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Derivation of the Rate Equations 3-5

The following describes a general derivation of the specific rate equations 3-5 in the text. The general postulated mechanism is:

$$TpCu + NO \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} TpCuNO$$

$$TpCuNO + xNO \xrightarrow{k_2} TpCuNO_2 + N_2O$$

where TpCu is the monomeric Cu(I) precusor (with any coordinated solvent not shown or explicitly considered) and x = 0 or 1. For the case where x = 0, the k_2 step is a unimolecular isomerization of some kind (see text), whereas when x = 1, the k_2 step involves attack of NO onto the TpCuNO complex. In both cases, subsequent steps are presumed to be fast (k_2 is rate-controlling). We also assume that k_1 and k_{-1} (and thus K_{eq}) are fast relative to k_2 (i.e., we have a rapid pre-equilibrium followed by a slow, rate-determining step, which is then followed by rapid steps that yield the final products). The overall rate expression is thus:

$$\text{rate} = k_2[TpCuNO][NO]^x$$

For a rapid pre-equilibrium, we define K_{eq} and $[Cu_{tot}]$ as follows:

$$K_{eq} = \frac{k_1}{k_{-1}} = \frac{[TpCuNO]}{[TpCu][NO]}$$

$$[Cu_{tot}] = [TpCu] + [TpCuNO]$$

We then rearrange the latter to give an expression in terms of [TpCu],

$$[TpCu] = [Cu_{tot}] - [TpCuNO]$$

and then substitute into the expression for K_{eq}:

$$\frac{k_1}{k_{-1}} = \frac{[TpCuNO]}{([Cu_{tot}] - [TpCuNO])[NO]}$$

This equation is then rearranged to give an expression for [TpCuNO] in terms of [NO], $[Cu_{tot}]$, and the rate constants k_1 and k_{-1}:

$$[TpCuNO] = \frac{k_1[NO][Cu_{tot}]}{k_{-1} + k_1[NO]}$$

By dividing top and bottom by k_{-1}, this same equation can be expressed using K_{eq}:

$$[\text{TpCuNO}] = \frac{K_{eq}[NO][Cu_{tot}]}{1 + K_{eq}[NO]}$$

Now we substitute this expression for [TpCuNO] into the overall rate expression:

$$\text{rate} = \frac{k_2[NO]^x K_{eq}[NO][Cu_{tot}]}{1 + K_{eq}[NO]}$$

which is equivalent to:

$$\text{rate} = \frac{k_2 K_{eq}[NO]^{x+1}[Cu_{tot}]}{1 + K_{eq}[NO]}$$

or, to put it in the same format as presented in the text,

$$\text{rate} = k_{obs}[Cu_{tot}]$$

$$k_{obs} = \frac{k_2 K_{eq}[NO]^{x+1}}{1 + K_{eq}[NO]}$$

When x = 0, this expression equals equation 4, and when x = 1, it equals equation 5.

CRYSTAL STRUCTURE REPORT

$C_{40}H_{48}BCuN_6O$

$Tp^{Ms,H}Cu(THF)$

Report prepared for:

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02 April 1998

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DATA COLLECTION

A crystal of the compound was attached to a glass fiber and mounted on the Enraf-Nonius CAD4 for a data collection at 177(2) K. Cell constants were determined from a set of 23 reflections determined from a random search routine. The data were corrected for Lorentz and polarization effects. 3 standard reflections were monitored hourly throughout the data collection which were used to calculate a correction for decay. Finally, a correction for absorption was determined empirically using DIFABS. Please refer to Table 1 for additional crystal and refinement information.

STRUCTURE SOLUTION AND REFINEMENT

The space group $R3c_h$ was determined based on systematic absences and intensity statistics.[1] A successful direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Several full-matrix least squares / difference Fourier cycles were performed which located the remainder of the non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters unless stated otherwise. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

The structure was re-refined and found as expected. The THF molecule in this structure is disordered. Three positions for this molecule are defined by the three-fold axis which the copper and boron atoms are positioned on. The THF oxygen atom is offset from the three-fold axis only slightly, causing unreasonable thermal parameters. Therefore, this oxygen atom was refined isotropically. All THF carbon atoms were refined anisotropically and the hydrogen atoms were placed in ideal positions and refined as riding atoms. The THF molecule was restrained using SAME.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Chemistry Department, The University of Minnesota. All calculations were preformed using SGI INDY R4400-SC or Pentium computers using the SHELXTL V5.0 suite of programs. All publications arising from this report must acknowledge the X-Ray Crystallographic Facility.

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1. SHELXTL-Plus V5.0, Siemens Industrial Automation, Inc., Madison, WI.

Some equations of interest:

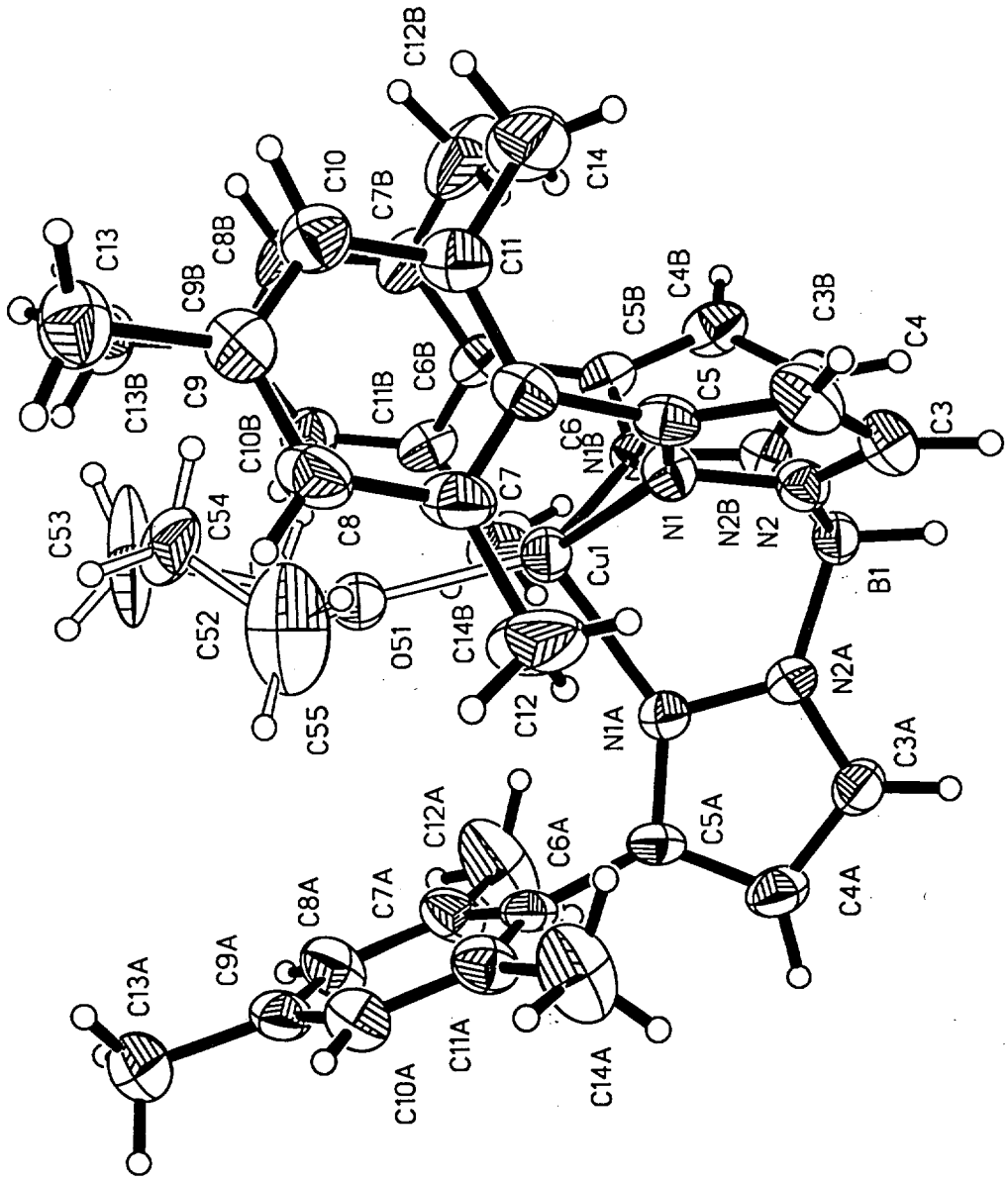
$$R_{int}=\Sigma|F_o^2-\langle F_o^2\rangle|/\Sigma|F_o^2|$$

$$R1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$$

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

where $w=q/\sigma^2(F_o^2)+(a*P)^2+b*P$

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



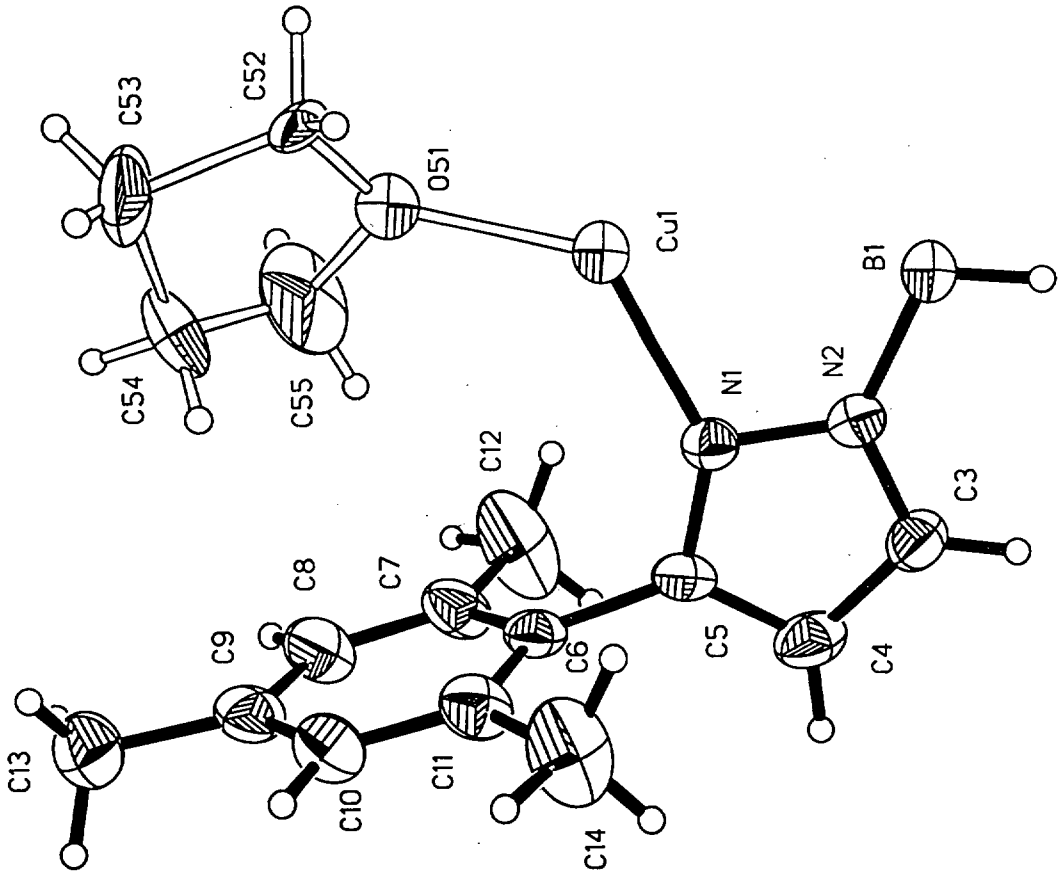

C52
C53
O51
Cu1
B1
C54
C55
N1
N2
C12
C3
C8
C7
C9
C6
C5
C4
C13
C10
C11
C14

Table 1. Crystal data, data collection, and solution and refinement for $Tp^{Ms,H}Cu(THF)$

Crystal Data	
Empirical formula	$C_{40}H_{48}BCuN_6O$
Crystal Habit, color	Prism, Colorless
Crystal size	0.600 x 0.500 x 0.300 mm
Crystal system	Rhombohedral
Space group	$R3c_h$
	a = 11.822(2) Å α = 90°
	b = 11.822(2) Å β = 90°
	c = 45.376(9) Å γ = 120°
Volume	5492(2) Å^3
Z	6
Formula weight	703.19
Density (calculated)	1.276 Mg/m^3
Absorption coefficient	0.637 mm^{-1}
F(000)	2232
Data Collection	
Diffractometer	Enraf-Nonius CAD4
Wavelength	0.71073 Å
Temperature	173(2) K
θ range for data collection	2.18 to 25.99°
Index ranges	$-14 \le h \le 14$, $-14 \le k \le 14$, $0 \le \ell \le 55$
Reflections collected	7289
Independent reflections	1225 (R_{int} = 0.065)
Solution and Refinement	
System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2)+(AP)^2+(BP)]^{-1}$, where $P = (Fo^2+2Fc^2))/3$, A = 0.0379, and B = 1.9906
Absorption correction	Semi-Empirical
Max. and min. transmission	1.31 and 0.79
Absolute structure parameter	-0.02(3)
Data / restraints / parameters	1225 / 1 / 173
R indices ($I>2\sigma(I)$ = 1077)	R1 = 0.0369, wR2 = 0.0891
R indices (all data)	R1 = 0.0438, wR2 = 0.0929
Goodness-of-fit on F^2	1.062
Largest diff. peak and hole	0.328 and -0.735 eÅ^{-3}

$Tp^{Ms,H}Cu(THF)$

Table 2. Atomic coordinates [x_3 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Cu(1)	10000	0	4999(1)	31(1)	1
N(1)	8402(3)	-1261(3)	5247(1)	28(1)	1
N(2)	8682(4)	-1118(4)	5541(1)	28(1)	1
C(3)	7656(4)	-2077(4)	5689(1)	35(1)	1
C(4)	6702(4)	-2847(4)	5492(1)	40(1)	1
C(5)	7208(4)	-2305(4)	5217(1)	30(1)	1
C(6)	6632(4)	-2691(4)	4915(1)	31(1)	1
C(7)	6801(4)	-3597(5)	4754(1)	43(1)	1
C(8)	6348(5)	-3856(5)	4463(1)	48(1)	1
C(9)	5772(4)	-3220(5)	4331(1)	40(1)	1
C(10)	5551(4)	-2383(4)	4500(1)	42(1)	1
C(11)	5984(4)	-2097(4)	4792(1)	39(1)	1
C(12)	7434(8)	-4304(7)	4890(2)	85(2)	1
C(13)	5366(6)	-3464(6)	4011(1)	53(1)	1
C(14)	5692(7)	-1189(6)	4969(1)	64(2)	1
B(1)	10000	0	5654(2)	29(2)	1
O(51)	10312(10)	-15(15)	4565(2)	36(3)	0.33
C(52)	10870(22)	962(21)	4383(5)	50(7)	0.33
C(53)	10211(81)	550(53)	4060(5)	107(34)	0.33
C(54)	9129(24)	-784(24)	4156(4)	53(6)	0.33
C(55)	9543(37)	-1282(31)	4399(9)	98(15)	0.33

Table 3. Bond lengths [Å] and angles [°] $Tp^{Ms,H}Cu(THF)$

Cu(1)-O(51)#1	2.004(7)	Cu(1)-O(51)#2	2.004(7)
Cu(1)-O(51)	2.004(7)	Cu(1)-N(1)	2.061(3)
Cu(1)-N(1)#2	2.061(3)	Cu(1)-N(1)#1	2.061(3)
N(1)-C(5)	1.339(5)	N(1)-N(2)	1.364(4)
N(2)-C(3)	1.352(5)	N(2)-B(1)	1.542(4)
C(3)-C(4)	1.370(6)	C(4)-C(5)	1.392(6)
C(5)-C(6)	1.495(5)	C(6)-C(11)	1.390(6)
C(6)-C(7)	1.391(6)	C(7)-C(8)	1.401(6)
C(7)-C(12)	1.506(7)	C(8)-C(9)	1.377(7)
C(9)-C(10)	1.376(6)	C(9)-C(13)	1.512(5)
C(10)-C(11)	1.399(7)	C(11)-C(14)	1.512(6)
B(1)-N(2)#2	1.542(4)	B(1)-N(2)#1	1.542(4)
O(51)-C(52)	1.30(3)	O(51)-C(55)	1.51(3)
C(52)-C(53)	1.62(4)	C(53)-C(54)	1.51(3)
C(54)-C(55)	1.45(5)		

O(51)#1-Cu(1)-O(51)#2	18.8(4)	O(51)#1-Cu(1)-O(51)	18.8(4)
O(51)#2-Cu(1)-O(51)	18.8(4)	O(51)#1-Cu(1)-N(1)	112.4(3)
O(51)#2-Cu(1)-N(1)	126.4(4)	O(51)-Cu(1)-N(1)	129.6(4)
O(51)#1-Cu(1)-N(1)#2	126.4(4)	O(51)#2-Cu(1)-N(1)#2	129.6(4)
O(51)-Cu(1)-N(1)#2	112.4(2)	N(1)-Cu(1)-N(1)#2	92.94(12)
O(51)#1-Cu(1)-N(1)#1	129.6(4)	O(51)#2-Cu(1)-N(1)#1	112.4(2)
O(51)-Cu(1)-N(1)#1	126.4(4)	N(1)-Cu(1)-N(1)#1	92.94(12)
N(1)#2-Cu(1)-N(1)#1	92.94(12)	C(5)-N(1)-N(2)	107.1(3)
C(5)-N(1)-Cu(1)	140.6(3)	N(2)-N(1)-Cu(1)	111.5(2)
C(3)-N(2)-N(1)	108.7(3)	C(3)-N(2)-B(1)	130.7(4)
N(1)-N(2)-B(1)	120.6(4)	N(2)-C(3)-C(4)	109.1(3)
C(3)-C(4)-C(5)	105.0(3)	N(1)-C(5)-C(4)	110.1(3)
N(1)-C(5)-C(6)	119.1(3)	C(4)-C(5)-C(6)	130.8(3)
C(11)-C(6)-C(7)	120.3(4)	C(11)-C(6)-C(5)	119.8(4)
C(7)-C(6)-C(5)	119.9(4)	C(6)-C(7)-C(8)	118.6(4)
C(6)-C(7)-C(12)	120.9(4)	C(8)-C(7)-C(12)	120.5(4)
C(9)-C(8)-C(7)	121.9(4)	C(10)-C(9)-C(8)	118.3(4)
C(10)-C(9)-C(13)	121.1(5)	C(8)-C(9)-C(13)	120.6(4)
C(9)-C(10)-C(11)	121.5(4)	C(6)-C(11)-C(10)	119.1(4)
C(6)-C(11)-C(14)	121.6(4)	C(10)-C(11)-C(14)	119.3(4)
N(2)#2-B(1)-N(2)#1	109.6(3)	N(2)#2-B(1)-N(2)	109.6(3)
N(2)#1-B(1)-N(2)	109.6(3)	C(52)-O(51)-C(55)	110.5(14)
C(52)-O(51)-Cu(1)	129.1(13)	C(55)-O(51)-Cu(1)	119(2)
O(51)-C(52)-C(53)	111(2)	C(54)-C(53)-C(52)	95(2)
C(55)-C(54)-C(53)	111(4)	C(54)-C(55)-O(51)	98(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y+2,-x+1,z #2 -y+1,x-y-1,z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2 U_{11}$ + ... + $2hka^*b^* U_{12}$]

	U11	U22	U33	U23	U13	U12
Cu(1)	32(1)	32(1)	27(1)	0	0	16(1)
N(1)	25(2)	27(2)	29(2)	0(1)	1(1)	10(1)
N(2)	25(2)	29(2)	30(2)	1(1)	3(1)	13(2)
C(3)	34(2)	32(2)	32(2)	1(2)	7(2)	13(2)
C(4)	30(2)	30(2)	49(2)	-3(2)	10(2)	7(2)
C(5)	19(2)	27(2)	40(2)	-5(2)	-1(2)	10(2)
C(6)	20(2)	28(2)	38(2)	-7(2)	1(2)	7(2)
C(7)	34(2)	52(3)	50(2)	-19(2)	-11(2)	27(2)
C(8)	41(3)	60(3)	50(2)	-27(2)	-9(2)	30(2)
C(9)	28(2)	36(2)	45(2)	-9(2)	-4(2)	8(2)
C(10)	41(2)	39(3)	45(2)	-3(2)	-6(2)	20(2)
C(11)	36(2)	33(2)	48(2)	-9(2)	-4(2)	17(2)
C(12)	117(6)	115(6)	79(4)	-52(4)	-43(4)	101(5)
C(13)	54(3)	56(3)	43(3)	-7(2)	-5(2)	22(3)
C(14)	94(5)	66(4)	63(3)	-21(3)	-17(3)	63(4)
B(1)	31(3)	31(3)	23(3)	0	0	16(1)
C(52)	33(12)	40(9)	26(8)	-10(7)	12(8)	-21(9)
C(53)	93(22)	117(43)	20(8)	-4(11)	-5(17)	-15(33)
C(54)	64(13)	54(10)	40(13)	-19(10)	-30(11)	30(11)
C(55)	113(26)	50(17)	73(19)	-36(14)	-28(16)	-3(16)

Table 5. Torsion angles [°] $Tp^{Ms,H}Cu(THF)$

O(51)#1-Cu(1)-N(1)-C(5)	5.9(7)	O(51)#2-Cu(1)-N(1)-C(5)	20.4(6)
O(51)-Cu(1)-N(1)-C(5)	-3.2(6)	N(1)#2-Cu(1)-N(1)-C(5)	-125.7(5)
N(1)#1-Cu(1)-N(1)-C(5)	141.2(5)	O(51)#1-Cu(1)-N(1)-N(2)	174.2(5)
O(51)#2-Cu(1)-N(1)-N(2)	-171.3(4)	O(51)-Cu(1)-N(1)-N(2)	165.1(4)
N(1)#2-Cu(1)-N(1)-N(2)	42.6(2)	N(1)#1-Cu(1)-N(1)-N(2)	-50.5(2)
C(5)-N(1)-N(2)-C(3)	0.0(5)	Cu(1)-N(1)-N(2)-C(3)	-172.3(3)
C(5)-N(1)-N(2)-B(1)	179.7(3)	Cu(1)-N(1)-N(2)-B(1)	7.4(4)
N(1)-N(2)-C(3)-C(4)	-0.2(5)	B(1)-N(2)-C(3)-C(4)	-179.8(3)
N(2)-C(3)-C(4)-C(5)	0.2(5)	N(2)-N(1)-C(5)-C(4)	0.1(5)
Cu(1)-N(1)-C(5)-C(4)	168.8(3)	N(2)-N(1)-C(5)-C(6)	179.3(3)
Cu(1)-N(1)-C(5)-C(6)	-12.1(7)	C(3)-C(4)-C(5)-N(1)	-0.2(5)
C(3)-C(4)-C(5)-C(6)	-179.2(4)	N(1)-C(5)-C(6)-C(11)	-84.6(5)
C(4)-C(5)-C(6)-C(11)	94.4(6)	N(1)-C(5)-C(6)-C(7)	92.4(5)
C(4)-C(5)-C(6)-C(7)	-88.7(6)	C(11)-C(6)-C(7)-C(8)	2.3(7)
C(5)-C(6)-C(7)-C(8)	-174.6(4)	C(11)-C(6)-C(7)-C(12)	-176.6(5)
C(5)-C(6)-C(7)-C(12)	6.5(7)	C(6)-C(7)-C(8)-C(9)	1.5(7)
C(12)-C(7)-C(8)-C(9)	-179.6(5)	C(7)-C(8)-C(9)-C(10)	-5.1(7)
C(7)-C(8)-C(9)-C(13)	176.3(5)	C(8)-C(9)-C(10)-C(11)	4.8(7)
C(13)-C(9)-C(10)-C(11)	-176.6(4)	C(7)-C(6)-C(11)-C(10)	-2.5(6)
C(5)-C(6)-C(11)-C(10)	174.4(4)	C(7)-C(6)-C(11)-C(14)	175.2(5)
C(5)-C(6)-C(11)-C(14)	-7.9(7)	C(9)-C(10)-C(11)-C(6)	-1.1(7)
C(9)-C(10)-C(11)-C(14)	-178.9(5)	C(3)-N(2)-B(1)-N(2)#2	114.4(6)
N(1)-N(2)-B(1)-N(2)#2	-65.2(4)	C(3)-N(2)-B(1)-N(2)#1	-125.3(5)
N(1)-N(2)-B(1)-N(2)#1	55.1(5)	O(51)#1-Cu(1)-O(51)-C(52)	114(3)
O(51)#2-Cu(1)-O(51)-C(52)	53(3)	N(1)-Cu(1)-O(51)-C(52)	141(2)
N(1)#2-Cu(1)-O(51)-C(52)	-105(2)	N(1)#1-Cu(1)-O(51)-C(52)	7(2)
O(51)#1-Cu(1)-O(51)-C(55)	-49(3)	O(51)#2-Cu(1)-O(51)-C(55)	-110(3)
N(1)-Cu(1)-O(51)-C(55)	-22(2)	N(1)#2-Cu(1)-O(51)-C(55)	92(2)
N(1)#1-Cu(1)-O(51)-C(55)	-156(2)	C(55)-O(51)-C(52)-C(53)	17(6)
Cu(1)-O(51)-C(52)-C(53)	-147(5)	O(51)-C(52)-C(53)-C(54)	7(7)
C(52)-C(53)-C(54)-C(55)	-30(6)	C(53)-C(54)-C(55)-O(51)	39(5)
C(52)-O(51)-C(55)-C(54)	-34(3)	Cu(1)-O(51)-C(55)-C(54)	132(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y+2,-x+1,z #2 -y+1,x-y-1,z

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) $Tp^{Ms,H}Cu(THF)$

	x	y	z	U(eq)	SOF
H(3A)	7606(4)	-2197(4)	5897(1)	42	1
H(4A)	5875(4)	-3589(4)	5533(1)	48	1
H(8A)	6440(5)	-4489(5)	4353(1)	57	1
H(10A)	5094(4)	-1990(4)	4417(1)	50	1
H(12A)	7470(8)	-4899(7)	4745(2)	127	1
H(12B)	6923(8)	-4806(7)	5061(2)	127	1
H(12C)	8322(8)	-3668(7)	4953(2)	127	1
H(13A)	5601(6)	-4083(6)	3927(1)	80	1
H(13B)	5814(6)	-2639(6)	3902(1)	80	1
H(13C)	4419(6)	-3828(6)	3996(1)	80	1
H(14A)	5233(7)	-871(6)	4844(1)	96	1
H(14B)	6513(7)	-447(6)	5039(1)	96	1
H(14C)	5142(7)	-1662(6)	5138(1)	96	1
H(1A)	10000	0	5874(2)	34	1
H(52A)	11812(22)	1253(21)	4369(5)	60	0.33
H(52B)	10784(22)	1701(21)	4458(5)	60	0.33
H(53A)	9879(81)	1121(53)	3989(5)	128	0.33
H(53B)	10800(81)	501(53)	3912(5)	128	0.33
H(54A)	8357(24)	-721(24)	4216(4)	63	0.33
H(54B)	8871(24)	-1398(24)	3988(4)	63	0.33
H(55A)	10097(37)	-1643(31)	4333(9)	117	0.33
H(55B)	8795(37)	-1947(31)	4515(9)	117	0.33

CRYSTAL STRUCTURE REPORT

$C_{17}H_{16}BCuF_9N_7$

$Tp^{CF3,CH3}Cu(CH_3CN)$

Report prepared for:
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DATA COLLECTION

A crystal of the compound was attached to a glass fiber and mounted on the Enraf-Nonius CAD4 for a data collection at 293(2) K. Cell constants were determined from a set of 25 reflections determined from a random search routine. The data were corrected for Lorentz and polarization effects. 3 standard reflections were monitored hourly throughout the data collection which were used to calculate a correction for decay. Finally, a correction for absorption was determined from a series of ψ scans. Please refer to Table 1 for additional crystal and refinement information.

STRUCTURE SOLUTION AND REFINEMENT

The space group $P2_1/c$ was determined based on systematic absences and intensity statistics.[1] A successful direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Several full-matrix least squares / difference Fourier cycles were performed which located the remainder of the non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters unless stated otherwise. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

The structure was re-refined and found as expected. Each of the disordered CF3 groups were refined as two parts. The C17 group was refined with each part half occupied. The C27 and C37 CF3 groups refined as .64/.36 and .40/.60 percent occupied respectively. The SAME and DELU restraints were used on the CF3 groups in order to maintain sensical bond lengths and angles. The EADP and EXYZ constraints were used on carbon atoms C17, C27, and C37 to keep the positional and displacement parameters of each part equivalent.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Chemistry Department, The University of Minnesota. All calculations were preformed using SGI INDY R4400-SC or Pentium computers using the SHELXTL V5.0 suite of programs. All publications arising from this report must acknowledge the X-Ray Crystallographic Facility.

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1. SHELXTL-Plus V5.0, Siemens Industrial Automation, Inc., Madison, WI.

Some equations of interest:

$$R_{int}=\sum|F_o^2-\langle F_o^2\rangle|/\sum|F_o^2|$$

$$R1=\sum||F_o|-|F_c||/\sum|F_o|$$

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

where $w=q/\sigma^2(F_o^2)+(a*p)^2+b*p$

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

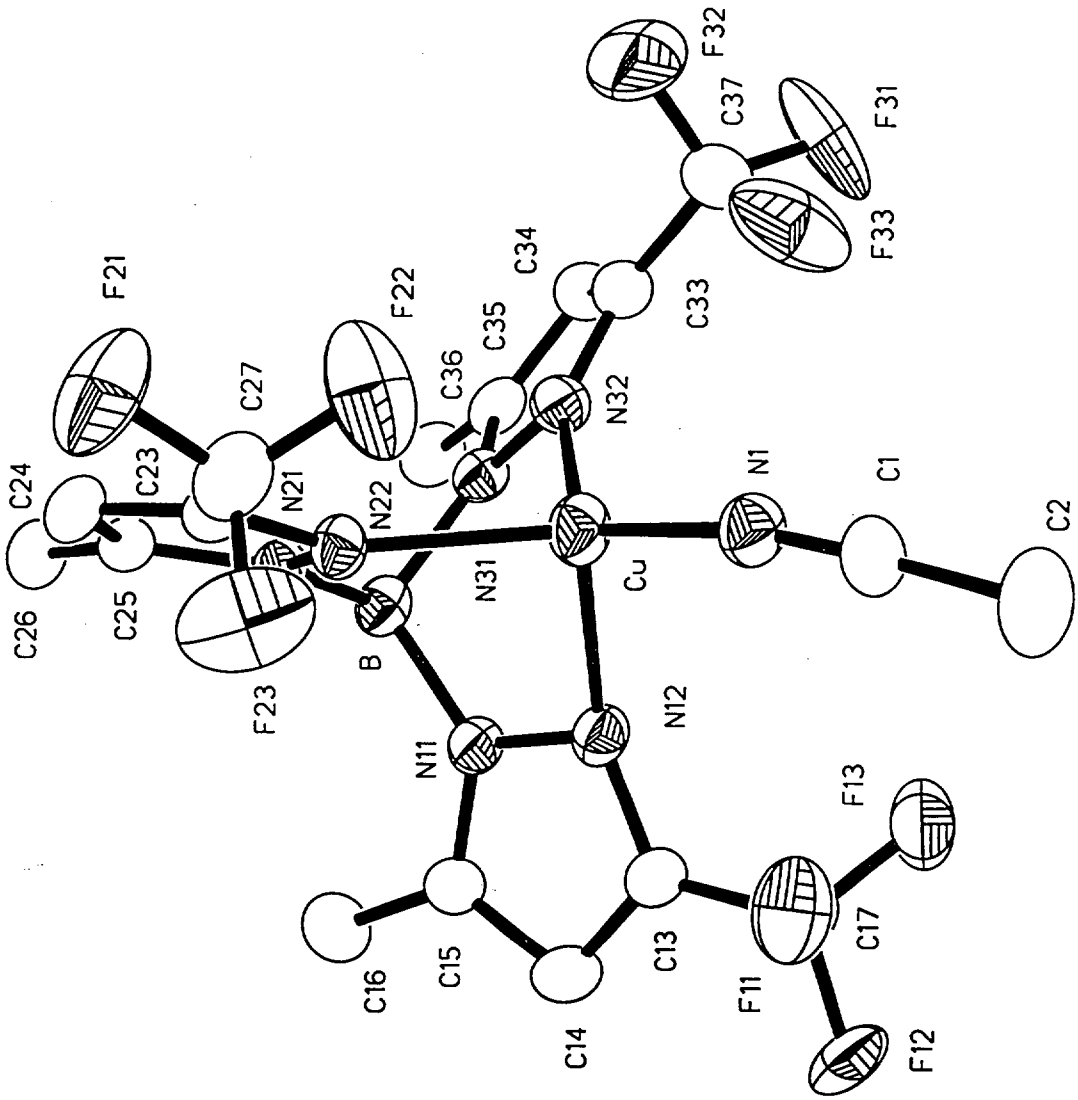
F32
C37
F31
F33
C33
C34
C35
C36
F21
F22
C27
N32
C24
C23
N21
N22
N1
C1
C2
C26
C25
N31
Cu
B
F23
N12
N11
F13
C17
C16
C15
C13
F11
C14
F12

Table 3. Crystal data, data collection, and solution and refinement for $Tp^{CF3,CH3}Cu(CH_3CN)$

Crystal Data	
Empirical formula	$C_{17}H_{16}BCuF_9N_7$
Crystal Habit, color	Block, Colorless
Crystal size	0.500 x 0.500 x 0.500 mm
Crystal system	Monoclinic
Space group	$P2_1/c$
	a = 11.936(2) Å α = 90°
	b = 8.954(2) Å β = 102.80(3)°
	c = 21.890(4) Å γ = 90°
Volume	2281.4(8) $Å^3$
Z	4
Formula weight	563.72
Density (calculated)	1.641 Mg/m^3
Absorption coefficient	1.051 mm^{-1}
F(000)	1128
Data Collection	
Diffractometer	Siemens SMART Platform CCD
Wavelength	0.71073 Å
Temperature	293(2) K
θ range for data collection	2.29 to 25.04°
Index ranges	$0 \le h \le 14$, $0 \le k \le 10$, $-25 \le \ell \le 25$
Reflections collected	4511
Independent reflections	4008 (R_{int} = 0.1723)
Solution and Refinement	
System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2)+(AP)^2+(BP)]^{-1}$, where P = $(Fo^2+2Fc^2))/3$, A = , and B =
Absorption correction	Semi-empirical from ψ-scans
Max. and min. transmission	1.00 and 0.92
Data / restraints / parameters	4005 / 337 / 402
R indices ($I>2\sigma(I)$ = 2368)	R1 = 0.0565, wR2 = 0.1474
R indices (all data)	R1 = 0.1202, wR2 = 0.1890
Goodness-of-fit on F^2	1.010
Largest diff. peak and hole	0.932 and -0.613 $eÅ^{-3}$

Table 2. Atomic coordinates [$x_3 10^4$] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

$Tp^{CF3,CH3}Cu(CH_3CN)$

	x	y	z	U(eq)	SOF
Cu	3233(1)	2556(1)	1160(1)	58(1)	1
C(17)	6458(5)	3351(7)	1582(3)	65(2)	0.50
F(11)	6337(24)	2015(16)	1305(9)	99(6)	0.50
F(12)	7508(13)	3741(30)	1604(13)	108(7)	0.50
F(13)	6348(28)	3088(36)	2159(8)	121(9)	0.50
C(17A)	6458(5)	3351(7)	1582(3)	65(2)	0.50
F(11A)	6555(25)	2111(21)	1269(10)	98(6)	0.50
F(12A)	7511(16)	3884(32)	1773(13)	99(6)	0.50
F(13A)	6170(26)	2880(29)	2108(9)	80(4)	0.50
C(27)	1826(5)	917(7)	-341(3)	70(2)	0.64(3)
F(21)	972(10)	410(13)	-755(8)	109(6)	0.64(3)
F(22)	1880(23)	117(9)	163(4)	119(7)	0.64(3)
F(23)	2750(12)	537(15)	-539(12)	124(7)	0.64(3)
C(27A)	1826(5)	917(7)	-341(3)	70(2)	0.36(3)
F(21A)	1046(32)	297(20)	-93(24)	146(16)	0.36(3)
F(22A)	2772(19)	308(20)	-82(20)	132(14)	0.36(3)
F(23A)	1577(47)	615(27)	-921(7)	169(20)	0.36(3)
C(37)	1464(5)	2694(7)	2330(3)	70(2)	0.40(3)
F(31)	1573(38)	3005(30)	2925(7)	153(12)	0.40(3)
F(32)	452(18)	2322(43)	2109(17)	178(14)	0.40(3)
F(33)	2175(28)	1614(31)	2322(16)	131(10)	0.40(3)
C(37A)	1464(5)	2694(7)	2330(3)	70(2)	0.60(3)
F(31A)	2369(11)	1952(21)	2580(12)	133(7)	0.60(3)
F(32A)	913(21)	2934(20)	2770(11)	153(9)	0.60(3)
F(33A)	801(15)	1685(14)	1970(6)	108(5)	0.60(3)
N(1)	3979(4)	815(5)	1514(2)	59(1)	1
N(11)	4032(3)	5543(5)	878(2)	45(1)	1
N(12)	4518(3)	4344(5)	1223(2)	51(1)	1
N(21)	2150(3)	4672(4)	214(2)	43(1)	1
N(22)	2390(4)	3182(5)	273(2)	47(1)	1
N(31)	2247(3)	5447(5)	1328(2)	46(1)	1
N(32)	2218(4)	4013(5)	1539(2)	48(1)	1
C(1)	4603(5)	-67(7)	1756(3)	63(2)	1
C(2)	5444(7)	-1178(9)	2037(4)	97(3)	1
C(13)	5636(4)	4456(6)	1241(3)	51(1)	1
C(14)	5880(5)	5688(7)	914(3)	62(2)	1
C(15)	4837(5)	6361(6)	685(3)	53(1)	1
C(16)	4573(6)	7721(7)	293(3)	76(2)	1
C(23)	1776(4)	2550(6)	-240(3)	48(1)	1
C(24)	1139(4)	3605(6)	-631(3)	52(1)	1
C(25)	1386(4)	4939(6)	-332(2)	46(1)	1
C(26)	929(5)	6463(6)	-528(3)	61(2)	1
C(33)	1687(4)	4068(7)	2007(3)	54(1)	1
C(34)	1383(5)	5531(7)	2116(3)	57(1)	1
C(35)	1738(4)	6368(6)	1672(3)	51(1)	1
C(36)	1635(5)	8015(7)	1563(3)	65(2)	1
B	2719(5)	5763(6)	741(3)	46(1)	1

Table 3. Bond lengths [Å] and angles [°] $Tp^{CF3,CH3}Cu(CH_3CN)$

Cu-N(1)	1.875(5)	Cu-N(22)	2.057(4)
Cu-N(32)	2.075(4)	Cu-N(12)	2.200(4)
C(17)-F(12)	1.291(13)	C(17)-F(13)	1.32(2)
C(17)-F(11)	1.335(14)	C(17)-C(13)	1.475(8)
C(17A)-F(11A)	1.32(2)	C(17A)-F(12A)	1.322(14)
C(17A)-F(13A)	1.34(2)	C(17A)-C(13)	1.475(8)
C(27)-F(21)	1.287(10)	C(27)-F(22)	1.306(10)
C(27)-F(23)	1.315(10)	C(27)-C(23)	1.482(8)
C(27A)-F(23A)	1.27(2)	C(27A)-F(22A)	1.269(13)
C(27A)-F(21A)	1.301(13)	C(27A)-C(23)	1.482(8)
C(37)-F(32)	1.243(14)	C(37)-F(33)	1.29(2)
C(37)-F(31)	1.310(14)	C(37)-C(33)	1.473(8)
C(37A)-F(31A)	1.283(13)	C(37A)-F(32A)	1.299(12)
C(37A)-F(33A)	1.338(11)	C(37A)-C(33)	1.473(8)
N(1)-C(1)	1.133(7)	N(11)-C(15)	1.349(7)
N(11)-N(12)	1.365(6)	N(11)-B	1.541(7)
N(12)-C(13)	1.330(6)	N(21)-C(25)	1.354(6)
N(21)-N(22)	1.365(6)	N(21)-B	1.548(7)
N(22)-C(23)	1.324(7)	N(31)-C(35)	1.349(7)
N(31)-N(32)	1.368(6)	N(31)-B	1.540(7)
N(32)-C(33)	1.318(7)	C(1)-C(2)	1.450(8)
C(13)-C(14)	1.380(8)	C(14)-C(15)	1.373(8)
C(15)-C(16)	1.482(8)	C(23)-C(24)	1.384(7)
C(24)-C(25)	1.363(7)	C(25)-C(26)	1.497(7)
C(33)-C(34)	1.394(8)	C(34)-C(35)	1.367(8)
C(35)-C(36)	1.495(8)		

N(1)-Cu-N(22)	134.8(2)	N(1)-Cu-N(32)	128.5(2)
N(22)-Cu-N(32)	90.0(2)	N(1)-Cu-N(12)	108.6(2)
N(22)-Cu-N(12)	92.8(2)	N(32)-Cu-N(12)	88.8(2)
F(12)-C(17)-F(13)	108.3(14)	F(12)-C(17)-F(11)	105.4(13)
F(13)-C(17)-F(11)	104.6(13)	F(12)-C(17)-C(13)	111.6(13)
F(13)-C(17)-C(13)	114(2)	F(11)-C(17)-C(13)	112.2(10)
F(11A)-C(17A)-F(12A)	106.3(13)	F(11A)-C(17A)-F(13A)	104.5(13)
F(12A)-C(17A)-F(13A)	104.4(13)	F(11A)-C(17A)-C(13)	115.1(11)
F(12A)-C(17A)-C(13)	113(2)	F(13A)-C(17A)-C(13)	112(2)
F(21)-C(27)-F(22)	106.6(8)	F(21)-C(27)-F(23)	105.6(9)
F(22)-C(27)-F(23)	104.4(8)	F(21)-C(27)-C(23)	113.6(7)
F(22)-C(27)-C(23)	114.2(7)	F(23)-C(27)-C(23)	111.6(7)
F(23A)-C(27A)-F(22A)	110.2(14)	F(23A)-C(27A)-F(21A)	107.2(13)
F(22A)-C(27A)-F(21A)	106.1(13)	F(23A)-C(27A)-C(23)	110.6(12)
F(22A)-C(27A)-C(23)	114.7(10)	F(21A)-C(27A)-C(23)	107.6(9)
F(32)-C(37)-F(33)	112(2)	F(32)-C(37)-F(31)	109(2)
F(33)-C(37)-F(31)	104.6(14)	F(32)-C(37)-C(33)	107.5(12)
F(33)-C(37)-C(33)	116(2)	F(31)-C(37)-C(33)	108.2(14)
F(31A)-C(37A)-F(32A)	106.7(12)	F(31A)-C(37A)-F(33A)	103.6(9)
F(32A)-C(37A)-F(33A)	102.6(10)	F(31A)-C(37A)-C(33)	114.4(11)
F(32A)-C(37A)-C(33)	113.2(10)	F(33A)-C(37A)-C(33)	115.2(8)
C(1)-N(1)-Cu	167.2(5)	C(15)-N(11)-N(12)	110.8(4)
C(15)-N(11)-B	129.3(4)	N(12)-N(11)-B	119.8(4)
C(13)-N(12)-N(11)	104.9(4)	C(13)-N(12)-Cu	137.5(4)
N(11)-N(12)-Cu	109.4(3)	C(25)-N(21)-N(22)	110.0(4)
C(25)-N(21)-B	130.2(4)	N(22)-N(21)-B	119.9(4)
C(23)-N(22)-N(21)	105.8(4)	C(23)-N(22)-Cu	138.3(4)
N(21)-N(22)-Cu	113.8(3)	C(35)-N(31)-N(32)	109.7(4)
C(35)-N(31)-B	130.3(4)	N(32)-N(31)-B	119.7(4)
C(33)-N(32)-N(31)	106.2(4)	C(33)-N(32)-Cu	139.3(4)
N(31)-N(32)-Cu	113.2(3)	N(1)-C(1)-C(2)	176.5(7)
N(12)-C(13)-C(14)	111.7(5)	N(12)-C(13)-C(17A)	121.0(5)

C(14)-C(13)-C(17A)	127.3(5)	N(12)-C(13)-C(17)	121.0(5)
C(14)-C(13)-C(17)	127.3(5)	C(15)-C(14)-C(13)	105.2(5)
N(11)-C(15)-C(14)	107.3(5)	N(11)-C(15)-C(16)	123.6(5)
C(14)-C(15)-C(16)	129.2(5)	N(22)-C(23)-C(24)	111.0(5)
N(22)-C(23)-C(27A)	121.0(5)	C(24)-C(23)-C(27A)	128.0(5)
N(22)-C(23)-C(27)	121.0(5)	C(24)-C(23)-C(27)	128.0(5)
C(25)-C(24)-C(23)	105.7(4)	N(21)-C(25)-C(24)	107.6(4)
N(21)-C(25)-C(26)	123.0(5)	C(24)-C(25)-C(26)	129.4(5)
N(32)-C(33)-C(34)	110.9(5)	N(32)-C(33)-C(37A)	120.7(5)
C(34)-C(33)-C(37A)	128.3(5)	N(32)-C(33)-C(37)	120.7(5)
C(34)-C(33)-C(37)	128.3(5)	C(35)-C(34)-C(33)	105.0(5)
N(31)-C(35)-C(34)	108.1(5)	N(31)-C(35)-C(36)	123.1(5)
C(34)-C(35)-C(36)	128.8(5)	N(31)-B-N(11)	111.0(4)
N(31)-B-N(21)	108.9(4)	N(11)-B-N(21)	109.0(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$ $Tp^{CF3,CH3}Cu(CH_3CN)$

	U11	U22	U33	U23	U13	U12
Cu	60(1)	46(1)	64(1)	12(1)	5(1)	10(1)
C(17)	45(3)	79(4)	68(4)	1(3)	6(3)	7(3)
F(11)	110(14)	65(6)	113(11)	28(6)	6(8)	39(7)
F(12)	36(6)	145(15)	141(18)	57(12)	13(7)	27(6)
F(13)	95(16)	202(25)	67(8)	51(10)	21(10)	66(14)
C(17A)	45(3)	79(4)	68(4)	1(3)	6(3)	7(3)
F(11A)	88(9)	103(11)	90(10)	-32(9)	-4(7)	23(7)
F(12A)	57(7)	112(10)	110(11)	-5(9)	-18(6)	-14(7)
F(13A)	63(7)	96(9)	73(7)	18(6)	-2(5)	10(7)
C(27)	69(4)	52(3)	81(4)	-7(3)	-1(3)	1(3)
F(21)	104(8)	51(5)	137(11)	-15(6)	-45(6)	-12(4)
F(22)	212(19)	43(4)	92(6)	12(3)	14(7)	13(8)
F(23)	107(8)	81(6)	193(19)	-47(10)	53(10)	4(6)
C(27A)	69(4)	52(3)	81(4)	-7(3)	-1(3)	1(3)
F(21A)	149(24)	54(9)	264(44)	20(16)	106(27)	-21(12)
F(22A)	127(17)	61(10)	170(27)	-14(15)	-46(17)	52(11)
F(23A)	339(56)	61(10)	84(8)	-32(8)	1(20)	-22(22)
C(37)	68(4)	76(4)	69(4)	8(3)	20(3)	-9(3)
F(31)	282(33)	136(16)	57(7)	36(8)	74(12)	14(19)
F(32)	105(10)	155(23)	246(27)	111(20)	-25(14)	-74(13)
F(33)	178(21)	68(10)	182(23)	41(13)	112(18)	25(14)
C(37A)	68(4)	76(4)	69(4)	8(3)	20(3)	-9(3)
F(31A)	83(7)	110(12)	181(17)	82(10)	-22(8)	-26(5)
F(32A)	234(19)	113(9)	161(15)	-8(10)	151(15)	-48(11)
F(33A)	147(9)	64(6)	94(7)	9(5)	-12(6)	-37(6)
N(1)	58(3)	48(3)	67(3)	14(2)	7(2)	7(2)
N(11)	41(2)	44(2)	50(2)	2(2)	8(2)	0(2)
N(12)	42(2)	51(2)	57(3)	8(2)	5(2)	3(2)
N(21)	41(2)	39(2)	48(3)	9(2)	7(2)	3(2)
N(22)	46(2)	44(2)	48(2)	4(2)	5(2)	5(2)
N(31)	40(2)	45(2)	52(2)	0(2)	9(2)	2(2)
N(32)	49(2)	42(2)	54(3)	5(2)	11(2)	0(2)
C(1)	67(4)	59(4)	58(4)	14(3)	6(3)	9(3)
C(2)	98(5)	100(6)	89(5)	25(5)	8(4)	50(5)
C(13)	42(3)	57(3)	51(3)	-4(3)	8(2)	2(2)
C(14)	47(3)	71(4)	71(4)	0(3)	18(3)	-8(3)
C(15)	49(3)	58(3)	54(3)	-2(3)	15(3)	-2(3)
C(16)	80(4)	64(4)	85(5)	25(4)	21(4)	-4(3)
C(23)	42(3)	47(3)	56(3)	-2(3)	8(2)	-2(2)
C(24)	43(3)	52(3)	53(3)	-3(3)	-5(2)	-5(2)
C(25)	38(3)	51(3)	49(3)	8(2)	6(2)	-2(2)
C(26)	56(3)	57(3)	64(4)	17(3)	1(3)	12(3)
C(33)	46(3)	65(4)	52(3)	2(3)	12(3)	-4(3)
C(34)	54(3)	67(4)	54(3)	-7(3)	19(3)	-3(3)
C(35)	40(3)	55(3)	55(3)	-11(3)	2(2)	0(2)
C(36)	59(4)	58(3)	76(4)	-10(3)	12(3)	5(3)
B	45(3)	37(3)	54(3)	2(3)	3(3)	2(2)

Table 5. Torsion angles [°] for $Tp^{CF3,CH3}Cu(CH_3CN)$

N(22)-Cu-N(1)-C(1)	119(2)	N(32)-Cu-N(1)-C(1)	-99(2)
N(12)-Cu-N(1)-C(1)	5(2)	C(15)-N(11)-N(12)-C(13)	0.6(6)
B-N(11)-N(12)-C(13)	178.3(4)	C(15)-N(11)-N(12)-Cu	-154.0(3)
B-N(11)-N(12)-Cu	23.7(5)	N(1)-Cu-N(12)-C(13)	27.9(6)
N(22)-Cu-N(12)-C(13)	-111.7(6)	N(32)-Cu-N(12)-C(13)	158.4(6)
N(1)-Cu-N(12)-N(11)	170.1(3)	N(22)-Cu-N(12)-N(11)	30.5(3)
N(32)-Cu-N(12)-N(11)	-59.4(3)	C(25)-N(21)-N(22)-C(23)	0.3(5)
B-N(21)-N(22)-C(23)	179.4(4)	C(25)-N(21)-N(22)-Cu	-166.6(3)
B-N(21)-N(22)-Cu	12.6(5)	N(1)-Cu-N(22)-C(23)	30.0(6)
N(32)-Cu-N(22)-C(23)	-121.3(5)	N(12)-Cu-N(22)-C(23)	150.0(5)
N(1)-Cu-N(22)-N(21)	-169.2(3)	N(32)-Cu-N(22)-N(21)	39.5(3)
N(12)-Cu-N(22)-N(21)	-49.3(3)	C(35)-N(31)-N(32)-C(33)	0.4(5)
B-N(31)-N(32)-C(33)	-174.6(4)	C(35)-N(31)-N(32)-Cu	-169.3(3)
B-N(31)-N(32)-Cu	15.6(5)	N(1)-Cu-N(32)-C(33)	-13.7(7)
N(22)-Cu-N(32)-C(33)	140.5(6)	N(12)-Cu-N(32)-C(33)	-126.6(6)
N(1)-Cu-N(32)-N(31)	151.1(3)	N(22)-Cu-N(32)-N(31)	-54.7(3)
N(12)-Cu-N(32)-N(31)	38.2(3)	Cu-N(1)-C(1)-C(2)	-59(13)
N(11)-N(12)-C(13)-C(14)	-0.3(6)	Cu-N(12)-C(13)-C(14)	142.9(5)
N(11)-N(12)-C(13)-C(17A)	179.4(5)	Cu-N(12)-C(13)-C(17A)	-37.4(8)
N(11)-N(12)-C(13)-C(17)	179.4(5)	Cu-N(12)-C(13)-C(17)	-37.4(8)
F(11A)-C(17A)-C(13)-N(12)	83(2)	F(12A)-C(17A)-C(13)-N(12)	-154.3(13)
F(13A)-C(17A)-C(13)-N(12)	-36.4(12)	F(11A)-C(17A)-C(13)-C(14)	-97(2)
F(12A)-C(17A)-C(13)-C(14)	25(2)	F(13A)-C(17A)-C(13)-C(14)	143.3(11)
F(11A)-C(17A)-C(13)-C(17)	0(100)	F(12A)-C(17A)-C(13)-C(17)	0(100)
F(13A)-C(17A)-C(13)-C(17)	0(100)	F(12)-C(17)-C(13)-N(12)	-172.8(14)
F(13)-C(17)-C(13)-N(12)	-50(2)	F(11)-C(17)-C(13)-N(12)	69(2)
F(12)-C(17)-C(13)-C(14)	7(2)	F(13)-C(17)-C(13)-C(14)	130.1(14)
F(11)-C(17)-C(13)-C(14)	-111(2)	F(12)-C(17)-C(13)-C(17A)	0(100)
F(13)-C(17)-C(13)-C(17A)	0(100)	F(11)-C(17)-C(13)-C(17A)	0(100)
N(12)-C(13)-C(14)-C(15)	0.0(7)	C(17A)-C(13)-C(14)-C(15)	-179.7(5)
C(17)-C(13)-C(14)-C(15)	-179.7(5)	N(12)-N(11)-C(15)-C(14)	-0.6(6)
B-N(11)-C(15)-C(14)	-178.1(5)	N(12)-N(11)-C(15)-C(16)	179.0(5)
B-N(11)-C(15)-C(16)	1.6(9)	C(13)-C(14)-C(15)-N(11)	0.4(6)
C(13)-C(14)-C(15)-C(16)	-179.2(6)	N(21)-N(22)-C(23)-C(24)	0.0(6)
Cu-N(22)-C(23)-C(24)	161.7(4)	N(21)-N(22)-C(23)-C(27A)	179.7(5)
Cu-N(22)-C(23)-C(27A)	-18.6(8)	N(21)-N(22)-C(23)-C(27)	179.7(5)
Cu-N(22)-C(23)-C(27)	-18.6(8)	F(23A)-C(27A)-C(23)-N(22)	-154(3)
F(22A)-C(27A)-C(23)-N(22)	-29(3)	F(21A)-C(27A)-C(23)-N(22)	89(3)
F(23A)-C(27A)-C(23)-C(24)	26(3)	F(22A)-C(27A)-C(23)-C(24)	151(3)
F(21A)-C(27A)-C(23)-C(24)	-91(3)	F(23A)-C(27A)-C(23)-C(27)	0(100)
F(22A)-C(27A)-C(23)-C(27)	0(100)	F(21A)-C(27A)-C(23)-C(27)	0(100)
F(21)-C(27)-C(23)-N(22)	161.5(11)	F(22)-C(27)-C(23)-N(22)	39(2)
F(23)-C(27)-C(23)-N(22)	-79.3(14)	F(21)-C(27)-C(23)-C(24)	-18.9(14)
F(22)-C(27)-C(23)-C(24)	-141.5(14)	F(23)-C(27)-C(23)-C(24)	100.4(14)
F(21)-C(27)-C(23)-C(27A)	0(100)	F(22)-C(27)-C(23)-C(27A)	0(100)
F(23)-C(27)-C(23)-C(27A)	0(100)	N(22)-C(23)-C(24)-C(25)	-0.2(6)
C(27A)-C(23)-C(24)-C(25)	-179.9(6)	C(27)-C(23)-C(24)-C(25)	-179.9(6)
N(22)-N(21)-C(25)-C(24)	-0.4(6)	B-N(21)-C(25)-C(24)	-179.5(5)
N(22)-N(21)-C(25)-C(26)	178.7(5)	B-N(21)-C(25)-C(26)	-0.4(8)
C(23)-C(24)-C(25)-N(21)	0.4(6)	C(23)-C(24)-C(25)-C(26)	-178.6(5)
N(31)-N(32)-C(33)-C(34)	-1.2(6)	Cu-N(32)-C(33)-C(34)	164.2(4)
N(31)-N(32)-C(33)-C(37A)	177.6(5)	Cu-N(32)-C(33)-C(37A)	-17.0(9)
N(31)-N(32)-C(33)-C(37)	177.6(5)	Cu-N(32)-C(33)-C(37)	-17.0(9)
F(31A)-C(37A)-C(33)-N(32)	59(2)	F(32A)-C(37A)-C(33)-N(32)	-178.6(14)
F(33A)-C(37A)-C(33)-N(32)	-61.0(12)	F(31A)-C(37A)-C(33)-C(34)	-122.5(14)
F(32A)-C(37A)-C(33)-C(34)	0(2)	F(33A)-C(37A)-C(33)-C(34)	117.6(11)
F(31A)-C(37A)-C(33)-C(37)	0(100)	F(32A)-C(37A)-C(33)-C(37)	0(100)
F(33A)-C(37A)-C(33)-C(37)	0(100)	F(32)-C(37)-C(33)-N(32)	-99(3)
F(33)-C(37)-C(33)-N(32)	27(2)	F(31)-C(37)-C(33)-N(32)	144(2)

F(32)-C(37)-C(33)-C(34)	80(3)	F(33)-C(37)-C(33)-C(34)	-154(2)
F(31)-C(37)-C(33)-C(34)	-37(2)	F(32)-C(37)-C(33)-C(37A)	0(100)
F(33)-C(37)-C(33)-C(37A)	0(100)	F(31)-C(37)-C(33)-C(37A)	0(100)
N(32)-C(33)-C(34)-C(35)	1.6(6)	C(37A)-C(33)-C(34)-C(35)	-177.1(6)
C(37)-C(33)-C(34)-C(35)	-177.1(6)	N(32)-N(31)-C(35)-C(34)	0.6(6)
B-N(31)-C(35)-C(34)	174.9(5)	N(32)-N(31)-C(35)-C(36)	179.5(5)
B-N(31)-C(35)-C(36)	-6.1(8)	C(33)-C(34)-C(35)-N(31)	-1.3(6)
C(33)-C(34)-C(35)-C(36)	179.9(5)	C(35)-N(31)-B-N(11)	115.1(5)
N(32)-N(31)-B-N(11)	-71.1(6)	C(35)-N(31)-B-N(21)	-125.0(5)
N(32)-N(31)-B-N(21)	48.9(6)	C(15)-N(11)-B-N(31)	-139.9(5)
N(12)-N(11)-B-N(31)	42.8(6)	C(15)-N(11)-B-N(21)	100.2(6)
N(12)-N(11)-B-N(21)	-77.1(5)	C(25)-N(21)-B-N(31)	111.2(5)
N(22)-N(21)-B-N(31)	-67.8(5)	C(25)-N(21)-B-N(11)	-127.6(5)
N(22)-N(21)-B-N(11)	53.4(6)		

Symmetry transformations used to generate equivalent atoms:

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Tp^{CF3,CH3}Cu(CH_3CN)$

	x	y	z	U(eq)	SOF
H(2A)	6097(7)	-1123(9)	1848(4)	146	1
H(2B)	5107(7)	-2155(9)	1970(4)	146	1
H(2C)	5685(7)	-994(9)	2479(4)	146	1
H(14A)	6596(5)	5997(7)	861(3)	75	1
H(16A)	3981(31)	7500(16)	-70(12)	114	1
H(16B)	5252(13)	8045(33)	164(20)	114	1
H(16C)	4316(41)	8498(18)	531(8)	114	1
H(24A)	644(4)	3438(6)	-1018(3)	62	1
H(26A)	519(31)	6839(20)	-229(11)	92	1
H(26B)	419(28)	6407(10)	-933(9)	92	1
H(26C)	1556(6)	7121(13)	-546(19)	92	1
H(34A)	1018(5)	5865(7)	2425(3)	69	1
H(36A)	2386(6)	8437(10)	1600(20)	97	1
H(36B)	1273(33)	8462(9)	1868(12)	97	1
H(36C)	1180(31)	8203(7)	1150(8)	97	1
H(37)	2534(5)	6792(6)	603(3)	56	1

CRYSTAL STRUCTURE REPORT

$C_{15}H_{13}BCuF_9N_7O_2$

$Tp^{CF3,CH3}Cu(NO_2)$

Report prepared for:
J. Schneider / Prof. W. Tolman

31 October 1997

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DATA COLLECTION

A crystal of the compound was attached to a glass fiber and mounted on the Siemens SMART system for a data collection at 173(2) K. An initial set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames are oriented such that orthogonal wedges of reciprocal space were surveyed. This produces orientation matrices determined from 85 reflections. Final cell constants are calculated from a set of 5237 strong reflections from the actual data collection. Please refer to Table 1 for additional crystal and refinement information.

The data collection technique used for this specimen is generally known as a hemisphere collection. Here a randomly oriented region of reciprocal space is surveyed to the extent of 1.3 hemispheres to a resolution of 0.84 Å. Three major swaths of frames are collected with 0.30^{o} steps in ω. In the event the lattice is triclinic some additional sets of frames are collected to better model the absorption correction.

STRUCTURE SOLUTION AND REFINEMENT

The space group Pnma was determined based on systematic absences and intensity statistics.[1] A successful direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Several full-matrix least squares / difference Fourier cycles were performed which located the remainder of the non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters unless stated otherwise. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

The complex was found as expected. A crystallographic mirror bisects the complex.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Chemistry Department, The University of Minnesota. All calculations were preformed using SGI INDY R4400-SC or Pentium computers using the SHELXTL V5.0 suite of programs. All publications arising from this report MUST either 1)include Victor G. Young, Jr. as a coauthor or 2)acknowledge both Victor G. Young, Jr. and the X-Ray Crystallographic Laboratory.

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1. SHELXTL-Plus V5.0, Siemens Industrial Automation, Inc., Madison, WI.

Some equations of interest:

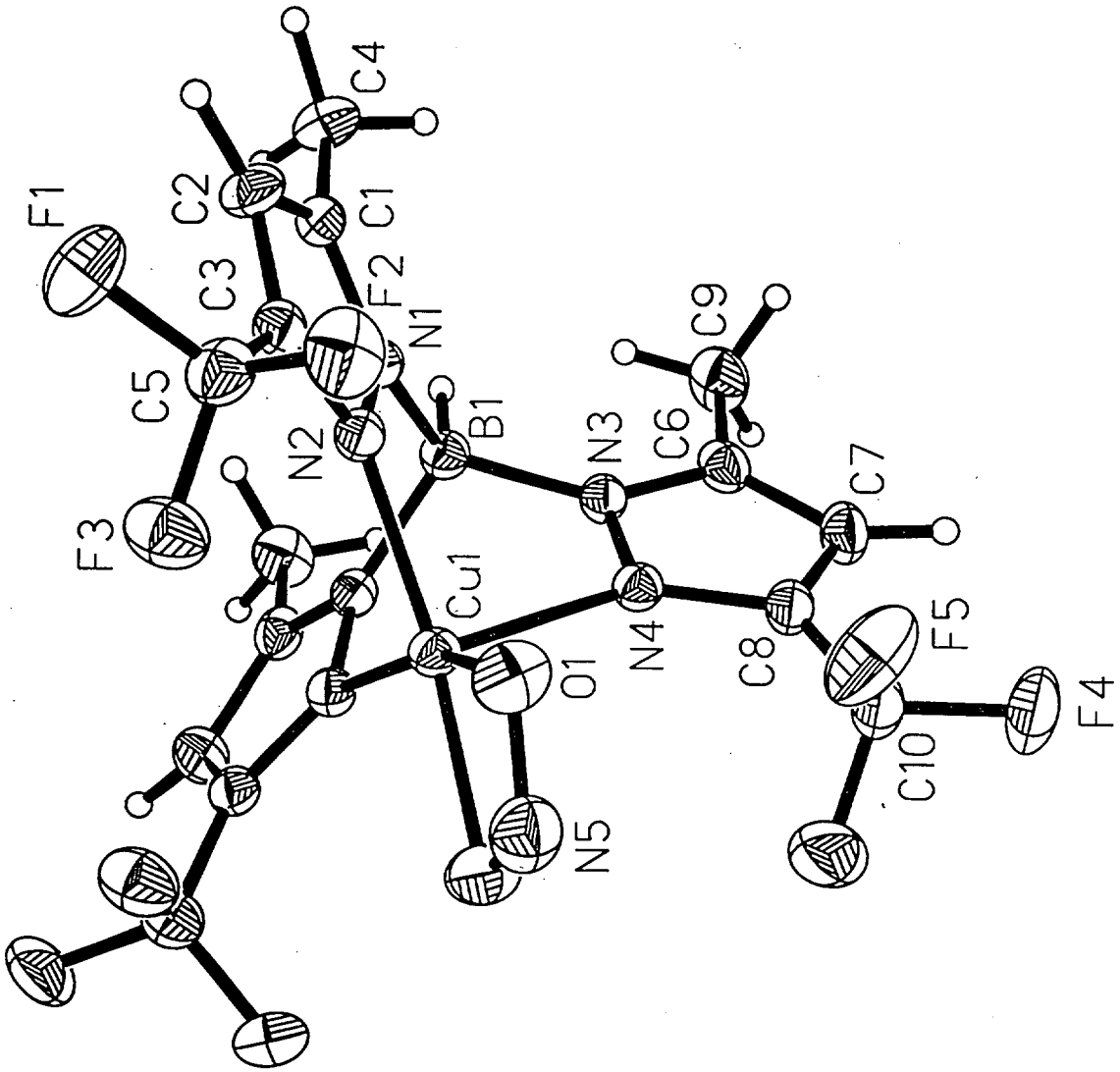
$$R_{int}=\sum|F_o^2-\langle F_o^2\rangle|/\sum|F_o^2|$$

$$R1=\sum||F_o|-|F_c||/\sum|F_o|$$

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

where $w=q/\sigma^2(F_o^2)+(a*P)^2+b*P$

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



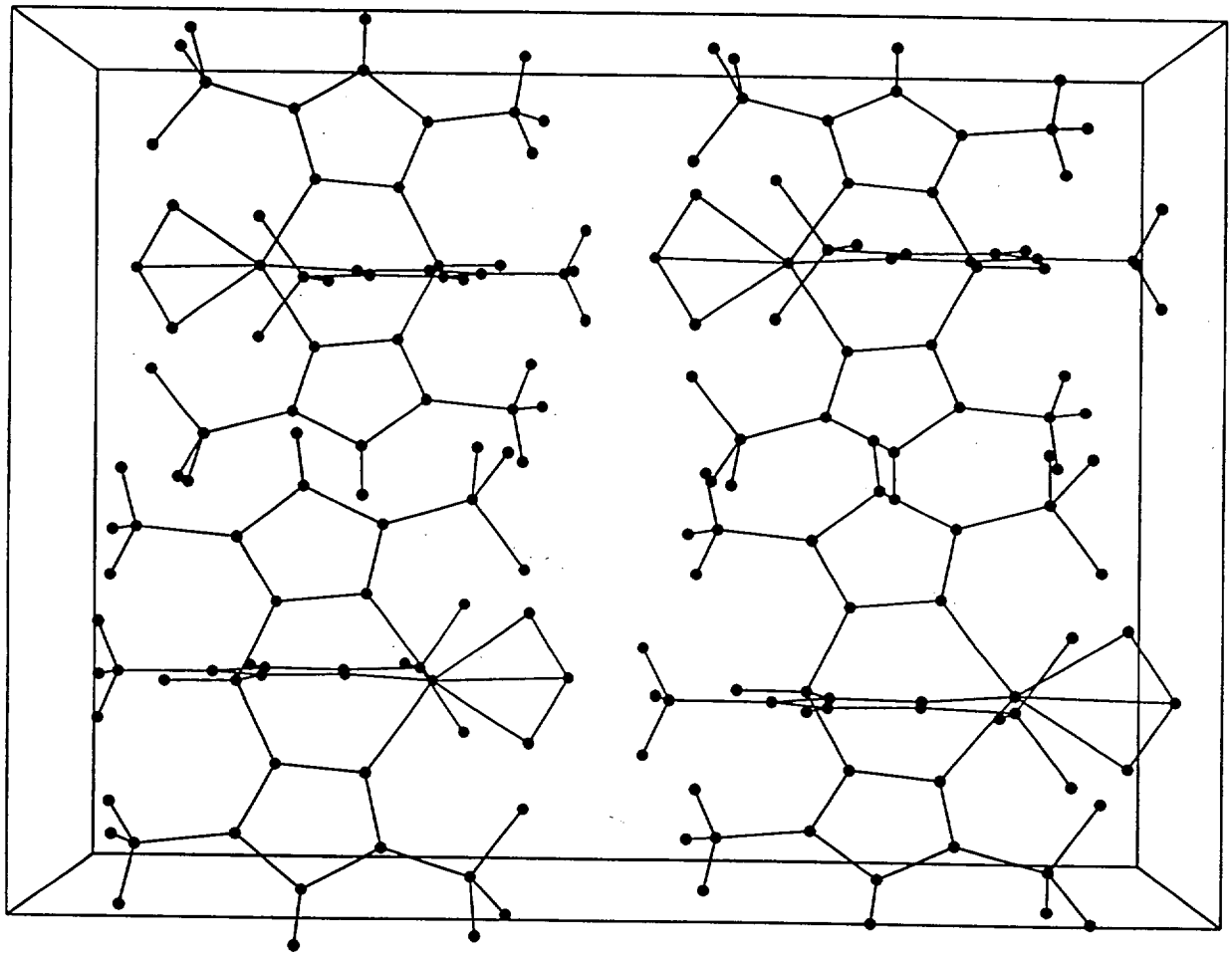


Table 1. Crystal data, data collection, and solution and refinement for $Tp^{CF3,CH3}Cu(NC$

Crystal Data	
Empirical formula	$C_{15}H_{13}BCuF_9N_7O_2$
Crystal Habit, color	Rhomb plate, Green
Crystal size	0.22 x 0.22 x 0.03 mm
Crystal system	Orthorhombic
Space group	Pnma
	a = 17.7811(5) Å α = 90°
	b = 13.4460(4) Å β = 90°
	c = 8.6908(2) Å γ = 90°
Volume	2077.84(10) $Å^3$
Z	4
Formula weight	568.67
Density (calculated)	1.818 Mg/m^3
Absorption coefficient	1.161 mm^{-1}
F(000)	1132
Data Collection	
Diffractometer	Siemens SMART Platform CCD
Wavelength	0.71073 Å
Temperature	173(2) K
θ range for data collection	2.29 to 25.06°
Index ranges	$0 \le h \le 21$, $0 \le k \le 16$, $0 \le \ell \le 10$
Reflections collected	10311
Independent reflections	1936 (R_{int} = 0.0342)
Solution and Refinement	
System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2)+(AP)^2+(BP)]^{-1}$, where P = $(Fo^2+2Fc^2))/3$, A = 0.0260, and B = 3.1256
Absorption correction	SADABS (Sheldrick, 1996)
Max. and min. transmission	1.000 and 0.824
Data / restraints / parameters	1936 / 0 / 176
R indices (I>2σ(I) = 1666)	R1 = 0.0374, wR2 = 0.0771
R indices (all data)	R1 = 0.0485, wR2 = 0.0810
Goodness-of-fit on F^2	1.093
Largest diff. peak and hole	0.425 and -0.405 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Cu(1)	8389(1)	2500	-1230(1)	21(1)	1
N(5)	9611(2)	2500	45(5)	38(1)	1
O(1)	9249(1)	1729(2)	-341(3)	37(1)	1
N(1)	7060(1)	1566(2)	-2405(3)	21(1)	1
N(2)	7827(1)	1466(2)	-2350(3)	21(1)	1
C(1)	6760(2)	816(2)	-3248(3)	24(1)	1
C(2)	7347(2)	231(2)	-3772(3)	29(1)	1
C(3)	7990(2)	662(2)	-3194(3)	23(1)	1
C(4)	5937(2)	705(2)	-3513(4)	33(1)	1
C(5)	8786(2)	365(2)	-3443(3)	30(1)	1
F(1)	8850(1)	-205(1)	-4698(2)	44(1)	1
F(2)	9075(1)	-156(1)	-2274(2)	40(1)	1
F(3)	9241(1)	1151(1)	-3645(2)	38(1)	1
N(3)	6822(2)	2500	74(4)	22(1)	1
N(4)	7545(2)	2500	613(4)	21(1)	1
C(6)	6322(2)	2500	1255(5)	26(1)	1
C(7)	6734(2)	2500	2603(5)	29(1)	1
C(8)	7475(2)	2500	2154(4)	24(1)	1
C(9)	5489(2)	2500	1036(5)	35(1)	1
C(10)	8159(3)	2500	3135(5)	31(1)	1
F(4)	7970(2)	2500	4620(3)	47(1)	1
F(5)	8598(1)	1708(2)	2914(2)	55(1)	1
B(1)	6682(3)	2500	-1680(5)	22(1)	1

Table 3. Bond lengths [Å] and angles [°] $Tp^{CF3,CH3}Cu(NO_2)$

Cu(1)-N(2)	1.970(2)	Cu(1)-N(2)#1	1.970(2)
Cu(1)-O(1)#1	2.003(2)	Cu(1)-O(1)	2.003(2)
Cu(1)-N(4)	2.195(3)	Cu(1)-N(5)	2.439(4)
N(5)-O(1)	1.265(3)	N(5)-O(1)#1	1.265(3)
N(1)-C(1)	1.357(3)	N(1)-N(2)	1.369(3)
N(1)-B(1)	1.557(3)	N(2)-C(3)	1.338(3)
C(1)-C(2)	1.384(4)	C(1)-C(4)	1.488(4)
C(2)-C(3)	1.377(4)	C(3)-C(5)	1.486(4)
C(5)-F(2)	1.337(3)	C(5)-F(1)	1.338(3)
C(5)-F(3)	1.342(3)	N(3)-C(6)	1.358(5)
N(3)-N(4)	1.368(4)	N(3)-B(1)	1.544(5)
N(4)-C(8)	1.345(5)	C(6)-C(7)	1.382(6)
C(6)-C(9)	1.492(6)	C(7)-C(8)	1.374(6)
C(8)-C(10)	1.485(6)	C(10)-F(5)#1	1.334(3)
C(10)-F(5)	1.334(3)	C(10)-F(4)	1.334(5)
B(1)-N(1)#1	1.557(3)		

N(2)-Cu(1)-N(2)#1	89.77(13)	N(2)-Cu(1)-O(1)#1	160.65(9)
N(2)#1-Cu(1)-O(1)#1	102.30(9)	N(2)-Cu(1)-O(1)	102.30(9)
N(2)#1-Cu(1)-O(1)	160.66(9)	O(1)#1-Cu(1)-O(1)	62.33(13)
N(2)-Cu(1)-N(4)	90.79(9)	N(2)#1-Cu(1)-N(4)	90.79(9)
O(1)#1-Cu(1)-N(4)	103.93(10)	O(1)-Cu(1)-N(4)	103.93(10)
N(2)-Cu(1)-N(5)	132.58(7)	N(2)#1-Cu(1)-N(5)	132.59(7)
O(1)#1-Cu(1)-N(5)	31.17(6)	O(1)-Cu(1)-N(5)	31.17(6)
N(4)-Cu(1)-N(5)	106.13(13)	O(1)-N(5)-O(1)#1	110.0(3)
O(1)-N(5)-Cu(1)	55.0(2)	O(1)#1-N(5)-Cu(1)	55.0(2)
N(5)-O(1)-Cu(1)	93.8(2)	C(1)-N(1)-N(2)	109.7(2)
C(1)-N(1)-B(1)	130.4(3)	N(2)-N(1)-B(1)	119.7(2)
C(3)-N(2)-N(1)	106.1(2)	C(3)-N(2)-Cu(1)	136.9(2)
N(1)-N(2)-Cu(1)	116.9(2)	N(1)-C(1)-C(2)	107.6(2)
N(1)-C(1)-C(4)	123.1(3)	C(2)-C(1)-C(4)	129.3(3)
C(3)-C(2)-C(1)	105.5(3)	N(2)-C(3)-C(2)	111.0(3)
N(2)-C(3)-C(5)	120.3(3)	C(2)-C(3)-C(5)	128.7(3)
F(2)-C(5)-F(1)	106.6(2)	F(2)-C(5)-F(3)	106.3(2)
F(1)-C(5)-F(3)	107.1(2)	F(2)-C(5)-C(3)	113.3(2)
F(1)-C(5)-C(3)	110.7(2)	F(3)-C(5)-C(3)	112.5(2)
C(6)-N(3)-N(4)	110.9(3)	C(6)-N(3)-B(1)	129.8(3)
N(4)-N(3)-B(1)	119.3(3)	C(8)-N(4)-N(3)	104.8(3)
C(8)-N(4)-Cu(1)	142.2(3)	N(3)-N(4)-Cu(1)	113.1(2)
N(3)-C(6)-C(7)	107.0(4)	N(3)-C(6)-C(9)	123.6(4)
C(7)-C(6)-C(9)	129.4(4)	C(8)-C(7)-C(6)	105.6(4)
N(4)-C(8)-C(7)	111.8(4)	N(4)-C(8)-C(10)	119.7(4)
C(7)-C(8)-C(10)	128.5(4)	F(5)#1-C(10)-F(5)	106.0(4)
F(5)#1-C(10)-F(4)	106.6(3)	F(5)-C(10)-F(4)	106.6(3)
F(5)#1-C(10)-C(8)	113.4(2)	F(5)-C(10)-C(8)	113.4(2)
F(4)-C(10)-C(8)	110.4(4)	N(3)-B(1)-N(1)#1	109.3(2)
N(3)-B(1)-N(1)	109.2(2)	N(1)#1-B(1)-N(1)	107.5(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z ,

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$] $Tp^{CF3,CH3}Cu(NO_2)$

	U11	U22	U33	U23	U13	U12
Cu(1)	24(1)	18(1)	22(1)	0	-2(1)	0
N(5)	33(2)	45(2)	36(2)	0	-3(2)	0
O(1)	38(1)	31(1)	42(1)	0(1)	-10(1)	5(1)
N(1)	24(1)	19(1)	20(1)	0(1)	-2(1)	-1(1)
N(2)	25(1)	19(1)	20(1)	0(1)	0(1)	1(1)
C(1)	33(2)	20(1)	20(1)	1(1)	-1(1)	-4(1)
C(2)	40(2)	20(1)	28(2)	-7(1)	-1(1)	0(1)
C(3)	30(2)	18(1)	21(1)	2(1)	1(1)	1(1)
C(4)	32(2)	32(2)	37(2)	-9(1)	-6(1)	-5(1)
C(5)	37(2)	23(2)	30(2)	-3(1)	-1(1)	4(1)
F(1)	48(1)	45(1)	39(1)	-18(1)	2(1)	13(1)
F(2)	43(1)	37(1)	41(1)	6(1)	-5(1)	13(1)
F(3)	31(1)	34(1)	49(1)	0(1)	8(1)	-1(1)
N(3)	25(2)	21(2)	19(2)	0	2(1)	0
N(4)	22(2)	19(2)	21(2)	0	-1(1)	0
C(6)	30(2)	21(2)	26(2)	0	7(2)	0
C(7)	36(3)	32(2)	20(2)	0	7(2)	0
C(8)	37(2)	18(2)	18(2)	0	1(2)	0
C(9)	26(2)	44(3)	35(3)	0	7(2)	0
C(10)	42(3)	30(2)	21(2)	0	-1(2)	0
F(4)	57(2)	64(2)	20(1)	0	-3(1)	0
F(5)	55(1)	59(1)	51(1)	-19(1)	-23(1)	26(1)
B(1)	25(2)	19(2)	22(2)	0	-1(2)	0

Table 5. Torsion angles [°] $Tp^{CF3,CH3}Cu(NO_2)$

N(2)-Cu(1)-N(5)-O(1)	-16.2(3)	N(2)#1-Cu(1)-N(5)-O(1)	-163.1(2)
O(1)#1-Cu(1)-N(5)-O(1)	-179.3(4)	O(1)-Cu(1)-N(5)-O(1)	0.0
N(4)-Cu(1)-N(5)-O(1)	90.4(2)	N(2)-Cu(1)-N(5)-O(1)#1	163.1(2)
N(2)#1-Cu(1)-N(5)-O(1)#1	16.2(3)	O(1)#1-Cu(1)-N(5)-O(1)#1	0.0
O(1)-Cu(1)-N(5)-O(1)#1	179.3(4)	N(4)-Cu(1)-N(5)-O(1)#1	-90.4(2)
O(1)#1-N(5)-O(1)-Cu(1)	-0.6(4)	Cu(1)-N(5)-O(1)-Cu(1)	0.0
N(2)-Cu(1)-O(1)-N(5)	167.9(2)	N(2)#1-Cu(1)-O(1)-N(5)	40.3(4)
O(1)#1-Cu(1)-O(1)-N(5)	0.4(2)	N(4)-Cu(1)-O(1)-N(5)	-98.2(2)
N(5)-Cu(1)-O(1)-N(5)	0.0	C(1)-N(1)-N(2)-C(3)	1.3(3)
B(1)-N(1)-N(2)-C(3)	-173.5(2)	C(1)-N(1)-N(2)-Cu(1)	178.3(2)
B(1)-N(1)-N(2)-Cu(1)	3.5(3)	N(2)#1-Cu(1)-N(2)-C(3)	127.1(2)
O(1)#1-Cu(1)-N(2)-C(3)	-2.1(5)	O(1)-Cu(1)-N(2)-C(3)	-37.6(3)
N(4)-Cu(1)-N(2)-C(3)	-142.1(3)	N(5)-Cu(1)-N(2)-C(3)	-29.1(3)
N(2)#1-Cu(1)-N(2)-N(1)	-48.6(2)	O(1)#1-Cu(1)-N(2)-N(1)	-177.8(2)
O(1)-Cu(1)-N(2)-N(1)	146.6(2)	N(4)-Cu(1)-N(2)-N(1)	42.2(2)
N(5)-Cu(1)-N(2)-N(1)	155.1(2)	N(2)-N(1)-C(1)-C(2)	-1.1(3)
B(1)-N(1)-C(1)-C(2)	173.0(3)	N(2)-N(1)-C(1)-C(4)	179.3(3)
B(1)-N(1)-C(1)-C(4)	-6.6(5)	N(1)-C(1)-C(2)-C(3)	0.5(3)
C(4)-C(1)-C(2)-C(3)	-180.0(3)	N(1)-N(2)-C(3)-C(2)	-1.0(3)
Cu(1)-N(2)-C(3)-C(2)	-177.1(2)	N(1)-N(2)-C(3)-C(5)	177.0(2)
Cu(1)-N(2)-C(3)-C(5)	0.9(4)	C(1)-C(2)-C(3)-N(2)	0.3(3)
C(1)-C(2)-C(3)-C(5)	-177.5(3)	N(2)-C(3)-C(5)-F(2)	82.1(3)
C(2)-C(3)-C(5)-F(2)	-100.3(4)	N(2)-C(3)-C(5)-F(1)	-158.2(2)
C(2)-C(3)-C(5)-F(1)	19.4(4)	N(2)-C(3)-C(5)-F(3)	-38.4(4)
C(2)-C(3)-C(5)-F(3)	139.1(3)	C(6)-N(3)-N(4)-C(8)	0.0
B(1)-N(3)-N(4)-C(8)	180.0	C(6)-N(3)-N(4)-Cu(1)	180.0
B(1)-N(3)-N(4)-Cu(1)	0.0	N(2)-Cu(1)-N(4)-C(8)	135.11(6)
N(2)#1-Cu(1)-N(4)-C(8)	-135.11(6)	O(1)#1-Cu(1)-N(4)-C(8)	-32.22(7)
O(1)-Cu(1)-N(4)-C(8)	32.22(7)	N(5)-Cu(1)-N(4)-C(8)	0.0
N(2)-Cu(1)-N(4)-N(3)	-44.89(6)	N(2)#1-Cu(1)-N(4)-N(3)	44.89(6)
O(1)#1-Cu(1)-N(4)-N(3)	147.78(7)	O(1)-Cu(1)-N(4)-N(3)	-147.78(7)
N(5)-Cu(1)-N(4)-N(3)	180.0	N(4)-N(3)-C(6)-C(7)	0.0
B(1)-N(3)-C(6)-C(7)	180.0	N(4)-N(3)-C(6)-C(9)	180.0
B(1)-N(3)-C(6)-C(9)	0.0	N(3)-C(6)-C(7)-C(8)	0.0
C(9)-C(6)-C(7)-C(8)	180.0	N(3)-N(4)-C(8)-C(7)	0.0
Cu(1)-N(4)-C(8)-C(7)	180.0	N(3)-N(4)-C(8)-C(10)	180.0
Cu(1)-N(4)-C(8)-C(10)	0.0	C(6)-C(7)-C(8)-N(4)	0.0
C(6)-C(7)-C(8)-C(10)	180.0	N(4)-C(8)-C(10)-F(5)#1	60.4(3)
C(7)-C(8)-C(10)-F(5)#1	-119.6(3)	N(4)-C(8)-C(10)-F(5)	-60.4(3)
C(7)-C(8)-C(10)-F(5)	119.6(3)	N(4)-C(8)-C(10)-F(4)	180.0
C(7)-C(8)-C(10)-F(4)	0.0	C(6)-N(3)-B(1)-N(1)#1	121.4(2)
N(4)-N(3)-B(1)-N(1)#1	-58.6(2)	C(6)-N(3)-B(1)-N(1)	-121.4(2)
N(4)-N(3)-B(1)-N(1)	58.6(2)	C(1)-N(1)-B(1)-N(3)	122.2(3)
N(2)-N(1)-B(1)-N(3)	-64.2(3)	C(1)-N(1)-B(1)-N(1)#1	-119.4(3)
N(2)-N(1)-B(1)-N(1)#1	54.2(4)		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) $Tp^{CF3,CH3}Cu(NO_2)$

	x	y	z	U(eq)	SOF
H(2A)	7314(2)	-346(2)	-4398(3)	35	1
H(4A)	5671(2)	750(15)	-2529(5)	50	1
H(4B)	5837(2)	56(7)	-3985(22)	50	1
H(4C)	5762(3)	1234(9)	-4201(19)	50	1
H(7A)	6545(2)	2500	3625(5)	35	1
H(9A)	5387(2)	2500	-48(5)	52	1
H(9B)	5274(2)	1918	1496(5)	52	0.50
H(9C)	5274(2)	3082	1496(5)	52	0.50
H(1A)	6086(3)	2500	-1917(5)	27	1