203000	-1.969746000
H	7.227222000	3.640499000	-2.916187000
C	8.401234000	3.687554000	-1.117369000
C	8.677696000	3.011346000	0.074391000
H	9.416677000	3.428834000	0.762437000
C	8.027452000	1.829165000	0.418677000
C	5.833957000	1.399670000	-2.694734000
H	5.330661000	2.206874000	-3.248642000
H	5.072206000	0.736454000	-2.264418000
H	6.403861000	0.806212000	-3.431892000
C	9.138832000	4.943910000	-1.478245000
H	10.098329000	4.705025000	-1.965774000
H	9.362068000	5.543965000	-0.584771000
H	8.556100000	5.563166000	-2.173653000
C	8.360852000	1.183153000	1.737256000
H	7.451096000	1.006459000	2.330985000
H	9.033557000	1.823291000	2.325657000
H	8.846905000	0.205105000	1.595794000
C	7.033547000	-1.285411000	0.437250000
C	6.770822000	-1.958083000	1.657981000
C	7.445924000	-3.139203000	1.969746000
H	7.227222000	-3.640499000	2.916187000
C	8.401234000	-3.687554000	1.117369000
C	8.677696000	-3.011346000	-0.074391000
H	9.416677000	-3.428834000	-0.762437000
C	8.027452000	-1.829165000	-0.418677000
C	5.833957000	-1.399670000	2.694734000
H	5.330661000	-2.206874000	3.248642000
H	5.072206000	-0.736454000	2.264418000
H	6.403861000	-0.806212000	3.431892000
C	9.138832000	-4.943910000	1.478245000
H	9.362068000	-5.543965000	0.584771000
H	8.556100000	-5.563166000	2.173653000

H	10.098329000	-4.705025000	1.965774000
C	8.360852000	-1.183153000	-1.737256000
H	9.033557000	-1.823291000	-2.325657000
H	8.846905000	-0.205105000	-1.595794000
H	7.451096000	-1.006459000	-2.330985000
B	6.252703000	0.000000000	0.000000000
C	4.150839000	-2.566474000	-0.187622000
H	5.073355000	-2.731077000	-0.761087000
H	4.310600000	-3.012159000	0.807652000
H	3.321446000	-3.100981000	-0.675968000

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Cu3CF3-Bz-Cu3CF3 dimer S0

Cu	-1.557745000	1.784616000	2.646851000
Cu	-1.108175000	-1.397926000	2.564598000
F	0.195835000	3.622637000	4.341997000
F	1.348293000	3.735079000	2.486034000
F	2.394827000	3.566589000	4.402828000
F	3.459236000	-1.939783000	3.577738000
F	1.674301000	-2.608015000	4.664701000
F	1.687252000	-2.605879000	2.480840000
F	-0.476386000	-4.201252000	2.735192000
F	-1.639368000	-5.972335000	2.188308000
F	-0.827744000	-4.662885000	0.619431000
N	0.101348000	1.064831000	3.243549000
N	0.303515000	-0.275211000	3.199756000
N	-2.589146000	-2.532394000	2.126455000
C	1.268804000	1.652840000	3.593852000
C	2.263178000	0.688209000	3.830219000
C	1.586395000	-0.512555000	3.556233000
C	1.307864000	3.136345000	3.707933000
C	2.104602000	-1.907776000	3.579630000
C	4.045960000	0.058741000	5.722090000
C	5.282133000	-0.628080000	5.838829000
C	5.581671000	-1.306666000	7.018889000
H	6.524855000	-1.850704000	7.086119000
C	4.717138000	-1.306507000	8.111678000
C	3.508324000	-0.621600000	7.995212000
H	2.820762000	-0.604628000	8.842360000
C	3.152215000	0.040807000	6.824367000
C	6.294700000	-0.695606000	4.721733000
H	5.827244000	-0.903127000	3.752537000
H	7.018902000	-1.498005000	4.914685000
H	6.853216000	0.247879000	4.620220000
C	5.076277000	-2.009939000	9.386799000
H	5.320918000	-1.278853000	10.171939000
H	5.946129000	-2.662701000	9.247446000
H	4.237346000	-2.621136000	9.748765000
C	1.829884000	0.767170000	6.811863000
H	1.930332000	1.800832000	6.455866000
H	1.409196000	0.804682000	7.825051000
H	1.099589000	0.260905000	6.164349000
C	4.800257000	1.716687000	3.743704000
C	5.163673000	1.524525000	2.392078000
C	6.294531000	2.158828000	1.882823000
H	6.593284000	1.954924000	0.857116000
C	7.042457000	3.055665000	2.644781000
C	6.642822000	3.292025000	3.959801000
H	7.199817000	4.011500000	4.565975000
C	5.563715000	2.618650000	4.528394000
C	4.407137000	0.583749000	1.491156000
H	4.627026000	0.801074000	0.435996000
H	3.327426000	0.671642000	1.649362000
H	4.691070000	-0.466697000	1.674943000

C	8.213606000	3.784082000	2.051469000
H	7.875322000	4.713578000	1.563520000
H	8.718434000	3.172214000	1.287989000
H	8.945811000	4.059926000	2.825742000
C	5.249150000	2.880780000	5.979103000
H	5.676335000	2.094328000	6.620341000
H	4.168558000	2.906194000	6.170654000
H	5.670881000	3.845808000	6.294678000
C	-2.657434000	-3.862916000	1.894372000
C	-3.989074000	-4.280212000	1.740315000
C	-1.408943000	-4.680167000	1.855376000
C	-5.710756000	-6.285131000	2.228272000
C	-6.785069000	-6.926808000	1.566047000
C	-7.867502000	-7.403903000	2.303049000
H	-8.702117000	-7.871970000	1.779149000
C	-7.910500000	-7.299957000	3.689923000
C	-6.837346000	-6.689413000	4.339157000
H	-6.851384000	-6.608283000	5.426191000
C	-5.751167000	-6.174004000	3.638685000
C	-6.819553000	-7.102157000	0.072376000
H	-6.464635000	-6.210591000	-0.455691000
H	-7.842597000	-7.317217000	-0.261033000
H	-6.174885000	-7.931829000	-0.247069000
C	-9.070521000	-7.842454000	4.473636000
H	-8.764656000	-8.723186000	5.057124000
H	-9.894151000	-8.141339000	3.814761000
H	-9.448144000	-7.089902000	5.178334000
C	-4.622953000	-5.556175000	4.426021000
H	-3.641295000	-5.902703000	4.079253000
H	-4.714258000	-5.815788000	5.487647000
H	-4.630701000	-4.460350000	4.346466000
B	3.705597000	0.840774000	4.417652000
B	-4.526047000	-5.709295000	1.407296000
F	-6.524170000	-1.588362000	1.574540000
F	-6.824916000	-3.710702000	1.075765000
F	-6.703569000	-3.075079000	3.178857000
N	-3.860560000	-2.036281000	2.092256000
C	-4.704295000	-3.080103000	1.901430000
C	-6.182915000	-2.875633000	1.929957000
C	-3.839329000	-6.497746000	0.260891000
C	-3.454340000	-7.843179000	0.458923000
C	-2.774506000	-8.519258000	-0.550511000
H	-2.451588000	-9.545314000	-0.374526000
C	-2.493765000	-7.919424000	-1.775245000
C	-2.916169000	-6.607955000	-1.980509000
H	-2.726679000	-6.129779000	-2.940737000
C	-3.567253000	-5.888053000	-0.986279000
C	-3.727324000	-8.571534000	1.746715000
H	-3.445966000	-7.975404000	2.621507000
H	-3.160422000	-9.509062000	1.781204000
H	-4.794741000	-8.813158000	1.854149000
C	-1.765056000	-8.660397000	-2.855956000
H	-2.435700000	-8.866557000	-3.702817000
H	-1.373680000	-9.614596000	-2.487358000
H	-0.923059000	-8.065404000	-3.234121000
C	-4.032168000	-4.494643000	-1.301509000
H	-5.035215000	-4.301425000	-0.905610000
H	-4.070123000	-4.333588000	-2.384097000
H	-3.360468000	-3.737390000	-0.870635000
Cu	-4.100700000	-0.142785000	1.987240000
F	-1.331369000	4.548401000	1.669749000
F	-2.487548000	5.264886000	3.386444000
F	-2.920109000	6.038180000	1.380720000

F	-7.589018000	2.936070000	1.072229000
F	-6.654712000	1.385821000	-0.164607000
F	-6.989979000	1.031495000	1.970607000
N	-3.204196000	2.537074000	2.056763000
N	-4.277656000	1.747237000	1.783087000
C	-3.571403000	3.823123000	1.849076000
C	-4.898132000	3.901364000	1.399699000
C	-5.290045000	2.555049000	1.383082000
C	-2.586536000	4.920352000	2.071017000
C	-6.627298000	1.983482000	1.058810000
C	-6.313458000	5.189745000	-0.474674000
C	-7.644062000	5.634319000	-0.685728000
C	-8.166325000	5.654256000	-1.979040000
H	-9.198317000	5.978570000	-2.123967000
C	-7.408802000	5.269616000	-3.088976000
C	-6.098811000	4.839823000	-2.877941000
H	-5.488591000	4.541142000	-3.734107000
C	-5.546039000	4.782480000	-1.599908000
C	-8.554514000	6.066883000	0.442773000
H	-8.478843000	5.398600000	1.311323000
H	-9.600491000	6.065026000	0.108216000
H	-8.313949000	7.082121000	0.796106000
C	-7.974486000	5.333360000	-4.479592000
H	-7.556976000	6.197092000	-5.022924000
H	-9.065416000	5.439213000	-4.460657000
H	-7.720148000	4.428767000	-5.050481000
C	-4.109054000	4.339903000	-1.485915000
H	-3.518506000	5.020257000	-0.858240000
H	-3.642077000	4.314430000	-2.477701000
H	-4.029300000	3.331928000	-1.052278000
C	-5.920545000	6.343259000	1.952146000
C	-6.311315000	6.121615000	3.296314000
C	-6.590718000	7.206440000	4.124091000
H	-6.922415000	7.017589000	5.145126000
C	-6.456364000	8.522332000	3.685729000
C	-6.032777000	8.736271000	2.376984000
H	-5.899341000	9.759771000	2.023801000
C	-5.780597000	7.681226000	1.503488000
C	-6.518622000	4.739488000	3.859760000
H	-6.838992000	4.799642000	4.906843000
H	-5.598900000	4.140757000	3.821025000
H	-7.293274000	4.192329000	3.303757000
C	-6.724624000	9.671945000	4.610659000
H	-5.849977000	9.856326000	5.253121000
H	-7.580505000	9.459121000	5.263559000
H	-6.933024000	10.592392000	4.053170000
C	-5.350298000	8.024345000	0.101196000
H	-6.191535000	7.955333000	-0.605655000
H	-4.565111000	7.355391000	-0.266665000
H	-4.962332000	9.051313000	0.068530000
B	-5.716315000	5.163741000	0.961954000
Cu	1.557745000	-1.784616000	-2.646851000
Cu	1.108175000	1.397926000	-2.564598000
F	-0.195835000	-3.622637000	-4.341997000
F	-1.348293000	-3.735079000	-2.486034000
F	-2.394827000	-3.566589000	-4.402828000
F	-3.459236000	1.939783000	-3.577738000
F	-1.674301000	2.608015000	-4.664701000
F	-1.687252000	2.605879000	-2.480840000
F	0.476386000	4.201252000	-2.735192000
F	1.639368000	5.972335000	-2.188308000
F	0.827744000	4.662885000	-0.619431000
N	-0.101348000	-1.064831000	-3.243549000

N	-0.303515000	0.275211000	-3.199756000
N	2.589146000	2.532394000	-2.126455000
C	-1.268804000	-1.652840000	-3.593852000
C	-2.263178000	-0.688209000	-3.830219000
C	-1.586395000	0.512555000	-3.556233000
C	-1.307864000	-3.136345000	-3.707933000
C	-2.104602000	1.907776000	-3.579630000
C	-4.045960000	-0.058741000	-5.722090000
C	-5.282133000	0.628080000	-5.838829000
C	-5.581671000	1.306666000	-7.018889000
H	-6.524855000	1.850704000	-7.086119000
C	-4.717138000	1.306507000	-8.111678000
C	-3.508324000	0.621600000	-7.995212000
H	-2.820762000	0.604628000	-8.842360000
C	-3.152215000	-0.040807000	-6.824367000
C	-6.294700000	0.695606000	-4.721733000
H	-5.827244000	0.903127000	-3.752537000
H	-7.018902000	1.498005000	-4.914685000
H	-6.853216000	-0.247879000	-4.620220000
C	-5.076277000	2.009939000	-9.386799000
H	-5.320918000	1.278853000	-10.171939000
H	-5.946129000	2.662701000	-9.247446000
H	-4.237346000	2.621136000	-9.748765000
C	-1.829884000	-0.767170000	-6.811863000
H	-1.930332000	-1.800832000	-6.455866000
H	-1.409196000	-0.804682000	-7.825051000
H	-1.099589000	-0.260905000	-6.164349000
C	-4.800257000	-1.716687000	-3.743704000
C	-5.163673000	-1.524525000	-2.392078000
C	-6.294531000	-2.158828000	-1.882823000
H	-6.593284000	-1.954924000	-0.857116000
C	-7.042457000	-3.055665000	-2.644781000
C	-6.642822000	-3.292025000	-3.959801000
H	-7.199817000	-4.011500000	-4.565975000
C	-5.563715000	-2.618650000	-4.528394000
C	-4.407137000	-0.583749000	-1.491156000
H	-4.627026000	-0.801074000	-0.435996000
H	-3.327426000	-0.671642000	-1.649362000
H	-4.691070000	0.466697000	-1.674943000
C	-8.213606000	-3.784082000	-2.051469000
H	-7.875322000	-4.713578000	-1.563520000
H	-8.718434000	-3.172214000	-1.287989000
H	-8.945811000	-4.059926000	-2.825742000
C	-5.249150000	-2.880780000	-5.979103000
H	-5.676335000	-2.094328000	-6.620341000
H	-4.168558000	-2.906194000	-6.170654000
H	-5.670881000	-3.845808000	-6.294678000
C	2.657434000	3.862916000	-1.894372000
C	3.989074000	4.280212000	-1.740315000
C	1.408943000	4.680167000	-1.855376000
C	5.710756000	6.285131000	-2.228272000
C	6.785069000	6.926808000	-1.566047000
C	7.867502000	7.403903000	-2.303049000
H	8.702117000	7.871970000	-1.779149000
C	7.910500000	7.299957000	-3.689923000
C	6.837346000	6.689413000	-4.339157000
H	6.851384000	6.608283000	-5.426191000
C	5.751167000	6.174004000	-3.638685000
C	6.819553000	7.102157000	-0.072376000
H	6.464635000	6.210591000	0.455691000
H	7.842597000	7.317217000	0.261033000
H	6.174885000	7.931829000	0.247069000
C	9.070521000	7.842454000	-4.473636000

H	8.764656000	8.723186000	-5.057124000
H	9.894151000	8.141339000	-3.814761000
H	9.448144000	7.089902000	-5.178334000
C	4.622953000	5.556175000	-4.426021000
H	3.641295000	5.902703000	-4.079253000
H	4.714258000	5.815788000	-5.487647000
H	4.630701000	4.460350000	-4.346466000
B	-3.705597000	-0.840774000	-4.417652000
B	4.526047000	5.709295000	-1.407296000
F	6.524170000	1.588362000	-1.574540000
F	6.824916000	3.710702000	-1.075765000
F	6.703569000	3.075079000	-3.178857000
N	3.860560000	2.036281000	-2.092256000
C	4.704295000	3.080103000	-1.901430000
C	6.182915000	2.875633000	-1.929957000
C	3.839329000	6.497746000	-0.260891000
C	3.454340000	7.843179000	-0.458923000
C	2.774506000	8.519258000	0.550511000
H	2.451588000	9.545314000	0.374526000
C	2.493765000	7.919424000	1.775245000
C	2.916169000	6.607955000	1.980509000
H	2.726679000	6.129779000	2.940737000
C	3.567253000	5.888053000	0.986279000
C	3.727324000	8.571534000	-1.746715000
H	3.445966000	7.975404000	-2.621507000
H	3.160422000	9.509062000	-1.781204000
H	4.794741000	8.813158000	-1.854149000
C	1.765056000	8.660397000	2.855956000
H	2.435700000	8.866557000	3.702817000
H	1.373680000	9.614596000	2.487358000
H	0.923059000	8.065404000	3.234121000
C	4.032168000	4.494643000	1.301509000
H	5.035215000	4.301425000	0.905610000
H	4.070123000	4.333588000	2.384097000
H	3.360468000	3.737390000	0.870635000
Cu	4.100700000	0.142785000	-1.987240000
F	1.331369000	-4.548401000	-1.669749000
F	2.487548000	-5.264886000	-3.386444000
F	2.920109000	-6.038180000	-1.380720000
F	7.589018000	-2.936070000	-1.072229000
F	6.654712000	-1.385821000	0.164607000
F	6.989979000	-1.031495000	-1.970607000
N	3.204196000	-2.537074000	-2.056763000
N	4.277656000	-1.747237000	-1.783087000
C	3.571403000	-3.823123000	-1.849076000
C	4.898132000	-3.901364000	-1.399699000
C	5.290045000	-2.555049000	-1.383082000
C	2.586536000	-4.920352000	-2.071017000
C	6.627298000	-1.983482000	-1.058810000
C	6.313458000	-5.189745000	0.474674000
C	7.644062000	-5.634319000	0.685728000
C	8.166325000	-5.654256000	1.979040000
H	9.198317000	-5.978570000	2.123967000
C	7.408802000	-5.269616000	3.088976000
C	6.098811000	-4.839823000	2.877941000
H	5.488591000	-4.541142000	3.734107000
C	5.546039000	-4.782480000	1.599908000
C	8.554514000	-6.066883000	-0.442773000
H	8.478843000	-5.398600000	-1.311323000
H	9.600491000	-6.065026000	-0.108216000
H	8.313949000	-7.082121000	-0.796106000
C	7.974486000	-5.333360000	4.479592000
H	7.556976000	-6.197092000	5.022924000

H	9.065416000	-5.439213000	4.460657000
H	7.720148000	-4.428767000	5.050481000
C	4.109054000	-4.339903000	1.485915000
H	3.518506000	-5.020257000	0.858240000
H	3.642077000	-4.314430000	2.477701000
H	4.029300000	-3.331928000	1.052278000
C	5.920545000	-6.343259000	-1.952146000
C	6.311315000	-6.121615000	-3.296314000
C	6.590718000	-7.206440000	-4.124091000
H	6.922415000	-7.017589000	-5.145126000
C	6.456364000	-8.522332000	-3.685729000
C	6.032777000	-8.736271000	-2.376984000
H	5.899341000	-9.759771000	-2.023801000
C	5.780597000	-7.681226000	-1.503488000
C	6.518622000	-4.739488000	-3.859760000
H	6.838992000	-4.799642000	-4.906843000
H	5.598900000	-4.140757000	-3.821025000
H	7.293274000	-4.192329000	-3.303757000
C	6.724624000	-9.671945000	-4.610659000
H	5.849977000	-9.856326000	-5.253121000
H	7.580505000	-9.459121000	-5.263559000
H	6.933024000	-10.592392000	-4.053170000
C	5.350298000	-8.024345000	-0.101196000
H	6.191535000	-7.955333000	0.605655000
H	4.565111000	-7.355391000	0.266665000
H	4.962332000	-9.051313000	-0.068530000
B	5.716315000	-5.163741000	-0.961954000
C	-0.261425000	1.370792000	0.038894000
H	-0.457111000	2.442872000	0.053727000
C	1.045282000	0.902384000	0.208093000
H	1.851324000	1.611314000	0.388448000
C	1.306003000	-0.468176000	0.170933000
H	2.317782000	-0.841595000	0.319860000
C	0.261425000	-1.370792000	-0.038894000
H	0.457111000	-2.442872000	-0.053727000
C	-1.045282000	-0.902384000	-0.208093000
H	-1.851324000	-1.611314000	-0.388448000
C	-1.306003000	0.468176000	-0.170933000
H	-2.317782000	0.841595000	-0.319860000

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Cu3CF3-Bz-CuCF3 dimer T1

Cu	-1.378271000	1.511069000	2.595227000
Cu	-0.880502000	-1.663941000	2.636538000
F	0.390234000	3.492925000	4.189386000
F	1.583418000	3.375137000	2.358770000
F	2.571947000	3.380227000	4.321945000
F	3.360172000	-2.320775000	4.165341000
F	1.859617000	-2.271690000	5.764109000
F	1.324843000	-3.058564000	3.798195000
F	-0.073779000	-4.256546000	1.799475000
F	-1.263930000	-6.101452000	1.806124000
F	-1.029730000	-4.943661000	-0.038817000
N	0.245843000	0.825187000	3.326625000
N	0.396214000	-0.513310000	3.499752000
N	-2.330951000	-2.741231000	1.973187000
C	1.407613000	1.426978000	3.674402000
C	2.352682000	0.483226000	4.108786000
C	1.635694000	-0.724604000	3.998268000
C	1.497695000	2.912801000	3.635651000
C	2.050448000	-2.086541000	4.430000000
C	4.299866000	-0.061999000	5.864982000
C	5.494179000	-0.827334000	5.873580000
C	5.856760000	-1.516734000	7.031200000

H	6.765142000	-2.122145000	7.019969000
C	5.102164000	-1.449093000	8.200633000
C	3.948458000	-0.664242000	8.194685000
H	3.353874000	-0.582310000	9.107891000
C	3.530480000	0.011164000	7.052015000
C	6.382958000	-0.970649000	4.665838000
H	5.824265000	-1.293880000	3.776171000
H	7.159986000	-1.722363000	4.852987000
H	6.882716000	-0.023895000	4.409733000
C	5.508842000	-2.199857000	9.434565000
H	5.635986000	-1.516198000	10.286919000
H	6.454316000	-2.736287000	9.282278000
H	4.738901000	-2.935788000	9.711723000
C	2.277365000	0.846313000	7.138070000
H	2.400456000	1.828441000	6.659410000
H	2.002977000	1.019143000	8.188982000
H	1.426522000	0.346681000	6.647249000
C	4.866128000	1.484176000	3.737522000
C	5.098708000	1.214884000	2.370732000
C	6.180797000	1.801449000	1.713390000
H	6.363024000	1.554943000	0.666626000
C	7.022111000	2.702608000	2.356731000
C	6.755034000	3.013023000	3.692591000
H	7.385559000	3.744863000	4.203661000
C	5.718142000	2.409487000	4.394532000
C	4.266875000	0.224569000	1.609270000
H	4.339073000	0.417831000	0.528828000
H	3.215783000	0.272562000	1.901019000
H	4.612799000	-0.807209000	1.781752000
C	8.161516000	3.361282000	1.639017000
H	7.979190000	4.441898000	1.535155000
H	8.301894000	2.943516000	0.635254000
H	9.099058000	3.241749000	2.201995000
C	5.530008000	2.768082000	5.845418000
H	5.933899000	1.982754000	6.504512000
H	4.469919000	2.892255000	6.104953000
H	6.048386000	3.708702000	6.078782000
C	-2.424293000	-4.050328000	1.641679000
C	-3.763775000	-4.482006000	1.641023000
C	-1.210113000	-4.841463000	1.303434000
C	-5.450127000	-6.510127000	2.139492000
C	-6.623463000	-7.066221000	1.547465000
C	-7.604702000	-7.644276000	2.348767000
H	-8.502997000	-8.050352000	1.879109000
C	-7.479978000	-7.696500000	3.735547000
C	-6.322095000	-7.158183000	4.315170000
H	-6.200835000	-7.213152000	5.399167000
C	-5.323575000	-6.563764000	3.553670000
C	-6.842945000	-7.005695000	0.065593000
H	-6.714498000	-5.979977000	-0.311216000
H	-7.853237000	-7.351856000	-0.195857000
H	-6.111659000	-7.628420000	-0.479827000
C	-8.555765000	-8.288079000	4.594275000
H	-8.140913000	-9.036212000	5.288166000
H	-9.331814000	-8.772611000	3.986472000
H	-9.038291000	-7.506003000	5.203687000
C	-4.097319000	-6.044424000	4.253965000
H	-3.177473000	-6.350492000	3.736167000
H	-4.054666000	-6.420644000	5.285555000
H	-4.092127000	-4.944302000	4.294768000
B	3.835978000	0.665017000	4.570838000
B	-4.352110000	-5.870634000	1.248223000
F	-6.282600000	-1.823145000	2.169792000

F	-6.652433000	-3.786602000	1.268575000
F	-6.305752000	-3.614321000	3.423447000
N	-3.597591000	-2.269137000	2.166155000
C	-4.453077000	-3.309213000	1.992957000
C	-5.915120000	-3.141957000	2.209110000
C	-3.833347000	-6.524101000	-0.065689000
C	-3.434632000	-7.893426000	-0.089185000
C	-2.980504000	-8.464647000	-1.273537000
H	-2.667118000	-9.510716000	-1.274049000
C	-2.902984000	-7.729368000	-2.458885000
C	-3.318790000	-6.390171000	-2.439245000
H	-3.298694000	-5.812412000	-3.365647000
C	-3.770647000	-5.780973000	-1.277180000
C	-3.489888000	-8.724748000	1.157523000
H	-2.934874000	-8.246912000	1.979054000
H	-3.068044000	-9.723504000	0.985231000
H	-4.527909000	-8.842069000	1.514466000
C	-2.370427000	-8.337893000	-3.718425000
H	-2.975674000	-8.041684000	-4.587323000
H	-2.355512000	-9.434067000	-3.660229000
H	-1.339133000	-7.993110000	-3.902826000
C	-4.281193000	-4.373119000	-1.351521000
H	-5.250899000	-4.279918000	-0.842829000
H	-4.408412000	-4.055022000	-2.394419000
H	-3.601313000	-3.659939000	-0.861478000
Cu	-3.895853000	-0.391726000	1.921198000
F	-1.081597000	4.216387000	1.877105000
F	-2.510584000	5.085711000	3.292053000
F	-2.524948000	5.714439000	1.186150000
F	-7.358208000	2.489142000	1.182373000
F	-6.528901000	1.841956000	-0.731659000
F	-6.506509000	0.474115000	0.971355000
N	-3.013307000	2.274065000	1.954642000
N	-4.065308000	1.490133000	1.589287000
C	-3.336103000	3.559276000	1.686569000
C	-4.608601000	3.646650000	1.109416000
C	-5.014167000	2.301137000	1.057357000
C	-2.372736000	4.649476000	2.007771000
C	-6.341338000	1.778378000	0.607394000
C	-5.969475000	4.848849000	-0.814590000
C	-7.332777000	5.145677000	-1.053543000
C	-7.848325000	5.006181000	-2.339370000
H	-8.907656000	5.211981000	-2.509210000
C	-7.046036000	4.626736000	-3.417750000
C	-5.697430000	4.377444000	-3.181858000
H	-5.053816000	4.105278000	-4.019532000
C	-5.152706000	4.465816000	-1.901394000
C	-8.250604000	5.603377000	0.049385000
H	-8.212623000	4.933788000	0.920300000
H	-9.290070000	5.638931000	-0.304797000
H	-7.976804000	6.607743000	0.408365000
C	-7.618677000	4.519492000	-4.800747000
H	-7.955028000	5.505371000	-5.160324000
H	-8.490088000	3.848078000	-4.815207000
H	-6.870274000	4.137932000	-5.508873000
C	-3.677118000	4.209147000	-1.735261000
H	-3.224849000	4.842780000	-0.962821000
H	-3.146948000	4.405730000	-2.673835000
H	-3.482788000	3.160580000	-1.457676000
C	-5.539786000	6.142349000	1.552418000
C	-5.835023000	5.995660000	2.931600000
C	-6.027382000	7.127340000	3.723582000
H	-6.280527000	6.997534000	4.777532000

C	-5.907570000	8.415618000	3.208761000
C	-5.590596000	8.556321000	1.858108000
H	-5.477937000	9.559288000	1.440914000
C	-5.418158000	7.455745000	1.023075000
C	-6.002789000	4.652685000	3.595303000
H	-6.520812000	4.769238000	4.557765000
H	-5.027683000	4.183395000	3.797147000
H	-6.585483000	3.952854000	2.984931000
C	-6.078951000	9.619236000	4.087746000
H	-5.103470000	9.939347000	4.489812000
H	-6.737401000	9.400915000	4.939942000
H	-6.502104000	10.463996000	3.527747000
C	-5.069921000	7.719292000	-0.418644000
H	-5.899716000	7.468112000	-1.094696000
H	-4.204102000	7.128025000	-0.745848000
H	-4.825336000	8.779930000	-0.559895000
B	-5.380997000	4.912882000	0.621937000
Cu	1.378271000	-1.511069000	-2.595227000
Cu	0.880502000	1.663941000	-2.636538000
F	-0.390234000	-3.492925000	-4.189386000
F	-1.583418000	-3.375137000	-2.358770000
F	-2.571947000	-3.380227000	-4.321945000
F	-3.360172000	2.320775000	-4.165341000
F	-1.859617000	2.271690000	-5.764109000
F	-1.324843000	3.058564000	-3.798195000
F	0.073779000	4.256546000	-1.799475000
F	1.263930000	6.101452000	-1.806124000
F	1.029730000	4.943661000	0.038817000
N	-0.245843000	-0.825187000	-3.326625000
N	-0.396214000	0.513310000	-3.499752000
N	2.330951000	2.741231000	-1.973187000
C	-1.407613000	-1.426978000	-3.674402000
C	-2.352682000	-0.483226000	-4.108786000
C	-1.635694000	0.724604000	-3.998268000
C	-1.497695000	-2.912801000	-3.635651000
C	-2.050448000	2.086541000	-4.430000000
C	-4.299866000	0.061999000	-5.864982000
C	-5.494179000	0.827334000	-5.873580000
C	-5.856760000	1.516734000	-7.031200000
H	-6.765142000	2.122145000	-7.019969000
C	-5.102164000	1.449093000	-8.200633000
C	-3.948458000	0.664242000	-8.194685000
H	-3.353874000	0.582310000	-9.107891000
C	-3.530480000	-0.011164000	-7.052015000
C	-6.382958000	0.970649000	-4.665838000
H	-5.824265000	1.293880000	-3.776171000
H	-7.159986000	1.722363000	-4.852987000
H	-6.882716000	0.023895000	-4.409733000
C	-5.508842000	2.199857000	-9.434565000
H	-5.635986000	1.516198000	-10.286919000
H	-6.454316000	2.736287000	-9.282278000
H	-4.738901000	2.935788000	-9.711723000
C	-2.277365000	-0.846313000	-7.138070000
H	-2.400456000	-1.828441000	-6.659410000
H	-2.002977000	-1.019143000	-8.188982000
H	-1.426522000	-0.346681000	-6.647249000
C	-4.866128000	-1.484176000	-3.737522000
C	-5.098708000	-1.214884000	-2.370732000
C	-6.180797000	-1.801449000	-1.713390000
H	-6.363024000	-1.554943000	-0.666626000
C	-7.022111000	-2.702608000	-2.356731000
C	-6.755034000	-3.013023000	-3.692591000
H	-7.385559000	-3.744863000	-4.203661000

C	-5.718142000	-2.409487000	-4.394532000
C	-4.266875000	-0.224569000	-1.609270000
H	-4.339073000	-0.417831000	-0.528828000
H	-3.215783000	-0.272562000	-1.901019000
H	-4.612799000	0.807209000	-1.781752000
C	-8.161516000	-3.361282000	-1.639017000
H	-7.979190000	-4.441898000	-1.535155000
H	-8.301894000	-2.943516000	-0.635254000
H	-9.099058000	-3.241749000	-2.201995000
C	-5.530008000	-2.768082000	-5.845418000
H	-5.933899000	-1.982754000	-6.504512000
H	-4.469919000	-2.892255000	-6.104953000
H	-6.048386000	-3.708702000	-6.078782000
C	2.424293000	4.050328000	-1.641679000
C	3.763775000	4.482006000	-1.641023000
C	1.210113000	4.841463000	-1.303434000
C	5.450127000	6.510127000	-2.139492000
C	6.623463000	7.066221000	-1.547465000
C	7.604702000	7.644276000	-2.348767000
H	8.502997000	8.050352000	-1.879109000
C	7.479978000	7.696500000	-3.735547000
C	6.322095000	7.158183000	-4.315170000
H	6.200835000	7.213152000	-5.399167000
C	5.323575000	6.563764000	-3.553670000
C	6.842945000	7.005695000	-0.065593000
H	6.714498000	5.979977000	0.311216000
H	7.853237000	7.351856000	0.195857000
H	6.111659000	7.628420000	0.479827000
C	8.555765000	8.288079000	-4.594275000
H	8.140913000	9.036212000	-5.288166000
H	9.331814000	8.772611000	-3.986472000
H	9.038291000	7.506003000	-5.203687000
C	4.097319000	6.044424000	-4.253965000
H	3.177473000	6.350492000	-3.736167000
H	4.054666000	6.420644000	-5.285555000
H	4.092127000	4.944302000	-4.294768000
B	-3.835978000	-0.665017000	-4.570838000
B	4.352110000	5.870634000	-1.248223000
F	6.282600000	1.823145000	-2.169792000
F	6.652433000	3.786602000	-1.268575000
F	6.305752000	3.614321000	-3.423447000
N	3.597591000	2.269137000	-2.166155000
C	4.453077000	3.309213000	-1.992957000
C	5.915120000	3.141957000	-2.209110000
C	3.833347000	6.524101000	0.065689000
C	3.434632000	7.893426000	0.089185000
C	2.980504000	8.464647000	1.273537000
H	2.667118000	9.510716000	1.274049000
C	2.902984000	7.729368000	2.458885000
C	3.318790000	6.390171000	2.439245000
H	3.298694000	5.812412000	3.365647000
C	3.770647000	5.780973000	1.277180000
C	3.489888000	8.724748000	-1.157523000
H	2.934874000	8.246912000	-1.979054000
H	3.068044000	9.723504000	-0.985231000
H	4.527909000	8.842069000	-1.514466000
C	2.370427000	8.337893000	3.718425000
H	2.975674000	8.041684000	4.587323000
H	2.355512000	9.434067000	3.660229000
H	1.339133000	7.993110000	3.902826000
C	4.281193000	4.373119000	1.351521000
H	5.250899000	4.279918000	0.842829000
H	4.408412000	4.055022000	2.394419000

H	3.601313000	3.659939000	0.861478000
Cu	3.895853000	0.391726000	-1.921198000
F	1.081597000	-4.216387000	-1.877105000
F	2.510584000	-5.085711000	-3.292053000
F	2.524948000	-5.714439000	-1.186150000
F	7.358208000	-2.489142000	-1.182373000
F	6.528901000	-1.841956000	0.731659000
F	6.506509000	-0.474115000	-0.971355000
N	3.013307000	-2.274065000	-1.954642000
N	4.065308000	-1.490133000	-1.589287000
C	3.336103000	-3.559276000	-1.686569000
C	4.608601000	-3.646650000	-1.109416000
C	5.014167000	-2.301137000	-1.057357000
C	2.372736000	-4.649476000	-2.007771000
C	6.341338000	-1.778378000	-0.607394000
C	5.969475000	-4.848849000	0.814590000
C	7.332777000	-5.145677000	1.053543000
C	7.848325000	-5.006181000	2.339370000
H	8.907656000	-5.211981000	2.509210000
C	7.046036000	-4.626736000	3.417750000
C	5.697430000	-4.377444000	3.181858000
H	5.053816000	-4.105278000	4.019532000
C	5.152706000	-4.465816000	1.901394000
C	8.250604000	-5.603377000	-0.049385000
H	8.212623000	-4.933788000	-0.920300000
H	9.290070000	-5.638931000	0.304797000
H	7.976804000	-6.607743000	-0.408365000
C	7.618677000	-4.519492000	4.800747000
H	7.955028000	-5.505371000	5.160324000
H	8.490088000	-3.848078000	4.815207000
H	6.870274000	-4.137932000	5.508873000
C	3.677118000	-4.209147000	1.735261000
H	3.224849000	-4.842780000	0.962821000
H	3.146948000	-4.405730000	2.673835000
H	3.482788000	-3.160580000	1.457676000
C	5.539786000	-6.142349000	-1.552418000
C	5.835023000	-5.995660000	-2.931600000
C	6.027382000	-7.127340000	-3.723582000
H	6.280527000	-6.997534000	-4.777532000
C	5.907570000	-8.415618000	-3.208761000
C	5.590596000	-8.556321000	-1.858108000
H	5.477937000	-9.559288000	-1.440914000
C	5.418158000	-7.455745000	-1.023075000
C	6.002789000	-4.652685000	-3.595303000
H	6.520812000	-4.769238000	-4.557765000
H	5.027683000	-4.183395000	-3.797147000
H	6.585483000	-3.952854000	-2.984931000
C	6.078951000	-9.619236000	-4.087746000
H	5.103470000	-9.939347000	-4.489812000
H	6.737401000	-9.400915000	-4.939942000
H	6.502104000	-10.463996000	-3.527747000
C	5.069921000	-7.719292000	0.418644000
H	5.899716000	-7.468112000	1.094696000
H	4.204102000	-7.128025000	0.745848000
H	4.825336000	-8.779930000	0.559895000
B	5.380997000	-4.912882000	-0.621937000
C	-0.099137000	1.392004000	-0.008108000
H	-0.181239000	2.479119000	0.006619000
C	1.126473000	0.780641000	0.278245000
H	1.992447000	1.401721000	0.501128000
C	1.225734000	-0.608861000	0.285397000
H	2.174592000	-1.093782000	0.508831000
C	0.099137000	-1.392004000	0.008108000

H	0.181239000	-2.479119000	-0.006619000
C	-1.126473000	-0.780641000	-0.278245000
H	-1.992447000	-1.401721000	-0.501128000
C	-1.225734000	0.608861000	-0.285397000
H	-2.174592000	1.093782000	-0.508831000

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Cu₃CH₃-Cu₃CH₃ dimer

Cu	0.907986000	-1.973616000	1.486014000
Cu	-1.017844000	0.626067000	1.084553000
Cu	2.163258000	0.971178000	1.240034000
N	-0.946373000	-2.090743000	1.875889000
N	-1.788578000	-1.056507000	1.490926000
N	-0.301972000	2.374929000	1.227876000
N	1.065189000	2.505802000	1.392980000
N	3.328074000	-0.515328000	1.415637000
N	2.797087000	-1.797596000	1.431703000
C	-1.673944000	-3.020897000	2.502179000
C	-3.039322000	-2.609692000	2.538656000
C	-3.033990000	-1.337390000	1.911777000
C	-1.004953000	-4.183156000	3.144522000
H	-1.334968000	-4.284014000	4.189178000
H	0.085017000	-4.042330000	3.133682000
H	-1.239713000	-5.131286000	2.646094000
C	-4.119715000	-0.340972000	1.748065000
H	-5.067342000	-0.820175000	1.470150000
H	-3.853978000	0.400599000	0.984559000
H	-4.295544000	0.191371000	2.695736000
C	-4.038753000	-4.939144000	3.266891000
C	-3.641932000	-5.763558000	2.188846000
C	-3.363970000	-7.112354000	2.404325000
H	-3.078368000	-7.738731000	1.555544000
C	-3.435328000	-7.684919000	3.676493000
C	-3.834233000	-6.870121000	4.736345000
H	-3.906381000	-7.296931000	5.740121000
C	-4.149625000	-5.519781000	4.547990000
C	-3.493273000	-5.226429000	0.792046000
H	-2.471535000	-4.855137000	0.608746000
H	-4.166010000	-4.382184000	0.600018000
H	-3.704994000	-6.011176000	0.051476000
C	-3.120689000	-9.139919000	3.881338000
H	-3.907680000	-9.774399000	3.442266000
H	-3.045981000	-9.384113000	4.948601000
H	-2.172375000	-9.412032000	3.395240000
C	-4.547054000	-4.691095000	5.740963000
H	-3.763246000	-3.957762000	5.989807000
H	-4.706003000	-5.323437000	6.625791000
H	-5.468939000	-4.125257000	5.540502000
C	-5.586334000	-2.659157000	3.392616000
C	-5.640503000	-1.577831000	4.307550000
C	-6.848479000	-0.922204000	4.548083000
H	-6.865935000	-0.089036000	5.256114000
C	-8.033583000	-1.304008000	3.918104000
C	-7.980145000	-2.370313000	3.022228000
H	-8.890854000	-2.682849000	2.507158000
C	-6.787910000	-3.046191000	2.752047000
C	-4.442792000	-1.136987000	5.107023000
H	-4.508172000	-0.067466000	5.349284000
H	-3.497064000	-1.329891000	4.588058000
H	-4.404280000	-1.682781000	6.064318000
C	-9.322454000	-0.591370000	4.210708000
H	-10.103921000	-0.857020000	3.486725000
H	-9.185350000	0.500233000	4.194278000
H	-9.694477000	-0.857825000	5.213335000

C	-6.813792000	-4.140150000	1.718321000
H	-7.844304000	-4.461976000	1.512832000
H	-6.231215000	-5.014821000	2.040699000
H	-6.382647000	-3.786152000	0.767205000
C	-0.888377000	3.549770000	1.513868000
C	0.114043000	4.493711000	1.866727000
C	1.326706000	3.751490000	1.804873000
C	-2.372051000	3.636982000	1.591373000
H	-2.836412000	2.835406000	1.000000000
H	-2.749185000	4.606175000	1.241351000
H	-2.695329000	3.515399000	2.639731000
C	2.722999000	4.132969000	2.144436000
H	2.949042000	3.875192000	3.192648000
H	2.888744000	5.210729000	2.030213000
H	3.431350000	3.589515000	1.503657000
C	1.024301000	6.740365000	2.978577000
C	1.711133000	7.868616000	2.475426000
C	2.722843000	8.467683000	3.230697000
H	3.251349000	9.331263000	2.819028000
C	3.066410000	7.998986000	4.498694000
C	2.359995000	6.906262000	5.006941000
H	2.593503000	6.542176000	6.010728000
C	1.362265000	6.268419000	4.270416000
C	1.416522000	8.423280000	1.106513000
H	1.789207000	7.743972000	0.321422000
H	1.908185000	9.396442000	0.962931000
H	0.333977000	8.541502000	0.944561000
C	4.168274000	8.644094000	5.289112000
H	3.972575000	8.584338000	6.368437000
H	4.290734000	9.700240000	5.011436000
H	5.127637000	8.135912000	5.098120000
C	0.646130000	5.102075000	4.903961000
H	-0.436934000	5.138253000	4.724412000
H	0.814686000	5.091668000	5.989897000
H	0.998627000	4.142091000	4.497788000
C	-1.304711000	6.694549000	1.502033000
C	-1.518899000	6.650690000	0.105297000
C	-2.685464000	7.184856000	-0.438245000
H	-2.834625000	7.146213000	-1.520250000
C	-3.682507000	7.741959000	0.364517000
C	-3.461226000	7.793934000	1.740691000
H	-4.224698000	8.231709000	2.389358000
C	-2.286736000	7.298416000	2.314568000
C	-0.509519000	6.039305000	-0.828064000
H	-0.475428000	4.943050000	-0.731534000
H	0.510925000	6.390763000	-0.615108000
H	-0.745188000	6.288100000	-1.871785000
C	-4.937273000	8.292795000	-0.247262000
H	-5.794333000	8.180551000	0.429578000
H	-5.168350000	7.773247000	-1.184026000
H	-4.826404000	9.366735000	-0.471859000
C	-2.128246000	7.357254000	3.810797000
H	-2.328822000	6.372184000	4.265202000
H	-2.832884000	8.074418000	4.254018000
H	-1.105642000	7.647719000	4.093129000
C	4.665053000	-0.602822000	1.432691000
C	5.041734000	-1.974612000	1.486451000
C	3.806489000	-2.676439000	1.500337000
C	5.485503000	0.639668000	1.453593000
H	4.824882000	1.520612000	1.453016000
H	6.156948000	0.703515000	0.585130000
H	6.119976000	0.681076000	2.353389000
C	3.521810000	-4.133476000	1.530101000

H	4.208204000	-4.692349000	0.878477000
H	2.493285000	-4.318198000	1.195933000
H	3.631532000	-4.551048000	2.542956000
C	6.638968000	-3.996713000	2.137951000
C	6.119556000	-4.324183000	3.413660000
C	6.194986000	-5.636121000	3.883360000
H	5.789866000	-5.869233000	4.872841000
C	6.771332000	-6.657015000	3.126160000
C	7.313613000	-6.323651000	1.885174000
H	7.780269000	-7.103828000	1.279576000
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C	7.822106000	-4.753510000	0.016731000
H	8.425233000	-5.601959000	-0.335213000
H	8.447383000	-3.849434000	0.011725000
H	7.011858000	-4.595735000	-0.711988000
C	7.613139000	-1.644438000	1.026557000
C	8.544574000	-1.119698000	1.950511000
C	9.451058000	-0.133204000	1.551451000
H	10.145649000	0.278918000	2.288623000
C	9.481175000	0.345041000	0.240768000
C	8.591741000	-0.213089000	-0.677290000
H	8.600180000	0.134376000	-1.709080000
C	7.662304000	-1.185180000	-0.309390000
C	8.530435000	-1.551591000	3.394168000
H	7.702834000	-1.070209000	3.941016000
H	9.464882000	-1.270540000	3.900613000
H	8.393664000	-2.639234000	3.485839000
C	10.419187000	1.445823000	-0.165013000
H	9.916262000	2.424462000	-0.091275000
H	10.756358000	1.322581000	-1.204371000
H	11.305803000	1.477854000	0.485160000
C	6.766088000	-1.739147000	-1.384952000
H	6.568718000	-0.978830000	-2.153764000
H	5.807913000	-2.093134000	-0.981696000
H	7.251286000	-2.593476000	-1.886083000
B	-4.232963000	-3.389659000	3.070221000
B	-0.053058000	5.984463000	2.129249000
B	6.446576000	-2.560171000	1.540002000
Cu	-0.856389529	2.103750843	-1.496996337
Cu	1.069440471	-0.495932157	-1.095535337
Cu	-2.111661529	-0.841043157	-1.251016337
N	0.997969471	2.220877843	-1.886871337
N	1.840174471	1.186641843	-1.501908337
N	0.353568471	-2.244794157	-1.238858337
N	-1.013592529	-2.375667157	-1.403962337
N	-3.276477529	0.645462843	-1.426619337
N	-2.745490529	1.927730843	-1.442685337
C	1.725540471	3.151031843	-2.513161337
C	3.090918471	2.739826843	-2.549638337
C	3.085586471	1.467524843	-1.922759337
C	1.056549471	4.313290843	-3.155504337
H	1.386564471	4.414148843	-4.200160337
H	-0.033420529	4.172464843	-3.144664337
H	1.291309471	5.261420843	-2.657076337
C	4.171311471	0.471106843	-1.759047337

H	5.118938471	0.950309843	-1.481132337
H	3.905574471	-0.270464157	-0.995541337
H	4.347140471	-0.061236157	-2.706718337
C	4.090349471	5.069278843	-3.277873337
C	3.693528471	5.893692843	-2.199828337
C	3.415566471	7.242488843	-2.415307337
H	3.129964471	7.868865843	-1.566526337
C	3.486924471	7.815053843	-3.687475337
C	3.885829471	7.000255843	-4.747327337
H	3.957977471	7.427065843	-5.751103337
C	4.201221471	5.649915843	-4.558972337
C	3.544869471	5.356563843	-0.803028337
H	2.523131471	4.985271843	-0.619728337
H	4.217606471	4.512318843	-0.611000337
H	3.756590471	6.141310843	-0.062458337
C	3.172285471	9.270053843	-3.892320337
H	3.959276471	9.904533843	-3.453248337
H	3.097577471	9.514247843	-4.959583337
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C	4.598650471	4.821229843	-5.751945337
H	3.814842471	4.087896843	-6.000789337
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H	5.520535471	4.255391843	-5.551484337
C	5.637930471	2.789291843	-3.403598337
C	5.692099471	1.707965843	-4.318532337
C	6.900075471	1.052338843	-4.559065337
H	6.917531471	0.219170843	-5.267096337
C	8.085179471	1.434142843	-3.929086337
C	8.031741471	2.500447843	-3.033210337
H	8.942450471	2.812983843	-2.518140337
C	6.839506471	3.176325843	-2.763029337
C	4.494388471	1.267121843	-5.118005337
H	4.559768471	0.197600843	-5.360266337
H	3.548660471	1.460025843	-4.599040337
H	4.455876471	1.812915843	-6.075300337
C	9.374050471	0.721504843	-4.221690337
H	10.155517471	0.987154843	-3.497707337
H	9.236946471	-0.370098157	-4.205260337
H	9.746073471	0.987959843	-5.224317337
C	6.865388471	4.270284843	-1.729303337
H	7.895900471	4.592110843	-1.523814337
H	6.282811471	5.144955843	-2.051681337
H	6.434243471	3.916286843	-0.778187337
C	0.939973471	-3.419635157	-1.524850337
C	-0.062446529	-4.363576157	-1.877709337
C	-1.275109529	-3.621355157	-1.815855337
C	2.423647471	-3.506847157	-1.602355337
H	2.888008471	-2.705271157	-1.010982337
H	2.800781471	-4.476040157	-1.252333337
H	2.746925471	-3.385264157	-2.650713337
C	-2.671402529	-4.002834157	-2.155418337
H	-2.897445529	-3.745057157	-3.203630337
H	-2.837147529	-5.080594157	-2.041195337
H	-3.379753529	-3.459380157	-1.514639337
C	-0.972704529	-6.610230157	-2.989559337
C	-1.659536529	-7.738481157	-2.486408337
C	-2.671246529	-8.337548157	-3.241679337
H	-3.199752529	-9.201128157	-2.830010337
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C	-2.308398529	-6.776127157	-5.017923337
H	-2.541906529	-6.412041157	-6.021710337
C	-1.310668529	-6.138284157	-4.281398337
C	-1.364925529	-8.293145157	-1.117495337

H	-1.737610529	-7.613837157	-0.332404337
H	-1.856588529	-9.266307157	-0.973913337
H	-0.282380529	-8.411367157	-0.955543337
C	-4.116677529	-8.513959157	-5.300094337
H	-3.920978529	-8.454203157	-6.379419337
H	-4.239137529	-9.570105157	-5.022418337
H	-5.076040529	-8.005777157	-5.109102337
C	-0.594533529	-4.971940157	-4.914943337
H	0.488530471	-5.008118157	-4.735394337
H	-0.763089529	-4.961533157	-6.000879337
H	-0.947030529	-4.011956157	-4.508770337
C	1.356307471	-6.564414157	-1.513015337
C	1.570495471	-6.520555157	-0.116279337
C	2.737060471	-7.054721157	0.427262663
H	2.886221471	-7.016078157	1.509267663
C	3.734103471	-7.611824157	-0.375499337
C	3.512822471	-7.663799157	-1.751673337
H	4.276294471	-8.101574157	-2.400340337
C	2.338332471	-7.168281157	-2.325550337
C	0.561115471	-5.909170157	0.817081663
H	0.527024471	-4.812915157	0.720551663
H	-0.459328529	-6.260628157	0.604125663
H	0.796784471	-6.157965157	1.860802663
C	4.988869471	-8.162660157	0.236279663
H	5.845929471	-8.050416157	-0.440560337
H	5.219946471	-7.643112157	1.173043663
H	4.878000471	-9.236600157	0.460876663
C	2.179842471	-7.227119157	-3.821779337
H	2.380418471	-6.242049157	-4.276184337
H	2.884480471	-7.944283157	-4.265000337
H	1.157238471	-7.517584157	-4.104111337
C	-4.613456529	0.732956843	-1.443673337
C	-4.990137529	2.104746843	-1.497433337
C	-3.754892529	2.806573843	-1.511319337
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H	-4.773285529	-1.390477157	-1.463998337
H	-6.105351529	-0.573380157	-0.596112337
H	-6.068379529	-0.550941157	-2.364371337
C	-3.470213529	4.263610843	-1.541083337
H	-4.156607529	4.822483843	-0.889459337
H	-2.441688529	4.448332843	-1.206915337
H	-3.579935529	4.681182843	-2.553938337
C	-6.587371529	4.126847843	-2.148933337
C	-6.067959529	4.454317843	-3.424642337
C	-6.143389529	5.766255843	-3.894342337
H	-5.738269529	5.999367843	-4.883823337
C	-6.719735529	6.787149843	-3.137142337
C	-7.262016529	6.453785843	-1.896156337
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H	-4.331711529	3.512291843	-4.313669337
H	-5.676078529	2.401337843	-4.040476337
H	-5.754496529	3.584831843	-5.370626337
C	-6.771793529	8.195706843	-3.656950337
H	-7.497148529	8.278574843	-4.483783337
H	-7.072726529	8.901212843	-2.870785337
H	-5.792804529	8.507473843	-4.050073337
C	-7.770509529	4.883644843	-0.027713337
H	-8.373636529	5.732093843	0.324230663
H	-8.395786529	3.979568843	-0.022707337
H	-6.960261529	4.725869843	0.701005663
C	-7.561542529	1.774572843	-1.037539337

C	-8.492977529	1.249832843	-1.961493337
C	-9.399461529	0.263338843	-1.562433337
H	-10.094052529	-0.148783157	-2.299605337
C	-9.429578529	-0.214906157	-0.251750337
C	-8.540144529	0.343223843	0.666307663
H	-8.548583529	-0.004241157	1.698097663
C	-7.610707529	1.315314843	0.298407663
C	-8.478838529	1.681725843	-3.405150337
H	-7.651237529	1.200343843	-3.951998337
H	-9.413285529	1.400674843	-3.911595337
H	-8.342067529	2.769368843	-3.496821337
C	-10.367590529	-1.315688157	0.154030663
H	-9.864665529	-2.294327157	0.080292663
H	-10.704761529	-1.192446157	1.193388663
H	-11.254206529	-1.347719157	-0.496142337
C	-6.714491529	1.869281843	1.373969663
H	-6.517121529	1.108964843	2.142781663
H	-5.756316529	2.223268843	0.970713663
H	-7.199689529	2.723610843	1.875100663
B	4.284559471	3.519793843	-3.081203337
B	0.104654471	-5.854328157	-2.140231337
B	-6.394979529	2.690305843	-1.550984337

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Cu₃CH₃-Cu₃CH₃ dimer T1

Cu	0.566052000	-1.972294000	1.203650000
Cu	-1.150680000	0.538500000	0.856752000
Cu	1.702024000	0.980976000	0.987965000
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N	-1.926712000	-0.907325000	1.893086000
N	-0.641053000	2.363519000	1.389734000
N	0.720924000	2.499083000	1.591987000
N	2.924593000	-0.495520000	1.071032000
N	2.446209000	-1.756877000	1.380781000
C	-1.908128000	-3.011447000	2.564673000
C	-3.190905000	-2.479007000	2.883743000
C	-3.122738000	-1.125265000	2.446969000
C	-1.293171000	-4.334840000	2.853578000
H	-1.644239000	-4.735759000	3.814814000
H	-0.198980000	-4.231275000	2.894261000
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C	-4.129031000	-0.036977000	2.500805000
H	-5.140057000	-0.423662000	2.317381000
H	-3.898824000	0.728740000	1.750265000
H	-4.143547000	0.448113000	3.489823000
C	-4.337058000	-4.805232000	3.015665000
C	-4.084000000	-5.298188000	1.711721000
C	-3.798928000	-6.653151000	1.518417000
H	-3.624903000	-7.021048000	0.500087000
C	-3.706904000	-7.546736000	2.592594000
C	-3.960999000	-7.055019000	3.877545000
H	-3.899208000	-7.736878000	4.732168000
C	-4.288415000	-5.708518000	4.099521000
C	-4.050187000	-4.388059000	0.508129000
H	-3.017703000	-4.058250000	0.307874000
H	-4.651062000	-3.478809000	0.652713000
H	-4.415781000	-4.910107000	-0.389160000
C	-3.340398000	-8.989263000	2.358650000
H	-4.044685000	-9.467656000	1.664986000
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H	-2.338494000	-9.073495000	1.906499000
C	-4.498196000	-5.209000000	5.506749000
H	-3.664885000	-4.559742000	5.817647000
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H	-5.41682000	-4.604057000	5.583874000
C	-5.696993000	-2.499830000	3.830851000
C	-5.590579000	-1.598544000	4.922481000
C	-6.691333000	-0.834621000	5.315549000
H	-6.580694000	-0.137674000	6.150007000
C	-7.928159000	-0.931701000	4.672501000
C	-8.038922000	-1.835912000	3.619412000
H	-8.990999000	-1.933335000	3.099756000
C	-6.958612000	-2.613175000	3.191691000
C	-4.325090000	-1.459943000	5.731296000
H	-4.238843000	-0.447380000	6.148011000
H	-3.429998000	-1.678977000	5.142004000
H	-4.333129000	-2.162367000	6.580965000
C	-9.100095000	-0.103074000	5.119445000
H	-9.880688000	-0.061595000	4.349120000
H	-8.791573000	0.925101000	5.361393000
H	-9.556504000	-0.531724000	6.027228000
C	-7.170527000	-3.493132000	1.989723000
H	-8.241266000	-3.687299000	1.833748000
H	-6.649367000	-4.453444000	2.091457000
H	-6.795632000	-3.003331000	1.078450000
C	-1.242686000	3.523283000	1.684937000
C	-0.257218000	4.459249000	2.110106000
C	0.963985000	3.733345000	2.054010000
C	-2.725187000	3.621184000	1.648150000
H	-3.147779000	2.735453000	1.157121000
H	-3.066762000	4.516410000	1.114333000
H	-3.131646000	3.672502000	2.669695000
C	2.343070000	4.138240000	2.426631000
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H	2.582113000	5.138813000	2.046466000
H	3.075120000	3.419189000	2.032783000
C	0.582877000	6.668697000	3.337065000
C	1.309708000	7.816655000	2.947475000
C	2.263635000	8.372214000	3.806494000
H	2.825705000	9.249409000	3.477385000
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C	1.753871000	6.734806000	5.473378000
H	1.903539000	6.327155000	6.475518000
C	0.816825000	6.135946000	4.631982000
C	1.136843000	8.440856000	1.588404000
H	1.695188000	7.876429000	0.829916000
H	1.519469000	9.467005000	1.577843000
H	0.086225000	8.456785000	1.281173000
C	3.538194000	8.443841000	5.982700000
H	3.211797000	8.408107000	7.030744000
H	3.749908000	9.488075000	5.714902000
H	4.482075000	7.881104000	5.911986000
C	0.052472000	4.947375000	5.163539000
H	-1.017573000	5.006217000	4.926620000
H	0.158580000	4.883811000	6.254683000
H	0.414460000	4.002490000	4.731525000
C	-1.627448000	6.643285000	1.650313000
C	-1.701823000	6.639871000	0.239538000
C	-2.854080000	7.102699000	-0.397820000
H	-2.895172000	7.099395000	-1.488410000
C	-3.964180000	7.547768000	0.321409000
C	-3.881878000	7.554493000	1.714470000
H	-4.739547000	7.898153000	2.298387000
C	-2.729864000	7.131463000	2.380885000
C	-0.556637000	6.147596000	-0.603546000
H	-0.345705000	5.077254000	-0.415637000
H	0.381511000	6.690708000	-0.374303000

H	-0.773798000	6.286102000	-1.677481000
C	-5.200168000	8.027190000	-0.382719000
H	-6.104835000	7.608919000	0.080590000
H	-5.184946000	7.734813000	-1.440082000
H	-5.280978000	9.125157000	-0.333810000
C	-2.711419000	7.125073000	3.883350000
H	-2.890278000	6.110303000	4.268526000
H	-3.495230000	7.776636000	4.294139000
H	-1.739083000	7.456262000	4.269901000
C	4.264670000	-0.537105000	1.015590000
C	4.698668000	-1.856893000	1.326746000
C	3.491587000	-2.577674000	1.544972000
C	5.020579000	0.717773000	0.753431000
H	4.383862000	1.421608000	0.197822000
H	5.933036000	0.527843000	0.174642000
H	5.320373000	1.199247000	1.698753000
C	3.263424000	-4.005311000	1.878272000
H	4.024984000	-4.651791000	1.425335000
H	2.275761000	-4.316608000	1.513832000
H	3.296327000	-4.176500000	2.964783000
C	6.337600000	-3.604424000	2.459246000
C	5.834851000	-3.611442000	3.783763000
C	5.973413000	-4.751290000	4.574962000
H	5.589784000	-4.736505000	5.599421000
C	6.587709000	-5.909994000	4.094112000
C	7.093392000	-5.894777000	2.794655000
H	7.594890000	-6.783404000	2.403700000
C	6.983175000	-4.767519000	1.978504000
C	5.144696000	-2.415287000	4.394163000
H	4.049944000	-2.492239000	4.290479000
H	5.436336000	-1.471872000	3.918603000
H	5.369055000	-2.347953000	5.468848000
C	6.714798000	-7.125983000	4.961972000
H	7.406561000	-6.940082000	5.794992000
H	7.093926000	-7.984549000	4.391125000
H	5.745371000	-7.396864000	5.402022000
C	7.498470000	-4.847217000	0.565729000
H	8.116585000	-5.741665000	0.414631000
H	8.095437000	-3.964364000	0.308417000
H	6.661606000	-4.895295000	-0.146900000
C	7.314371000	-1.590119000	0.858266000
C	8.285045000	-0.939593000	1.654837000
C	9.289385000	-0.181868000	1.053319000
H	10.022283000	0.320958000	1.685359000
C	9.390595000	-0.055100000	-0.332404000
C	8.447360000	-0.715845000	-1.115562000
H	8.507768000	-0.646999000	-2.202489000
C	7.419616000	-1.472514000	-0.547559000
C	8.231268000	-0.999399000	3.155951000
H	7.415499000	-0.377020000	3.544434000
H	9.162631000	-0.626091000	3.593573000
H	8.061528000	-2.025577000	3.514386000
C	10.486326000	0.769690000	-0.939447000
H	10.248216000	1.843827000	-0.873151000
H	10.642030000	0.517380000	-1.995498000
H	11.436212000	0.613600000	-0.408251000
C	6.493980000	-2.205029000	-1.484196000
H	6.322593000	-1.618533000	-2.397756000
H	5.528912000	-2.421128000	-1.013583000
H	6.937324000	-3.169558000	-1.787191000
B	-4.438002000	-3.256634000	3.281553000
B	-0.426259000	5.947520000	2.382902000
B	6.123802000	-2.356104000	1.531221000

Cu	-0.566052000	1.972294000	-1.203650000
Cu	1.150680000	-0.538500000	-0.856752000
Cu	-1.702024000	-0.980976000	-0.987965000
N	1.175210000	2.059401000	-1.976023000
N	1.926712000	0.907325000	-1.893086000
N	0.641053000	-2.363519000	-1.389734000
N	-0.720924000	-2.499083000	-1.591987000
N	-2.924593000	0.495520000	-1.071032000
N	-2.446209000	1.756877000	-1.380781000
C	1.908128000	3.011447000	-2.564673000
C	3.190905000	2.479007000	-2.883743000
C	3.122738000	1.125265000	-2.446969000
C	1.293171000	4.334840000	-2.853578000
H	1.644239000	4.735759000	-3.814814000
H	0.198980000	4.231275000	-2.894261000
H	1.539445000	5.081048000	-2.084281000
C	4.129031000	0.036977000	-2.500805000
H	5.140057000	0.423662000	-2.317381000
H	3.898824000	-0.728740000	-1.750265000
H	4.143547000	-0.448113000	-3.489823000
C	4.337058000	4.805232000	-3.015665000
C	4.084000000	5.298188000	-1.711721000
C	3.798928000	6.653151000	-1.518417000
H	3.624903000	7.021048000	-0.500087000
C	3.706904000	7.546736000	-2.592594000
C	3.960999000	7.055019000	-3.877545000
H	3.899208000	7.736878000	-4.732168000
C	4.288415000	5.708518000	-4.099521000
C	4.050187000	4.388059000	-0.508129000
H	3.017703000	4.058250000	-0.307874000
H	4.651062000	3.478809000	-0.652713000
H	4.415781000	4.910107000	0.389160000
C	3.340398000	8.989263000	-2.358650000
H	4.044685000	9.467656000	-1.664986000
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H	2.338494000	9.073495000	-1.906499000
C	4.498196000	5.209000000	-5.506749000
H	3.664885000	4.559742000	-5.817647000
H	4.558870000	6.042282000	-6.223677000
H	5.416820000	4.604057000	-5.583874000
C	5.696993000	2.499830000	-3.830851000
C	5.590579000	1.598544000	-4.922481000
C	6.691333000	0.834621000	-5.315549000
H	6.580694000	0.137674000	-6.150007000
C	7.928159000	0.931701000	-4.672501000
C	8.038922000	1.835912000	-3.619412000
H	8.990999000	1.933335000	-3.099756000
C	6.958612000	2.613175000	-3.191691000
C	4.325090000	1.459943000	-5.731296000
H	4.238843000	0.447380000	-6.148011000
H	3.429998000	1.678977000	-5.142004000
H	4.333129000	2.162367000	-6.580965000
C	9.100095000	0.103074000	-5.119445000
H	9.880688000	0.061595000	-4.349120000
H	8.791573000	-0.925101000	-5.361393000
H	9.556504000	0.531724000	-6.027228000
C	7.170527000	3.493132000	-1.989723000
H	8.241266000	3.687299000	-1.833748000
H	6.649367000	4.453444000	-2.091457000
H	6.795632000	3.003331000	-1.078450000
C	1.242686000	-3.523283000	-1.684937000
C	0.257218000	-4.459249000	-2.110106000
C	-0.963985000	-3.733345000	-2.054010000

C	2.725187000	-3.621184000	-1.648150000
H	3.147779000	-2.735453000	-1.157121000
H	3.066762000	-4.516410000	-1.114333000
H	3.131646000	-3.672502000	-2.669695000
C	-2.343070000	-4.138240000	-2.426631000
H	-2.458582000	-4.177017000	-3.520905000
H	-2.582113000	-5.138813000	-2.046466000
H	-3.075120000	-3.419189000	-2.032783000
C	-0.582877000	-6.668697000	-3.337065000
C	-1.309708000	-7.816655000	-2.947475000
C	-2.263635000	-8.372214000	-3.806494000
H	-2.825705000	-9.249409000	-3.477385000
C	-2.503532000	-7.845102000	-5.073677000
C	-1.753871000	-6.734806000	-5.473378000
H	-1.903539000	-6.327155000	-6.475518000
C	-0.816825000	-6.135946000	-4.631982000
C	-1.136843000	-8.440856000	-1.588404000
H	-1.695188000	-7.876429000	-0.829916000
H	-1.519469000	-9.467005000	-1.577843000
H	-0.086225000	-8.456785000	-1.281173000
C	-3.538194000	-8.443841000	-5.982700000
H	-3.211797000	-8.408107000	-7.030744000
H	-3.749908000	-9.488075000	-5.714902000
H	-4.482075000	-7.881104000	-5.911986000
C	-0.052472000	-4.947375000	-5.163539000
H	1.017573000	-5.006217000	-4.926620000
H	-0.158580000	-4.883811000	-6.254683000
H	-0.414460000	-4.002490000	-4.731525000
C	1.627448000	-6.643285000	-1.650313000
C	1.701823000	-6.639871000	-0.239538000
C	2.854080000	-7.102699000	0.397820000
H	2.895172000	-7.099395000	1.488410000
C	3.964180000	-7.547768000	-0.321409000
C	3.881878000	-7.554493000	-1.714470000
H	4.739547000	-7.898153000	-2.298387000
C	2.729864000	-7.131463000	-2.380885000
C	0.556637000	-6.147596000	0.603546000
H	0.345705000	-5.077254000	0.415637000
H	-0.381511000	-6.690708000	0.374303000
H	0.773798000	-6.286102000	1.677481000
C	5.200168000	-8.027190000	0.382719000
H	6.104835000	-7.608919000	-0.080590000
H	5.184946000	-7.734813000	1.440082000
H	5.280978000	-9.125157000	0.333810000
C	2.711419000	-7.125073000	-3.883350000
H	2.890278000	-6.110303000	-4.268526000
H	3.495230000	-7.776636000	-4.294139000
H	1.739083000	-7.456262000	-4.269901000
C	-4.264670000	0.537105000	-1.015590000
C	-4.698668000	1.856893000	-1.326746000
C	-3.491587000	2.577674000	-1.544972000
C	-5.020579000	-0.717773000	-0.753431000
H	-4.383862000	-1.421608000	-0.197822000
H	-5.933036000	-0.527843000	-0.174642000
H	-5.320373000	-1.199247000	-1.698753000
C	-3.263424000	4.005311000	-1.878272000
H	-4.024984000	4.651791000	-1.425335000
H	-2.275761000	4.316608000	-1.513832000
H	-3.296327000	4.176500000	-2.964783000
C	-6.337600000	3.604424000	-2.459246000
C	-5.834851000	3.611442000	-3.783763000
C	-5.973413000	4.751290000	-4.574962000
H	-5.589784000	4.736505000	-5.599421000

C	-6.587709000	5.909994000	-4.094112000
C	-7.093392000	5.894777000	-2.794655000
H	-7.594890000	6.783404000	-2.403700000
C	-6.983175000	4.767519000	-1.978504000
C	-5.144696000	2.415287000	-4.394163000
H	-4.049944000	2.492239000	-4.290479000
H	-5.436336000	1.471872000	-3.918603000
H	-5.369055000	2.347953000	-5.468848000
C	-6.714798000	7.125983000	-4.961972000
H	-7.406561000	6.940082000	-5.794992000
H	-7.093926000	7.984549000	-4.391125000
H	-5.745371000	7.396864000	-5.402022000
C	-7.498470000	4.847217000	-0.565729000
H	-8.116585000	5.741665000	-0.414631000
H	-8.095437000	3.964364000	-0.308417000
H	-6.661606000	4.895295000	0.146900000
C	-7.314371000	1.590119000	-0.858266000
C	-8.285045000	0.939593000	-1.654837000
C	-9.289385000	0.181868000	-1.053319000
H	-10.022283000	-0.320958000	-1.685359000
C	-9.390595000	0.055100000	0.332404000
C	-8.447360000	0.715845000	1.115562000
H	-8.507768000	0.646999000	2.202489000
C	-7.419616000	1.472514000	0.547559000
C	-8.231268000	0.999399000	-3.155951000
H	-7.415499000	0.377020000	-3.544434000
H	-9.162631000	0.626091000	-3.593573000
H	-8.061528000	2.025577000	-3.514386000
C	-10.486326000	-0.769690000	0.939447000
H	-10.248216000	-1.843827000	0.873151000
H	-10.642030000	-0.517380000	1.995498000
H	-11.436212000	-0.613600000	0.408251000
C	-6.493980000	2.205029000	1.484196000
H	-6.322593000	1.618533000	2.397756000
H	-5.528912000	2.421128000	1.013583000
H	-6.937324000	3.169558000	1.787191000
B	4.438002000	3.256634000	-3.281553000
B	0.426259000	-5.947520000	-2.382902000
B	-6.123802000	2.356104000	-1.531221000

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Cu3CF3-Cu3CF3

Cu	-1.497534000	1.963030000	2.229562000
Cu	-1.016909000	-1.235275000	1.967792000
F	0.142167000	3.535271000	4.314077000
F	1.287834000	4.010621000	2.508743000
F	2.342014000	3.523119000	4.380007000
F	3.499343000	-1.824767000	3.044481000
F	1.572689000	-2.627776000	3.688579000
F	1.943601000	-2.274359000	1.568606000
F	-0.292044000	-3.914340000	2.145624000
F	-1.473969000	-5.755229000	1.996632000
F	-0.883196000	-4.676925000	0.183564000
N	0.183460000	1.222947000	2.644797000
N	0.411639000	-0.102569000	2.447669000
N	-2.498040000	-2.376181000	1.700846000
C	1.286000000	1.753995000	3.231726000
C	2.264418000	0.769601000	3.440216000
C	1.644919000	-0.383522000	2.932446000
C	1.274512000	3.202069000	3.602892000
C	2.170706000	-1.771133000	2.816028000
C	3.886254000	0.035688000	5.457392000
C	5.114398000	-0.652987000	5.640725000
C	5.335416000	-1.365863000	6.816836000

H	6.275354000	-1.907806000	6.934842000
C	4.401011000	-1.404186000	7.845133000
C	3.195714000	-0.730369000	7.658744000
H	2.446961000	-0.750317000	8.451712000
C	2.915223000	-0.035570000	6.486291000
C	6.203504000	-0.693559000	4.602283000
H	5.816239000	-0.841282000	3.589924000
H	6.892489000	-1.522032000	4.815641000
H	6.788873000	0.238605000	4.588854000
C	4.681488000	-2.138675000	9.121475000
H	4.901493000	-1.428134000	9.932502000
H	5.542796000	-2.809853000	9.015678000
H	3.813715000	-2.737557000	9.429940000
C	1.582057000	0.661341000	6.392363000
H	1.683410000	1.718366000	6.111558000
H	1.068108000	0.625764000	7.361498000
H	0.929811000	0.179310000	5.648654000
C	4.789762000	1.753930000	3.598396000
C	5.218720000	1.592091000	2.260325000
C	6.392253000	2.203590000	1.831060000
H	6.743790000	2.020780000	0.815291000
C	7.107116000	3.070132000	2.650917000
C	6.641941000	3.279493000	3.949932000
H	7.179907000	3.968610000	4.603285000
C	5.528621000	2.609397000	4.446580000
C	4.497142000	0.711203000	1.282454000
H	4.952932000	0.826737000	0.288319000
H	3.429365000	0.965811000	1.204305000
H	4.576479000	-0.352224000	1.552163000
C	8.302750000	3.808055000	2.124942000
H	7.986123000	4.750973000	1.652957000
H	8.830395000	3.223001000	1.363160000
H	9.005616000	4.057567000	2.928429000
C	5.158156000	2.821048000	5.892560000
H	5.581946000	2.024827000	6.526170000
H	4.074422000	2.815433000	6.055566000
H	5.551831000	3.781921000	6.250699000
C	-2.559834000	-3.718141000	1.547819000
C	-3.888177000	-4.166319000	1.561686000
C	-1.311510000	-4.524073000	1.455831000
C	-5.536163000	-6.204230000	2.230625000
C	-6.627075000	-6.886130000	1.637432000
C	-7.642595000	-7.404232000	2.443706000
H	-8.492528000	-7.905039000	1.972836000
C	-7.603224000	-7.296368000	3.831514000
C	-6.514475000	-6.640941000	4.410947000
H	-6.464430000	-6.558280000	5.498619000
C	-5.492859000	-6.087048000	3.640017000
C	-6.751451000	-7.060764000	0.145859000
H	-6.478731000	-6.148070000	-0.404454000
H	-7.785715000	-7.325801000	-0.120923000
H	-6.084479000	-7.858720000	-0.218754000
C	-8.693107000	-7.877888000	4.687725000
H	-8.316639000	-8.737958000	5.266021000
H	-9.542089000	-8.223268000	4.080096000
H	-9.064879000	-7.131899000	5.402828000
C	-4.336530000	-5.419850000	4.345480000
H	-3.364068000	-5.733887000	3.937922000
H	-4.347610000	-5.671677000	5.415692000
H	-4.387600000	-4.324356000	4.255581000
B	3.649769000	0.870987000	4.166315000
B	-4.409109000	-5.622847000	1.335315000
F	-6.509468000	-1.532784000	1.639805000

F	-6.791199000	-3.663178000	1.170335000
F	-6.460905000	-3.040786000	3.258470000
N	-3.773810000	-1.906669000	1.819081000
C	-4.608239000	-2.975231000	1.763956000
C	-6.086599000	-2.811268000	1.955111000
C	-3.761345000	-6.457620000	0.199338000
C	-3.298830000	-7.771880000	0.449313000
C	-2.650374000	-8.472341000	-0.567502000
H	-2.260135000	-9.470624000	-0.354767000
C	-2.481476000	-7.932539000	-1.845360000
C	-2.995312000	-6.659917000	-2.100453000
H	-2.899426000	-6.228856000	-3.101788000
C	-3.609619000	-5.913362000	-1.101258000
C	-3.451606000	-8.440666000	1.794637000
H	-3.111079000	-7.802181000	2.621475000
H	-2.864470000	-9.368345000	1.826228000
H	-4.508044000	-8.693676000	1.998172000
C	-1.770069000	-8.690245000	-2.926363000
H	-2.460460000	-8.940152000	-3.746553000
H	-1.336112000	-9.622763000	-2.543907000
H	-0.956085000	-8.083787000	-3.350469000
C	-4.166088000	-4.560399000	-1.449116000
H	-5.145784000	-4.388187000	-0.981700000
H	-4.296363000	-4.453864000	-2.536007000
H	-3.499765000	-3.749945000	-1.111848000
Cu	-4.047413000	-0.018131000	1.727093000
F	-1.353142000	4.726597000	1.593415000
F	-2.616306000	5.414596000	3.248331000
F	-2.956207000	6.181468000	1.217476000
F	-7.589638000	3.008632000	0.856194000
F	-6.636355000	1.390327000	-0.283598000
F	-6.974312000	1.160427000	1.868963000
N	-3.189100000	2.672540000	1.818001000
N	-4.251581000	1.863734000	1.557705000
C	-3.587271000	3.955490000	1.654325000
C	-4.925295000	4.013816000	1.241368000
C	-5.288020000	2.660262000	1.196669000
C	-2.635127000	5.070866000	1.925521000
C	-6.619631000	2.062388000	0.902041000
C	-6.381717000	5.349497000	-0.567766000
C	-7.724953000	5.767244000	-0.742783000
C	-8.280237000	5.785848000	-2.024174000
H	-9.322547000	6.086949000	-2.142699000
C	-7.546472000	5.430360000	-3.155112000
C	-6.219679000	5.041452000	-2.978789000
H	-5.625265000	4.763781000	-3.851466000
C	-5.630709000	4.989535000	-1.715149000
C	-8.611245000	6.170714000	0.410452000
H	-8.500688000	5.506528000	1.279069000
H	-9.664417000	6.148890000	0.100040000
H	-8.382856000	7.190158000	0.761726000
C	-8.153156000	5.480303000	-4.531028000
H	-7.788333000	6.366149000	-5.078766000
H	-9.249178000	5.539271000	-4.485276000
H	-7.877912000	4.589445000	-5.116273000
C	-4.178512000	4.595650000	-1.636393000
H	-3.582556000	5.308238000	-1.047667000
H	-3.745022000	4.547437000	-2.643966000
H	-4.058422000	3.605165000	-1.174106000
C	-5.946389000	6.426813000	1.890242000
C	-6.261098000	6.155043000	3.249826000
C	-6.503264000	7.207371000	4.130835000
H	-6.771686000	6.982657000	5.167663000

C	-6.408563000	8.539738000	3.726946000
C	-6.064800000	8.802867000	2.399155000
H	-5.966111000	9.840072000	2.068510000
C	-5.843575000	7.780690000	1.477086000
C	-6.412637000	4.751186000	3.783357000
H	-6.740502000	4.774954000	4.830628000
H	-5.466184000	4.194478000	3.739806000
H	-7.159727000	4.177644000	3.215900000
C	-6.632284000	9.652601000	4.710588000
H	-5.725299000	9.811548000	5.319774000
H	-7.460100000	9.418455000	5.399814000
H	-6.865886000	10.596423000	4.195016000
C	-5.484858000	8.179451000	0.066932000
H	-6.363512000	8.141551000	-0.597430000
H	-4.723213000	7.523171000	-0.374736000
H	-5.095393000	9.207275000	0.052922000
B	-5.762824000	5.281741000	0.857617000
Cu	1.497534000	-1.963030000	-2.229562000
Cu	1.016909000	1.235275000	-1.967792000
F	-0.142167000	-3.535271000	-4.314077000
F	-1.287834000	-4.010621000	-2.508743000
F	-2.342014000	-3.523119000	-4.380007000
F	-3.499343000	1.824767000	-3.044481000
F	-1.572689000	2.627776000	-3.688579000
F	-1.943601000	2.274359000	-1.568606000
F	0.292044000	3.914340000	-2.145624000
F	1.473969000	5.755229000	-1.996632000
F	0.883196000	4.676925000	-0.183564000
N	-0.183460000	-1.222947000	-2.644797000
N	-0.411639000	0.102569000	-2.447669000
N	2.498040000	2.376181000	-1.700846000
C	-1.286000000	-1.753995000	-3.231726000
C	-2.264418000	-0.769601000	-3.440216000
C	-1.644919000	0.383522000	-2.932446000
C	-1.274512000	-3.202069000	-3.602892000
C	-2.170706000	1.771133000	-2.816028000
C	-3.886254000	-0.035688000	-5.457392000
C	-5.114398000	0.652987000	-5.640725000
C	-5.335416000	1.365863000	-6.816836000
H	-6.275354000	1.907806000	-6.934842000
C	-4.401011000	1.404186000	-7.845133000
C	-3.195714000	0.730369000	-7.658744000
H	-2.446961000	0.750317000	-8.451712000
C	-2.915223000	0.035570000	-6.486291000
C	-6.203504000	0.693559000	-4.602283000
H	-5.816239000	0.841282000	-3.589924000
H	-6.892489000	1.522032000	-4.815641000
H	-6.788873000	-0.238605000	-4.588854000
C	-4.681488000	2.138675000	-9.121475000
H	-4.901493000	1.428134000	-9.932502000
H	-5.542796000	2.809853000	-9.015678000
H	-3.813715000	2.737557000	-9.429940000
C	-1.582057000	-0.661341000	-6.392363000
H	-1.683410000	-1.718366000	-6.111558000
H	-1.068108000	-0.625764000	-7.361498000
H	-0.929811000	-0.179310000	-5.648654000
C	-4.789762000	-1.753930000	-3.598396000
C	-5.218720000	-1.592091000	-2.260325000
C	-6.392253000	-2.203590000	-1.831060000
H	-6.743790000	-2.020780000	-0.815291000
C	-7.107116000	-3.070132000	-2.650917000
C	-6.641941000	-3.279493000	-3.949932000
H	-7.179907000	-3.968610000	-4.603285000

C	-5.528621000	-2.609397000	-4.446580000
C	-4.497142000	-0.711203000	-1.282454000
H	-4.952932000	-0.826737000	-0.288319000
H	-3.429365000	-0.965811000	-1.204305000
H	-4.576479000	0.352224000	-1.552163000
C	-8.302750000	-3.808055000	-2.124942000
H	-7.986123000	-4.750973000	-1.652957000
H	-8.830395000	-3.223001000	-1.363160000
H	-9.005616000	-4.057567000	-2.928429000
C	-5.158156000	-2.821048000	-5.892560000
H	-5.581946000	-2.024827000	-6.526170000
H	-4.074422000	-2.815433000	-6.055566000
H	-5.551831000	-3.781921000	-6.250699000
C	2.559834000	3.718141000	-1.547819000
C	3.888177000	4.166319000	-1.561686000
C	1.311510000	4.524073000	-1.455831000
C	5.536163000	6.204230000	-2.230625000
C	6.627075000	6.886130000	-1.637432000
C	7.642595000	7.404232000	-2.443706000
H	8.492528000	7.905039000	-1.972836000
C	7.603224000	7.296368000	-3.831514000
C	6.514475000	6.640941000	-4.410947000
H	6.464430000	6.558280000	-5.498619000
C	5.492859000	6.087048000	-3.640017000
C	6.751451000	7.060764000	-0.145859000
H	6.478731000	6.148070000	0.404454000
H	7.785715000	7.325801000	0.120923000
H	6.084479000	7.858720000	0.218754000
C	8.693107000	7.877888000	-4.687725000
H	8.316639000	8.737958000	-5.266021000
H	9.542089000	8.223268000	-4.080096000
H	9.064879000	7.131899000	-5.402828000
C	4.336530000	5.419850000	-4.345480000
H	3.364068000	5.733887000	-3.937922000
H	4.347610000	5.671677000	-5.415692000
H	4.387600000	4.324356000	-4.255581000
B	-3.649769000	-0.870987000	-4.166315000
B	4.409109000	5.622847000	-1.335315000
F	6.509468000	1.532784000	-1.639805000
F	6.791199000	3.663178000	-1.170335000
F	6.460905000	3.040786000	-3.258470000
N	3.773810000	1.906669000	-1.819081000
C	4.608239000	2.975231000	-1.763956000
C	6.086599000	2.811268000	-1.955111000
C	3.761345000	6.457620000	-0.199338000
C	3.298830000	7.771880000	-0.449313000
C	2.650374000	8.472341000	0.567502000
H	2.260135000	9.470624000	0.354767000
C	2.481476000	7.932539000	1.845360000
C	2.995312000	6.659917000	2.100453000
H	2.899426000	6.228856000	3.101788000
C	3.609619000	5.913362000	1.101258000
C	3.451606000	8.440666000	-1.794637000
H	3.111079000	7.802181000	-2.621475000
H	2.864470000	9.368345000	-1.826228000
H	4.508044000	8.693676000	-1.998172000
C	1.770069000	8.690245000	2.926363000
H	2.460460000	8.940152000	3.746553000
H	1.336112000	9.622763000	2.543907000
H	0.956085000	8.083787000	3.350469000
C	4.166088000	4.560399000	1.449116000
H	5.145784000	4.388187000	0.981700000
H	4.296363000	4.453864000	2.536007000

H	3.499765000	3.749945000	1.111848000
Cu	4.047413000	0.018131000	-1.727093000
F	1.353142000	-4.726597000	-1.593415000
F	2.616306000	-5.414596000	-3.248331000
F	2.956207000	-6.181468000	-1.217476000
F	7.589638000	-3.008632000	-0.856194000
F	6.636355000	-1.390327000	0.283598000
F	6.974312000	-1.160427000	-1.868963000
N	3.189100000	-2.672540000	-1.818001000
N	4.251581000	-1.863734000	-1.557705000
C	3.587271000	-3.955490000	-1.654325000
C	4.925295000	-4.013816000	-1.241368000
C	5.288020000	-2.660262000	-1.196669000
C	2.635127000	-5.070866000	-1.925521000
C	6.619631000	-2.062388000	-0.902041000
C	6.381717000	-5.349497000	0.567766000
C	7.724953000	-5.767244000	0.742783000
C	8.280237000	-5.785848000	2.024174000
H	9.322547000	-6.086949000	2.142699000
C	7.546472000	-5.430360000	3.155112000
C	6.219679000	-5.041452000	2.978789000
H	5.625265000	-4.763781000	3.851466000
C	5.630709000	-4.989535000	1.715149000
C	8.611245000	-6.170714000	-0.410452000
H	8.500688000	-5.506528000	-1.279069000
H	9.664417000	-6.148890000	-0.100040000
H	8.382856000	-7.190158000	-0.761726000
C	8.153156000	-5.480303000	4.531028000
H	7.788333000	-6.366149000	5.078766000
H	9.249178000	-5.539271000	4.485276000
H	7.877912000	-4.589445000	5.116273000
C	4.178512000	-4.595650000	1.636393000
H	3.582556000	-5.308238000	1.047667000
H	3.745022000	-4.547437000	2.643966000
H	4.058422000	-3.605165000	1.174106000
C	5.946389000	-6.426813000	-1.890242000
C	6.261098000	-6.155043000	-3.249826000
C	6.503264000	-7.207371000	-4.130835000
H	6.771686000	-6.982657000	-5.167663000
C	6.408563000	-8.539738000	-3.726946000
C	6.064800000	-8.802867000	-2.399155000
H	5.966111000	-9.840072000	-2.068510000
C	5.843575000	-7.780690000	-1.477086000
C	6.412637000	-4.751186000	-3.783357000
H	6.740502000	-4.774954000	-4.830628000
H	5.466184000	-4.194478000	-3.739806000
H	7.159727000	-4.177644000	-3.215900000
C	6.632284000	-9.652601000	-4.710588000
H	5.725299000	-9.811548000	-5.319774000
H	7.460100000	-9.418455000	-5.399814000
H	6.865886000	-10.596423000	-4.195016000
C	5.484858000	-8.179451000	-0.066932000
H	6.363512000	-8.141551000	0.597430000
H	4.723213000	-7.523171000	0.374736000
H	5.095393000	-9.207275000	-0.052922000
B	5.762824000	-5.281741000	-0.857617000

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Cu3CF3-Cu3CF3-T1

Cu	-0.968736755	1.690415262	1.479265945
Cu	-0.622919755	-1.498644738	1.803729945
F	0.273504245	3.473371262	3.673823945
F	1.596078245	3.749363262	1.938420945
F	2.432969245	3.597405262	3.958054945

F	3.475911245	-1.982912738	4.015306945
F	1.656279245	-2.008072738	5.218699945
F	1.617226245	-2.857936738	3.210000945
F	-0.015157755	-4.126414738	1.802333945
F	-1.270444755	-5.420610738	3.053256945
F	-1.085941755	-5.808552738	0.911513945
N	0.649816245	0.984969262	2.213643945
N	0.778326245	-0.354159738	2.451102945
N	-2.203639755	-2.574990738	1.573161945
C	1.560435245	1.632045262	2.988031945
C	2.305525245	0.727058262	3.758873945
C	1.751166245	-0.510661738	3.384564945
C	1.483289245	3.110624262	3.129225945
C	2.123100245	-1.835732738	3.949864945
C	3.381218245	0.404149262	6.194662945
C	4.515098245	-0.230522738	6.785537945
C	4.442074245	-0.724396738	8.086439945
H	5.316852245	-1.216222738	8.516532945
C	3.275922245	-0.629570738	8.842232945
C	2.160598245	-0.011220738	8.258067945
H	1.243890245	0.085757262	8.844323945
C	2.187991245	0.489075262	6.963328945
C	5.787524245	-0.411799738	6.014864945
H	5.600734245	-0.884770738	5.039323945
H	6.498212245	-1.036210738	6.572837945
H	6.275248245	0.555248262	5.800003945
C	3.200172245	-1.168860738	10.237868945
H	3.036819245	-0.354091738	10.962072945
H	4.124691245	-1.692868738	10.517766945
H	2.360739245	-1.872376738	10.342429945
C	0.954594245	1.169655262	6.435245945
H	1.186891245	2.160153262	6.017484945
H	0.213572245	1.303833262	7.234701945
H	0.482572245	0.584447262	5.632777945
C	4.684459245	1.855558262	4.286956945
C	5.289290245	1.635543262	3.019515945
C	6.394665245	2.381996262	2.628324945
H	6.856460245	2.178267262	1.662126945
C	6.927980245	3.388354262	3.436689945
C	6.335297245	3.611956262	4.684650945
H	6.731550245	4.402898262	5.325658945
C	5.241039245	2.876722262	5.120200945
C	4.811823245	0.548926262	2.105171945
H	5.550580245	0.367740262	1.320875945
H	3.851713245	0.827526262	1.634153945
H	4.635577245	-0.395765738	2.637261945
C	8.076541245	4.229158262	2.973657945
H	7.780016245	5.288414262	2.909106945
H	8.432531245	3.912711262	1.984417945
H	8.919884245	4.170146262	3.681000945
C	4.641404245	3.193040262	6.458940945
H	4.803395245	2.371544262	7.178721945
H	3.551549245	3.327716262	6.388111945
H	5.084556245	4.106880262	6.878905945
C	-2.356193755	-3.918204738	1.607782945
C	-3.717218755	-4.271097738	1.653253945
C	-1.186081755	-4.822211738	1.818800945
C	-5.334350755	-6.330625738	2.573884945
C	-6.296260755	-7.288894738	2.132060945
C	-6.954545755	-8.089930738	3.051073945
H	-7.688569755	-8.811019738	2.691737945
C	-6.694159755	-8.007264738	4.420874945
C	-5.811719755	-7.029871738	4.856428945

H	-5.619641755	-6.924207738	5.926150945
C	-5.152972755	-6.172631738	3.971525945
C	-6.677730755	-7.433362738	0.684059945
H	-6.957541755	-6.462763738	0.256264945
H	-7.537881755	-8.105678738	0.582629945
H	-5.857557755	-7.834130738	0.076211945
C	-7.345186755	-8.951662738	5.384717945
H	-6.720018755	-9.847138738	5.522576945
H	-8.323093755	-9.284184738	5.016676945
H	-7.483112755	-8.487325738	6.370288945
C	-4.258132755	-5.143192738	4.604277945
H	-3.614389755	-5.611922738	5.363499945
H	-4.879443755	-4.387921738	5.110996945
H	-3.616508755	-4.621005738	3.891071945
B	3.472196245	1.003292262	4.765373945
B	-4.356645755	-5.702251738	1.550651945
F	-6.170552755	-1.531353738	1.411933945
F	-6.558385755	-3.673183738	1.129811945
F	-6.174524755	-2.876416738	3.129561945
N	-3.445760755	-2.012274738	1.560158945
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C	-5.803650755	-2.775866738	1.819606945
C	-3.818616755	-6.543450738	0.342555945
C	-3.136483755	-7.762372738	0.571741945
C	-2.494166755	-8.394624738	-0.489659055
H	-1.929293755	-9.308737738	-0.295806055
C	-2.525620755	-7.880225738	-1.788775055
C	-3.264903755	-6.724171738	-2.018183055
H	-3.334120755	-6.321219738	-3.029126055
C	-3.901826755	-6.048247738	-0.980391055
C	-3.033799755	-8.371511738	1.944878945
H	-2.680139755	-7.644653738	2.690624945
H	-2.329908755	-9.214666738	1.937944945
H	-4.009716755	-8.741513738	2.293370945
C	-1.762537755	-8.548411738	-2.891893055
H	-1.980114755	-8.085660738	-3.863718055
H	-2.008869755	-9.617897738	-2.953582055
H	-0.677094755	-8.465129738	-2.710214055
C	-4.730976755	-4.843008738	-1.300568055
H	-5.754292755	-4.954740738	-0.913065055
H	-4.797108755	-4.684013738	-2.383329055
H	-4.318645755	-3.927151738	-0.854680055
Cu	-3.646212755	-0.130654738	1.177783945
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F	-2.159831755	5.322194262	2.910480945
F	-2.239890755	5.998243262	0.831354945
F	-7.124187755	3.014207262	1.387745945
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F	-6.465082755	0.943417262	1.124388945
N	-2.673924755	2.528964262	1.195293945
N	-3.804483755	1.789465262	0.980726945
C	-3.041934755	3.826580262	1.308539945
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C	-4.847157755	2.655833262	0.917402945
C	-2.058050755	4.902988262	1.619676945
C	-6.257590755	2.224827262	0.695011945
C	-6.150971755	5.532718262	-0.201247055
C	-7.464663755	6.035109262	-0.033592055
C	-8.263015755	6.269067262	-1.154336055
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C	-8.054952755	6.313407262	1.326226945
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H	-8.203791755	7.112548262	-4.279504055
H	-9.657461755	6.666077262	-3.353415055
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H	-4.105462755	7.556676262	-0.214624055
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B	-5.232621755	5.304863262	1.032539945
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H	6.957541755	6.462763738	-0.256264945
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C	3.818616755	6.543450738	-0.342555945
C	3.136483755	7.762372738	-0.571741945

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H	1.929293755	9.308737738	0.295806055
C	2.525620755	7.880225738	1.788775055
C	3.264903755	6.724171738	2.018183055
H	3.334120755	6.321219738	3.029126055
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H	2.680139755	7.644653738	-2.690624945
H	2.329908755	9.214666738	-1.937944945
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H	0.677094755	8.465129738	2.710214055
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H	5.754292755	4.954740738	0.913065055
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Cu	3.646212755	0.130654738	-1.177783945
F	0.789426755	-4.472080262	-1.431994945
F	2.159831755	-5.322194262	-2.910480945
F	2.239890755	-5.998243262	-0.831354945
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H	9.282242755	-6.635353262	1.010525055
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H	7.645621755	-7.238265262	-1.762267945
C	8.654370755	-6.331334262	3.648843055
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