

Inorganic Chemistry

including bioinorganic chemistry

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Table of bond angles involving the nonhydrogen atoms for [CuCl(Me2tpa)]ClO4
(cont.)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	C(15)	C(16)	122(2)				
C(15)	C(16)	C(17)	120(2)				
C(16)	C(17)	C(18)	117(2)				
C(17)	C(18)	C(19)	122(2)				
N(4)	C(19)	C(18)	120(1)				
N(4)	C(19)	C(20)	118(1)				
C(18)	C(19)	C(20)	122(2)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table of bond angles involving the hydrogen atoms for [CuCl(Me2tpa)]ClO4

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(1)	108.08	C(12)	C(13)	H(12)	109.43
N(1)	C(1)	H(2)	108.09	C(12)	C(13)	H(13)	109.46
C(2)	C(1)	H(1)	108.07	C(12)	C(13)	H(14)	109.47
C(2)	C(1)	H(2)	108.07	H(12)	C(13)	H(13)	109.47
H(1)	C(1)	H(2)	109.48	H(12)	C(13)	H(14)	109.47
C(2)	C(3)	H(3)	119.87	H(13)	C(13)	H(14)	109.53
C(4)	C(3)	H(3)	119.84	N(1)	C(14)	H(15)	108.86
C(3)	C(4)	H(4)	122.67	N(1)	C(14)	H(16)	108.79
C(5)	C(4)	H(4)	122.65	C(15)	C(14)	H(15)	108.88
C(4)	C(5)	H(5)	118.52	C(15)	C(14)	H(16)	108.81
C(6)	C(5)	H(5)	118.53	H(15)	C(14)	H(16)	109.36
N(2)	C(6)	H(6)	119.55	C(15)	C(16)	H(17)	120.21
C(5)	C(6)	H(6)	119.54	C(17)	C(16)	H(17)	120.13
N(1)	C(7)	H(7)	109.54	C(16)	C(17)	H(18)	121.40
N(1)	C(7)	H(8)	109.56	C(18)	C(17)	H(18)	121.27
C(8)	C(7)	H(7)	109.49	C(17)	C(18)	H(19)	119.23
C(8)	C(7)	H(8)	109.52	C(19)	C(18)	H(19)	119.10
H(7)	C(7)	H(8)	109.44	C(19)	C(20)	H(20)	110.18
C(8)	C(9)	H(9)	119.66	C(19)	C(20)	H(21)	110.16
C(10)	C(9)	H(9)	119.73	C(19)	C(20)	H(22)	109.05
C(9)	C(10)	H(10)	122.59	H(20)	C(20)	H(21)	110.13
C(11)	C(10)	H(10)	122.60	H(20)	C(20)	H(22)	108.65
C(10)	C(11)	H(11)	118.99	H(21)	C(20)	H(22)	108.63
C(12)	C(11)	H(11)	119.01				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table of torsion or conformation angles for [CuCl(Me2tpa)]ClO4

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
Cu	N(1)	C(1)	C(2)	12(2)	N(1)	Cu	N(3)	C(12)	158(1)
Cu	N(1)	C(7)	C(8)	-44(1)	N(1)	Cu	N(4)	C(15)	1(1)
Cu	N(1)	C(14)	C(15)	-43(1)	N(1)	Cu	N(4)	C(19)	157(1)
Cu	N(2)	C(2)	C(1)	0(2)	N(1)	C(1)	C(2)	N(2)	-8(2)
Cu	N(2)	C(2)	C(3)	174(1)	N(1)	C(1)	C(2)	C(3)	177(1)
Cu	N(2)	C(6)	C(5)	-176(1)	N(1)	C(7)	C(8)	N(3)	25(2)
Cu	N(3)	C(8)	C(7)	8(2)	N(1)	C(7)	C(8)	C(9)	-151(1)
Cu	N(3)	C(8)	C(9)	-176(1)	N(1)	C(14)	C(15)	N(4)	47(2)
Cu	N(3)	C(12)	C(11)	173(1)	N(1)	C(14)	C(15)	C(16)	-138(2)
Cu	N(3)	C(12)	C(13)	-9(2)	N(2)	Cu	N(1)	C(1)	-8.9(9)
Cu	N(4)	C(15)	C(14)	-25(1)	N(2)	Cu	N(1)	C(7)	-130.9(9)
Cu	N(4)	C(15)	C(16)	160(1)	N(2)	Cu	N(1)	C(14)	113(1)
Cu	N(4)	C(19)	C(18)	-157(1)	N(2)	Cu	N(3)	C(8)	8(2)
Cu	N(4)	C(19)	C(20)	24(2)	N(2)	Cu	N(3)	C(12)	-167(1)
Cl(1)Cu	N(1)	C(1)		71(2)	N(2)	Cu	N(4)	C(15)	-82(1)
Cl(1)Cu	N(1)	C(7)		-51(2)	N(2)	Cu	N(4)	C(19)	73(1)
Cl(1)Cu	N(1)	C(14)		-167.6(9)	N(2)	C(2)	C(3)	C(4)	3(3)
Cl(1)Cu	N(2)	C(2)		-159(1)	N(2)	C(6)	C(5)	C(4)	0(3)
Cl(1)Cu	N(2)	C(6)		18(1)	N(3)	Cu	N(1)	C(1)	159(1)
Cl(1)Cu	N(3)	C(8)		136.3(9)	N(3)	Cu	N(1)	C(7)	37.4(8)
Cl(1)Cu	N(3)	C(12)		-39(1)	N(3)	Cu	N(1)	C(14)	-79.0(9)
Cl(1)Cu	N(4)	C(15)		-175.8(9)	N(3)	Cu	N(2)	C(2)	-30(2)
Cl(1)Cu	N(4)	C(19)		-20(1)	N(3)	Cu	N(2)	C(6)	147(1)
N(1)	Cu	N(2)	C(2)	5(1)	N(3)	Cu	N(4)	C(15)	79(1)
N(1)	Cu	N(2)	C(6)	-178(1)	N(3)	Cu	N(4)	C(19)	-126(1)
N(1)	Cu	N(3)	C(8)	-27(1)	N(3)	C(8)	C(9)	C(10)	3(3)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Table of torsion or conformation angles for [CuCl(Me2tpa)]ClO₄⁴ (cont.)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
N(3)	C(12)	C(11)	C(10)	1(3)	C(8)	C(9)	C(10)	C(11)	-4(2)
N(4)	Cu	N(1)	C(1)	-99.5(9)	C(9)	C(8)	N(3)	C(12)	0(2)
N(4)	Cu	N(1)	C(7)	138.5(9)	C(9)	C(10)	C(11)	C(12)	2(3)
N(4)	Cu	N(1)	C(14)	22.1(9)	C(10)	C(11)	C(12)	C(13)	-177(1)
N(4)	Cu	N(2)	C(2)	86(1)	C(14)	C(15)	N(4)	C(19)	176(1)
N(4)	Cu	N(2)	C(6)	-97(1)	C(14)	C(15)	C(16)	C(17)	-174(2)
N(4)	Cu	N(3)	C(8)	-106(1)	C(15)	N(4)	C(19)	C(18)	-3(2)
N(4)	Cu	N(3)	C(12)	79(1)	C(15)	N(4)	C(19)	C(20)	178(1)
N(4)	C(15)	C(16)	C(17)	0(3)	C(15)	C(16)	C(17)	C(18)	1(3)
N(4)	C(19)	C(18)	C(17)	3(3)	C(16)	C(15)	N(4)	C(19)	1(2)
C(1)	N(1)	C(7)	C(8)	-161(1)	C(16)	C(17)	C(18)	C(19)	-2(3)
C(1)	N(1)	C(14)	C(15)	76(1)	C(17)	C(18)	C(19)	C(20)	-177(2)
C(1)	C(2)	N(2)	C(6)	-177(1)					
C(1)	C(2)	C(3)	C(4)	177(2)					
C(2)	N(2)	C(6)	C(5)	1(2)					
C(2)	C(1)	N(1)	C(7)	126(1)					
C(2)	C(1)	N(1)	C(14)	-106(1)					
C(2)	C(3)	C(4)	C(5)	-1(3)					
C(3)	C(2)	N(2)	C(6)	-3(2)					
C(3)	C(4)	C(5)	C(6)	0(3)					
C(7)	N(1)	C(14)	C(15)	-154(1)					
C(7)	C(8)	N(3)	C(12)	-176(1)					
C(7)	C(8)	C(9)	C(10)	179(1)					
C(8)	N(3)	C(12)	C(11)	-2(2)					
C(8)	N(3)	C(12)	C(13)	176(1)					
C(8)	C(7)	N(1)	C(14)	70(1)					

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

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Table of Least-Squares Planes

----- Plane number 1 -----

Atoms Defining Plane	Distance	esd
N(1)	0.0000	
N(2)	0.0000	
N(3)	0.0000	

Additional Atoms	Distance
Cu	-0.2350
Cl(1)	0.1512

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

----- Plane number 2 -----

Atoms Defining Plane	Distance	esd
Cl(1)	0.0034	0.0037
N(1)	0.0468	0.0112
N(2)	-0.0354	0.0106
N(3)	-0.0331	0.0102

Additional Atoms	Distance
Cu	-0.2814

Mean deviation from plane is 0.0297 angstroms
Chi-squared: 38.5

Dihedral angles between least-squares planes

plane	plane	angle
2	1	2.61

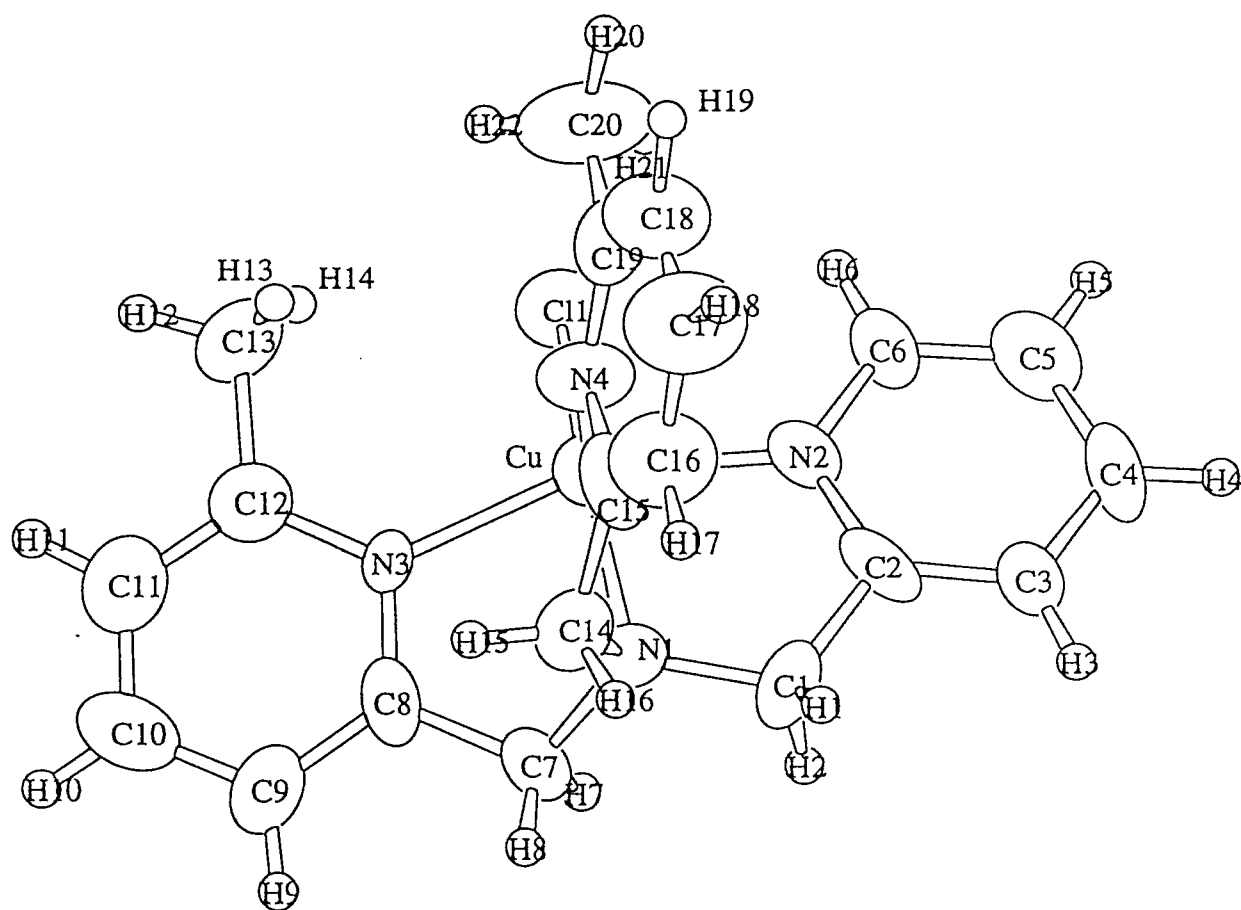


Table of information on collected data and refinement for 4

formula	C ₄₂ H ₄₈ N ₈ O ₄ Cl ₄ Cu ₂
fw	997.80
Color, Habit	blue, prismatic
Dimensions	0.40x0.30x0.10 mm
space group (No.)	<i>P</i> 2 ₁ /a (14)
<i>a</i>	15.698(6) Å
<i>b</i>	14.687(7) Å
<i>c</i>	19.475(4) Å
β	97.13(2) deg
<i>V</i>	4455(2) Å ³
<i>D</i> _{calc}	1.49 gcm ⁻³
<i>Z</i>	4
μ	12.45 cm ⁻¹
Radiation	graphite monochromated MoKα (λ =0.71069Å)
Diffractionmeter	Rigaku AFC5R
T	23 °C
Scan type	ω-2θ
2θ _{max}	50.0
Reflections Measured	+h, +k, ±l
No. of reflections measured(total)	8515
No. of observation (<i>F</i> _o >3σ(<i>F</i> _o))	3735
No. of variables	541
Reflection/Parameter Ratio	6.95
<i>R</i> / <i>R</i> _w	0.054/0.038
trans coef.	0.75-1.15
Goodness of fit indicator	2.30
Maximum peak in Final Diff. Map	0.70 e ⁻ / Å ³

Table of atomic coordinates and B(eq) for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

atom	x	y	z	B(eq)
Cu(1)	0.24116(6)	0.14239(8)	0.09820(6)	4.14(3)
Cu(2)	0.70724(5)	0.13456(7)	0.49045(5)	3.44(2)
Cl(1)	0.1244(1)	0.1582(2)	0.0204(1)	5.11(6)
Cl(2)	0.6174(1)	0.2445(2)	0.4388(1)	5.75(7)
Cl(3)	0.6932(1)	-0.0261(1)	0.4949(1)	4.05(6)
Cl(4)	0.9113(2)	0.3770(2)	0.8342(1)	5.40(7)
O(1)	0.9412(6)	0.2984(6)	0.8194(7)	22.6(5)
O(2)	0.9261(6)	0.390(1)	0.8989(4)	20.5(5)
O(3)	0.8282(5)	0.3794(6)	0.8148(6)	16.2(4)
O(4)	0.9576(5)	0.4446(5)	0.8062(4)	11.4(3)
N(1)	0.3724(3)	0.1239(5)	0.0933(3)	3.8(2)
N(2)	0.2778(4)	0.2756(4)	0.0923(4)	3.9(2)
N(3)	0.2444(5)	0.0040(5)	0.0951(4)	4.5(2)
N(4)	0.2786(4)	0.1379(5)	0.2087(3)	4.3(2)
N(5)	0.8328(4)	0.1632(4)	0.5428(3)	3.0(2)
N(6)	0.6758(4)	0.1535(4)	0.5866(3)	3.3(2)
N(7)	0.7718(3)	0.1307(4)	0.4072(3)	3.3(2)
N(8)	0.9825(4)	0.0975(5)	0.6675(3)	4.1(2)
C(1)	0.3965(5)	0.1999(6)	0.0495(4)	4.4(2)
C(2)	0.3562(5)	0.2868(6)	0.0704(4)	3.9(2)
C(3)	0.3945(5)	0.3695(7)	0.0631(5)	5.4(3)
C(4)	0.3510(6)	0.4474(6)	0.0769(5)	5.7(3)
C(5)	0.2714(6)	0.4381(7)	0.0990(5)	5.5(3)
C(6)	0.2371(5)	0.3519(7)	0.1052(4)	4.4(2)
C(7)	0.1506(5)	0.3451(7)	0.1302(5)	7.4(3)
C(8)	0.3820(5)	0.0360(6)	0.0601(5)	5.1(3)
C(9)	0.3180(6)	-0.0314(7)	0.0795(4)	4.8(3)
C(10)	0.3350(6)	-0.1233(7)	0.0750(5)	5.8(3)
C(11)	0.2722(8)	-0.1837(6)	0.0901(5)	6.9(4)
C(12)	0.1969(7)	-0.1498(8)	0.1067(5)	7.0(3)
C(13)	0.1849(6)	-0.0582(7)	0.1089(5)	6.1(3)
C(14)	0.1019(6)	-0.0240(7)	0.1301(6)	9.0(4)
C(15)	0.4168(5)	0.1282(7)	0.1645(4)	5.4(3)
C(16)	0.3635(5)	0.1217(6)	0.2221(4)	3.9(2)
C(17)	0.4029(5)	0.1040(6)	0.2864(5)	5.2(3)
C(18)	0.3556(6)	0.1034(7)	0.3413(5)	6.5(3)
C(19)	0.2692(6)	0.1195(6)	0.3286(5)	5.5(3)
C(20)	0.2321(5)	0.1375(7)	0.2618(5)	4.7(2)
C(21)	0.1386(6)	0.1567(8)	0.2506(5)	8.3(3)
C(22)	0.8174(5)	0.2193(5)	0.6029(4)	4.5(2)
C(23)	0.7409(5)	0.1828(6)	0.6335(4)	3.8(2)
C(24)	0.7370(6)	0.1860(7)	0.7035(5)	5.8(3)
C(25)	0.6621(7)	0.1614(7)	0.7266(4)	7.1(3)
C(26)	0.5936(6)	0.1347(7)	0.6812(5)	5.9(3)
C(27)	0.6026(5)	0.1304(6)	0.6117(4)	4.3(2)
C(28)	0.5303(5)	0.0986(6)	0.5600(4)	5.2(3)
C(29)	0.8711(5)	0.2126(5)	0.4885(5)	4.5(2)
C(30)	0.8513(5)	0.1669(6)	0.4193(4)	3.9(2)
C(31)	0.9083(5)	0.1672(6)	0.3698(5)	5.1(3)
C(32)	0.8797(6)	0.1307(8)	0.3063(5)	6.3(3)
C(33)	0.7991(6)	0.0960(6)	0.2926(4)	5.1(3)
C(34)	0.7461(5)	0.0967(6)	0.3444(4)	4.0(2)
C(35)	0.6579(5)	0.0583(7)	0.3303(4)	6.0(3)
C(36)	0.8788(5)	0.0779(5)	0.5646(4)	3.7(2)
C(37)	0.9707(5)	0.0906(5)	0.5992(4)	3.5(2)
C(38)	1.0375(5)	0.0941(6)	0.5588(4)	4.3(2)

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Table of atomic coordinates and B(eq) for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4
(cont.)

atom	x	y	z	B(eq)
C(39)	1.1205(5)	0.1052(6)	0.5909(5)	4.3(2)
C(40)	1.1330(5)	0.1129(6)	0.6616(5)	4.7(3)
C(41)	1.0635(5)	0.1093(6)	0.6982(4)	4.5(2)
C(42)	1.0750(5)	0.1193(8)	0.7740(5)	7.5(3)
H(1)	0.3768	0.1871	0.0024	5.0
H(2)	0.4571	0.2064	0.0552	5.0
H(3)	0.4501	0.3730	0.0489	5.0
H(4)	0.3751	0.5060	0.0713	5.0
H(5)	0.2401	0.4905	0.1099	5.0
H(6)	0.1305	0.4048	0.1384	5.0
H(7)	0.1561	0.3116	0.1723	5.0
H(8)	0.1120	0.3156	0.0965	5.0
H(9)	0.3741	0.0440	0.0114	5.0
H(10)	0.4382	0.0134	0.0742	5.0
H(11)	0.3880	-0.1442	0.0621	5.0
H(12)	0.2816	-0.2476	0.0887	5.0
H(13)	0.1527	-0.1901	0.1169	5.0
H(14)	0.0671	-0.0747	0.1387	5.0
H(15)	0.0735	0.0119	0.0941	5.0
H(16)	0.1138	0.0111	0.1709	5.0
H(17)	0.4466	0.1845	0.1693	5.0
H(18)	0.4570	0.0795	0.1697	5.0
H(19)	0.4629	0.0922	0.2937	5.0
H(20)	0.3823	0.0921	0.3870	5.0
H(21)	0.2349	0.1180	0.3655	5.0
H(22)	0.1163	0.1535	0.2937	5.0
H(23)	0.1111	0.1125	0.2199	5.0
H(24)	0.1295	0.2156	0.2314	5.0
H(25)	0.8665	0.2172	0.6368	5.0
H(26)	0.8067	0.2804	0.5886	5.0
H(27)	0.7852	0.2047	0.7347	5.0
H(28)	0.6574	0.1631	0.7748	5.0
H(29)	0.5406	0.1192	0.6971	5.0
H(30)	0.4823	0.0841	0.5833	5.0
H(31)	0.5153	0.1452	0.5272	5.0
H(32)	0.5478	0.0458	0.5373	5.0
H(33)	0.9316	0.2148	0.5005	5.0
H(34)	0.8488	0.2728	0.4854	5.0
H(35)	0.9646	0.1915	0.3796	5.0
H(36)	0.9167	0.1296	0.2712	5.0
H(37)	0.7795	0.0717	0.2482	5.0
H(38)	0.6491	0.0360	0.2841	5.0
H(39)	0.6173	0.1043	0.3361	5.0
H(40)	0.6520	0.0096	0.3615	5.0
H(41)	0.8473	0.0475	0.5964	5.0
H(42)	0.8805	0.0410	0.5247	5.0
H(43)	1.0263	0.0891	0.5099	5.0
H(44)	1.1676	0.1073	0.5646	5.0
H(45)	1.1892	0.1207	0.6852	5.0
H(46)	1.1343	0.1261	0.7896	5.0
H(47)	1.0539	0.0661	0.7940	5.0
H(48)	1.0444	0.1708	0.7863	5.0

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Table of anisotropic parameters for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

atom	U11	U22	U33	U12	U13	U23
Cu(1)	0.0454(6)	0.0544(8)	0.0583(8)	0.0019(7)	0.0090(5)	-0.0009(8)
Cu(2)	0.0429(5)	0.0473(7)	0.0400(6)	0.0021(6)	0.0036(5)	-0.0032(7)
Cl(1)	0.060(1)	0.062(2)	0.069(2)	-0.004(1)	-0.005(1)	-0.001(2)
Cl(2)	0.074(2)	0.081(2)	0.066(2)	0.032(1)	0.017(1)	0.018(2)
Cl(3)	0.055(1)	0.045(1)	0.056(2)	-0.004(1)	0.011(1)	-0.003(1)
Cl(4)	0.074(2)	0.052(2)	0.082(2)	-0.006(2)	0.020(2)	0.003(2)
O(1)	0.22(1)	0.072(7)	0.61(2)	-0.015(7)	0.24(1)	-0.10(1)
O(2)	0.22(1)	0.48(2)	0.081(7)	-0.08(1)	0.015(7)	0.02(1)
O(3)	0.075(5)	0.139(8)	0.39(1)	-0.017(6)	-0.025(7)	-0.03(1)
O(4)	0.150(7)	0.131(7)	0.150(8)	-0.051(6)	0.000(6)	0.060(7)
N(1)	0.043(4)	0.054(5)	0.051(5)	0.006(4)	0.014(3)	0.000(5)
N(2)	0.052(5)	0.039(5)	0.058(5)	0.010(4)	0.007(4)	-0.002(4)
N(3)	0.062(5)	0.052(6)	0.058(5)	-0.002(4)	0.017(4)	0.007(5)
N(4)	0.061(4)	0.057(5)	0.050(5)	-0.001(5)	0.022(4)	-0.004(5)
N(5)	0.050(4)	0.037(5)	0.026(4)	-0.002(3)	0.001(3)	-0.003(4)
N(6)	0.045(4)	0.041(5)	0.038(4)	0.006(4)	0.007(3)	-0.006(4)
N(7)	0.038(3)	0.038(4)	0.049(4)	-0.001(4)	0.007(3)	0.002(4)
N(8)	0.047(4)	0.054(5)	0.054(5)	-0.000(4)	-0.000(4)	0.009(4)
C(1)	0.041(5)	0.063(7)	0.062(7)	-0.003(5)	0.009(5)	0.001(6)
C(2)	0.051(6)	0.055(7)	0.041(6)	-0.001(5)	0.008(5)	-0.001(5)
C(3)	0.062(6)	0.070(8)	0.075(7)	-0.009(7)	0.010(5)	-0.009(7)
C(4)	0.086(8)	0.050(7)	0.077(8)	-0.018(6)	0.002(6)	-0.008(6)
C(5)	0.070(7)	0.056(7)	0.082(8)	0.016(6)	0.004(6)	-0.014(7)
C(6)	0.040(5)	0.059(7)	0.067(6)	-0.010(6)	-0.004(4)	-0.007(7)
C(7)	0.071(7)	0.074(8)	0.13(1)	0.005(6)	0.010(6)	-0.030(8)
C(8)	0.073(7)	0.059(7)	0.067(7)	0.020(6)	0.024(5)	-0.006(6)
C(9)	0.076(7)	0.064(8)	0.043(6)	0.009(6)	0.010(5)	0.004(6)
C(10)	0.103(8)	0.052(8)	0.065(7)	0.024(7)	0.013(6)	-0.003(7)
C(11)	0.15(1)	0.032(7)	0.077(9)	0.011(7)	-0.013(8)	0.019(6)
C(12)	0.106(9)	0.059(8)	0.095(9)	-0.019(8)	-0.004(7)	0.016(8)
C(13)	0.084(8)	0.068(8)	0.078(8)	0.013(7)	0.011(6)	0.014(7)
C(14)	0.105(9)	0.09(1)	0.16(1)	-0.034(7)	0.034(8)	0.034(9)
C(15)	0.065(6)	0.087(8)	0.052(6)	0.007(6)	0.009(5)	0.002(7)
C(16)	0.057(5)	0.047(6)	0.044(6)	0.002(5)	0.008(4)	0.008(5)
C(17)	0.073(6)	0.073(8)	0.056(7)	0.020(6)	0.020(5)	0.013(6)
C(18)	0.103(8)	0.09(1)	0.056(7)	0.029(7)	0.003(6)	0.013(7)
C(19)	0.099(7)	0.061(8)	0.054(7)	-0.004(6)	0.033(6)	0.012(6)
C(20)	0.059(6)	0.057(7)	0.066(7)	-0.001(6)	0.015(5)	0.007(7)
C(21)	0.086(7)	0.16(1)	0.077(8)	-0.002(8)	0.030(6)	-0.008(9)
C(22)	0.056(6)	0.045(6)	0.066(7)	0.006(5)	-0.010(5)	-0.014(6)
C(23)	0.064(6)	0.035(6)	0.046(6)	0.011(5)	0.002(5)	-0.008(5)
C(24)	0.098(8)	0.082(8)	0.038(6)	0.000(7)	0.007(6)	-0.009(6)
C(25)	0.15(1)	0.10(1)	0.028(6)	-0.008(9)	0.017(6)	-0.008(6)
C(26)	0.106(8)	0.063(7)	0.063(7)	-0.008(7)	0.048(6)	-0.005(7)
C(27)	0.061(5)	0.049(6)	0.054(6)	0.007(6)	0.011(5)	-0.012(6)
C(28)	0.060(6)	0.065(7)	0.073(7)	0.008(5)	0.018(5)	-0.000(6)
C(29)	0.037(5)	0.037(6)	0.096(8)	0.000(4)	-0.001(5)	0.009(6)
C(30)	0.052(5)	0.046(6)	0.048(6)	0.005(5)	0.002(5)	0.002(5)
C(31)	0.045(5)	0.063(7)	0.089(8)	-0.005(5)	0.024(5)	0.015(6)
C(32)	0.097(7)	0.087(9)	0.064(7)	0.007(8)	0.040(6)	0.005(8)
C(33)	0.088(7)	0.070(8)	0.037(6)	0.003(6)	0.017(5)	-0.004(5)
C(34)	0.050(5)	0.059(7)	0.042(6)	-0.000(5)	0.001(5)	-0.002(5)
C(35)	0.069(6)	0.098(8)	0.056(7)	-0.006(6)	-0.003(5)	-0.014(7)
C(36)	0.054(5)	0.038(6)	0.047(6)	0.005(5)	0.004(4)	0.003(5)
C(37)	0.047(5)	0.035(5)	0.049(6)	0.004(4)	0.001(4)	-0.002(5)
C(38)	0.055(5)	0.047(6)	0.059(7)	0.008(5)	0.004(5)	-0.002(5)

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Table of anisotropic parameters for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4
(cont.)

atom	U11	U22	U33	U12	U13	U23
C(39)	0.047(5)	0.053(7)	0.065(7)	0.006(5)	0.013(5)	-0.002(6)
C(40)	0.047(5)	0.048(7)	0.081(8)	-0.005(5)	0.001(5)	0.004(6)
C(41)	0.060(6)	0.071(8)	0.037(6)	0.003(5)	0.003(5)	0.005(5)
C(42)	0.065(6)	0.13(1)	0.087(8)	-0.006(7)	-0.002(6)	0.032(8)

Table of bond lengths involving the nonhydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

atom	atom	distance	atom	atom	distance
Cu(1)	Cl(1)	2.240(2)	N(6)	C(23)	1.355(9)
Cu(1)	N(1)	2.092(6)	N(6)	C(27)	1.347(9)
Cu(1)	N(2)	2.047(7)	N(7)	C(30)	1.350(8)
Cu(1)	N(3)	2.035(7)	N(7)	C(34)	1.336(9)
Cu(1)	N(4)	2.161(6)	N(8)	C(37)	1.324(9)
Cu(2)	Cl(2)	2.292(2)	N(8)	C(41)	1.347(9)
Cu(2)	Cl(3)	2.373(2)	C(1)	C(2)	1.50(1)
Cu(2)	N(5)	2.145(6)	C(2)	C(3)	1.37(1)
Cu(2)	N(6)	2.014(6)	C(3)	C(4)	1.38(1)
Cu(2)	N(7)	2.017(6)	C(4)	C(5)	1.38(1)
Cl(4)	O(1)	1.292(8)	C(5)	C(6)	1.39(1)
Cl(4)	O(2)	1.266(8)	C(6)	C(7)	1.50(1)
Cl(4)	O(3)	1.314(7)	C(8)	C(9)	1.49(1)
Cl(4)	O(4)	1.381(7)	C(9)	C(10)	1.38(1)
N(1)	C(1)	1.481(9)	C(10)	C(11)	1.38(1)
N(1)	C(8)	1.46(1)	C(11)	C(12)	1.36(1)
N(1)	C(15)	1.474(9)	C(12)	C(13)	1.36(1)
N(2)	C(2)	1.362(9)	C(13)	C(14)	1.50(1)
N(2)	C(6)	1.33(1)	C(15)	C(16)	1.48(1)
N(3)	C(9)	1.34(1)	C(16)	C(17)	1.35(1)
N(3)	C(13)	1.36(1)	C(17)	C(18)	1.38(1)
N(4)	C(16)	1.347(8)	C(18)	C(19)	1.37(1)
N(4)	C(20)	1.336(9)	C(19)	C(20)	1.38(1)
N(5)	C(22)	1.475(9)	C(20)	C(21)	1.48(1)
N(5)	C(29)	1.471(9)	C(22)	C(23)	1.50(1)
N(5)	C(36)	1.481(9)	C(23)	C(24)	1.37(1)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

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Table of bond lengths involving the nonhydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

(cont.)

atom	atom	distance	atom	atom	distance
C(24)	C(25)	1.36(1)			
C(25)	C(26)	1.36(1)			
C(26)	C(27)	1.38(1)			
C(27)	C(28)	1.50(1)			
C(29)	C(30)	1.50(1)			
C(30)	C(31)	1.39(1)			
C(31)	C(32)	1.37(1)			
C(32)	C(33)	1.36(1)			
C(33)	C(34)	1.38(1)			
C(34)	C(35)	1.49(1)			
C(36)	C(37)	1.526(9)			
C(37)	C(38)	1.386(9)			
C(38)	C(39)	1.383(9)			
C(39)	C(40)	1.37(1)			
C(40)	C(41)	1.38(1)			
C(41)	C(42)	1.47(1)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table of bond lengths involving the hydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.950	C(22)	H(25)	0.951
C(1)	H(2)	0.949	C(22)	H(26)	0.949
C(3)	H(3)	0.950	C(24)	H(27)	0.950
C(4)	H(4)	0.951	C(25)	H(28)	0.951
C(5)	H(5)	0.951	C(26)	H(29)	0.951
C(7)	H(6)	0.952	C(28)	H(30)	0.952
C(7)	H(7)	0.951	C(28)	H(31)	0.945
C(7)	H(8)	0.941	C(28)	H(32)	0.950
C(8)	H(9)	0.950	C(29)	H(33)	0.950
C(8)	H(10)	0.951	C(29)	H(34)	0.950
C(10)	H(11)	0.949	C(31)	H(35)	0.950
C(11)	H(12)	0.951	C(32)	H(36)	0.950
C(12)	H(13)	0.952	C(33)	H(37)	0.951
C(14)	H(14)	0.950	C(35)	H(38)	0.951
C(14)	H(15)	0.944	C(35)	H(39)	0.946
C(14)	H(16)	0.948	C(35)	H(40)	0.950
C(15)	H(17)	0.950	C(36)	H(41)	0.950
C(15)	H(18)	0.950	C(36)	H(42)	0.950
C(17)	H(19)	0.950	C(38)	H(43)	0.950
C(18)	H(20)	0.951	C(39)	H(44)	0.950
C(19)	H(21)	0.950	C(40)	H(45)	0.950
C(21)	H(22)	0.949	C(42)	H(46)	0.949
C(21)	H(23)	0.949	C(42)	H(47)	0.952
C(21)	H(24)	0.946	C(42)	H(48)	0.943

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table of bond angles involving the nonhydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Cu(1)	N(1)	135.3(2)	Cu(1)	N(1)	C(1)	104.6(5)
Cl(1)	Cu(1)	N(2)	94.3(2)	Cu(1)	N(1)	C(8)	106.9(5)
Cl(1)	Cu(1)	N(3)	96.0(2)	Cu(1)	N(1)	C(15)	107.8(5)
Cl(1)	Cu(1)	N(4)	140.8(2)	C(1)	N(1)	C(8)	111.3(7)
N(1)	Cu(1)	N(2)	80.6(3)	C(1)	N(1)	C(15)	112.7(7)
N(1)	Cu(1)	N(3)	80.9(3)	C(8)	N(1)	C(15)	113.0(7)
N(1)	Cu(1)	N(4)	83.9(2)	Cu(1)	N(2)	C(2)	113.8(6)
N(2)	Cu(1)	N(3)	161.0(3)	Cu(1)	N(2)	C(6)	130.6(6)
N(2)	Cu(1)	N(4)	92.4(3)	C(2)	N(2)	C(6)	115.6(7)
N(3)	Cu(1)	N(4)	89.6(3)	Cu(1)	N(3)	C(9)	114.9(6)
Cl(2)	Cu(2)	Cl(3)	131.44(9)	Cu(1)	N(3)	C(13)	130.3(7)
Cl(2)	Cu(2)	N(5)	123.3(2)	C(9)	N(3)	C(13)	114.8(8)
Cl(2)	Cu(2)	N(6)	95.9(2)	Cu(1)	N(4)	C(16)	109.8(5)
Cl(2)	Cu(2)	N(7)	90.6(2)	Cu(1)	N(4)	C(20)	131.6(6)
Cl(3)	Cu(2)	N(5)	105.1(2)	C(16)	N(4)	C(20)	118.1(7)
Cl(3)	Cu(2)	N(6)	93.9(2)	Cu(2)	N(5)	C(22)	104.8(4)
Cl(3)	Cu(2)	N(7)	93.4(2)	Cu(2)	N(5)	C(29)	100.9(4)
N(5)	Cu(2)	N(6)	81.2(2)	Cu(2)	N(5)	C(36)	110.9(4)
N(5)	Cu(2)	N(7)	82.2(2)	C(22)	N(5)	C(29)	114.6(6)
N(6)	Cu(2)	N(7)	163.1(2)	C(22)	N(5)	C(36)	111.6(6)
O(1)	Cl(4)	O(2)	109.3(8)	C(29)	N(5)	C(36)	113.2(6)
O(1)	Cl(4)	O(3)	109.5(6)	Cu(2)	N(6)	C(23)	114.8(5)
O(1)	Cl(4)	O(4)	109.3(6)	Cu(2)	N(6)	C(27)	128.5(6)
O(2)	Cl(4)	O(3)	109.5(6)	C(23)	N(6)	C(27)	116.2(7)
O(2)	Cl(4)	O(4)	104.2(7)	Cu(2)	N(7)	C(30)	113.2(5)
O(3)	Cl(4)	O(4)	114.8(6)	Cu(2)	N(7)	C(34)	128.4(5)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

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Table of bond angles involving the nonhydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

(cont.)

atom	atom	atom	angle	atom	atom	atom	angle
C(30)	N(7)	C(34)	118.4(7)	C(16)	C(17)	C(18)	119.4(8)
C(37)	N(8)	C(41)	117.5(7)	C(17)	C(18)	C(19)	118.5(9)
N(1)	C(1)	C(2)	109.7(7)	C(18)	C(19)	C(20)	119.6(8)
N(2)	C(2)	C(1)	114.2(8)	N(4)	C(20)	C(19)	121.5(8)
N(2)	C(2)	C(3)	124.3(8)	N(4)	C(20)	C(21)	120.7(8)
C(1)	C(2)	C(3)	121.3(8)	C(19)	C(20)	C(21)	117.8(8)
C(2)	C(3)	C(4)	118.9(8)	N(5)	C(22)	C(23)	109.4(7)
C(3)	C(4)	C(5)	118.0(9)	N(6)	C(23)	C(22)	114.8(7)
C(4)	C(5)	C(6)	119.6(9)	N(6)	C(23)	C(24)	123.9(8)
N(2)	C(6)	C(5)	123.5(8)	C(22)	C(23)	C(24)	121.1(8)
N(2)	C(6)	C(7)	118.7(9)	C(23)	C(24)	C(25)	117.8(9)
C(5)	C(6)	C(7)	117.7(9)	C(24)	C(25)	C(26)	120.5(9)
N(1)	C(8)	C(9)	111.5(7)	C(25)	C(26)	C(27)	118.8(9)
N(3)	C(9)	C(8)	115.3(8)	N(6)	C(27)	C(26)	122.7(8)
N(3)	C(9)	C(10)	125.0(9)	N(6)	C(27)	C(28)	116.3(7)
C(8)	C(9)	C(10)	119.5(9)	C(26)	C(27)	C(28)	121.0(8)
C(9)	C(10)	C(11)	117.7(9)	N(5)	C(29)	C(30)	111.5(7)
C(10)	C(11)	C(12)	119(1)	N(7)	C(30)	C(29)	114.6(7)
C(11)	C(12)	C(13)	120(1)	N(7)	C(30)	C(31)	122.5(8)
N(3)	C(13)	C(12)	124(1)	C(29)	C(30)	C(31)	122.7(8)
N(3)	C(13)	C(14)	118.1(9)	C(30)	C(31)	C(32)	117.2(8)
C(12)	C(13)	C(14)	118(1)	C(31)	C(32)	C(33)	121.0(8)
N(1)	C(15)	C(16)	117.6(7)	C(32)	C(33)	C(34)	119.0(8)
N(4)	C(16)	C(15)	118.7(7)	N(7)	C(34)	C(33)	121.9(8)
N(4)	C(16)	C(17)	122.8(8)	N(7)	C(34)	C(35)	118.7(7)
C(15)	C(16)	C(17)	118.4(8)	C(33)	C(34)	C(35)	119.4(8)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

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Table of bond angles involving the nonhydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

				(cont.)			
atom	atom	atom	angle	atom	atom	atom	angle
N(5)	C(36)	C(37)	115.1(6)				
N(8)	C(37)	C(36)	117.3(7)				
N(8)	C(37)	C(38)	123.1(7)				
C(36)	C(37)	C(38)	119.6(7)				
C(37)	C(38)	C(39)	119.0(8)				
C(38)	C(39)	C(40)	118.2(8)				
C(39)	C(40)	C(41)	119.5(8)				
N(8)	C(41)	C(40)	122.7(8)				
N(8)	C(41)	C(42)	116.7(8)				
C(40)	C(41)	C(42)	120.6(8)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table of bond angles involving the hydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(1)	109.37	C(11)	C(12)	H(13)	120.00
N(1)	C(1)	H(2)	109.38	C(13)	C(12)	H(13)	120.07
C(2)	C(1)	H(1)	109.39	C(13)	C(14)	H(14)	108.91
C(2)	C(1)	H(2)	109.44	C(13)	C(14)	H(15)	109.20
H(1)	C(1)	H(2)	109.53	C(13)	C(14)	H(16)	108.99
C(2)	C(3)	H(3)	120.69	H(14)	C(14)	H(15)	109.92
C(4)	C(3)	H(3)	120.44	H(14)	C(14)	H(16)	109.64
C(3)	C(4)	H(4)	121.10	H(15)	C(14)	H(16)	110.16
C(5)	C(4)	H(4)	120.94	N(1)	C(15)	H(17)	107.31
C(4)	C(5)	H(5)	120.11	N(1)	C(15)	H(18)	107.35
C(6)	C(5)	H(5)	120.24	C(16)	C(15)	H(17)	107.48
C(6)	C(7)	H(6)	108.91	C(16)	C(15)	H(18)	107.49
C(6)	C(7)	H(7)	108.93	H(17)	C(15)	H(18)	109.46
C(6)	C(7)	H(8)	109.55	C(16)	C(17)	H(19)	120.33
H(6)	C(7)	H(7)	109.22	C(18)	C(17)	H(19)	120.25
H(6)	C(7)	H(8)	110.08	C(17)	C(18)	H(20)	120.67
H(7)	C(7)	H(8)	110.13	C(19)	C(18)	H(20)	120.82
N(1)	C(8)	H(9)	109.00	C(18)	C(19)	H(21)	120.09
N(1)	C(8)	H(10)	108.93	C(20)	C(19)	H(21)	120.29
C(9)	C(8)	H(9)	109.02	C(20)	C(21)	H(22)	109.10
C(9)	C(8)	H(10)	108.98	C(20)	C(21)	H(23)	109.04
H(9)	C(8)	H(10)	109.40	C(20)	C(21)	H(24)	109.26
C(9)	C(10)	H(11)	121.09	H(22)	C(21)	H(23)	109.60
C(11)	C(10)	H(11)	121.17	H(22)	C(21)	H(24)	109.93
C(10)	C(11)	H(12)	120.70	H(23)	C(21)	H(24)	109.90
C(12)	C(11)	H(12)	120.72	N(5)	C(22)	H(25)	109.51

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

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Table of bond angles involving the hydrogen atoms
for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

(cont.)

atom	atom	atom	angle	atom	atom	atom	angle
N(5)	C(22)	H(26)	109.62	C(34)	C(33)	H(37)	120.56
C(23)	C(22)	H(25)	109.37	C(34)	C(35)	H(38)	109.22
C(23)	C(22)	H(26)	109.48	C(34)	C(35)	H(39)	109.45
H(25)	C(22)	H(26)	109.47	C(34)	C(35)	H(40)	109.22
C(23)	C(24)	H(27)	121.12	H(38)	C(35)	H(39)	109.76
C(25)	C(24)	H(27)	121.03	H(38)	C(35)	H(40)	109.40
C(24)	C(25)	H(28)	119.81	H(39)	C(35)	H(40)	109.79
C(26)	C(25)	H(28)	119.73	N(5)	C(36)	H(41)	108.03
C(25)	C(26)	H(29)	120.69	N(5)	C(36)	H(42)	108.06
C(27)	C(26)	H(29)	120.55	C(37)	C(36)	H(41)	108.06
C(27)	C(28)	H(30)	109.12	C(37)	C(36)	H(42)	108.07
C(27)	C(28)	H(31)	109.51	H(41)	C(36)	H(42)	109.46
C(27)	C(28)	H(32)	109.24	C(37)	C(38)	H(43)	120.46
H(30)	C(28)	H(31)	109.76	C(39)	C(38)	H(43)	120.55
H(30)	C(28)	H(32)	109.30	C(38)	C(39)	H(44)	120.88
H(31)	C(28)	H(32)	109.89	C(40)	C(39)	H(44)	120.94
N(5)	C(29)	H(33)	109.00	C(39)	C(40)	H(45)	120.27
N(5)	C(29)	H(34)	108.99	C(41)	C(40)	H(45)	120.20
C(30)	C(29)	H(33)	108.91	C(41)	C(42)	H(46)	109.02
C(30)	C(29)	H(34)	108.89	C(41)	C(42)	H(47)	108.90
H(33)	C(29)	H(34)	109.49	C(41)	C(42)	H(48)	109.39
C(30)	C(31)	H(35)	121.47	H(46)	C(42)	H(47)	109.40
C(32)	C(31)	H(35)	121.37	H(46)	C(42)	H(48)	110.16
C(31)	C(32)	H(36)	119.49	H(47)	C(42)	H(48)	109.95
C(33)	C(32)	H(36)	119.48				
C(32)	C(33)	H(37)	120.49				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

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Table of torsion or conformation angles for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
Cu(1)N(1)	C(1)	C(2)		43.9(7)	Cl(1)Cu(1)N(1)	C(1)			54.0(6)
Cu(1)N(1)	C(8)	C(9)		-35.0(8)	Cl(1)Cu(1)N(1)	C(8)			-64.1(6)
Cu(1)N(1)	C(15)	C(16)		14(1)	Cl(1)Cu(1)N(1)	C(15)			174.1(5)
Cu(1)N(2)	C(2)	C(1)		4.8(9)	Cl(1)Cu(1)N(2)	C(2)			-118.9(6)
Cu(1)N(2)	C(2)	C(3)		-179.3(7)	Cl(1)Cu(1)N(2)	C(6)			59.8(8)
Cu(1)N(2)	C(6)	C(5)		179.7(7)	Cl(1)Cu(1)N(3)	C(9)			123.6(6)
Cu(1)N(2)	C(6)	C(7)		2(1)	Cl(1)Cu(1)N(3)	C(13)			-59.1(8)
Cu(1)N(3)	C(9)	C(8)		-6(1)	Cl(1)Cu(1)N(4)	C(16)			177.1(5)
Cu(1)N(3)	C(9)	C(10)		179.4(8)	Cl(1)Cu(1)N(4)	C(20)			6(1)
Cu(1)N(3)	C(13)	C(12)		-177.9(8)	Cl(2)Cu(2)N(5)	C(22)			65.3(5)
Cu(1)N(3)	C(13)	C(14)		0(1)	Cl(2)Cu(2)N(5)	C(29)			-54.0(5)
Cu(1)N(4)	C(16)	C(15)		12(1)	Cl(2)Cu(2)N(5)	C(36)			-174.2(4)
Cu(1)N(4)	C(16)	C(17)		-171.5(8)	Cl(2)Cu(2)N(6)	C(23)			-116.4(6)
Cu(1)N(4)	C(20)	C(19)		169.3(7)	Cl(2)Cu(2)N(6)	C(27)			72.6(7)
Cu(1)N(4)	C(20)	C(21)		-11(1)	Cl(2)Cu(2)N(7)	C(30)			109.1(5)
Cu(2)N(5)	C(22)	C(23)		40.1(7)	Cl(2)Cu(2)N(7)	C(34)			-71.9(7)
Cu(2)N(5)	C(29)	C(30)		-43.9(7)	Cl(3)Cu(2)N(5)	C(22)			-117.8(5)
Cu(2)N(5)	C(36)	C(37)		177.0(5)	Cl(3)Cu(2)N(5)	C(29)			123.0(4)
Cu(2)N(6)	C(23)	C(22)		15.4(9)	Cl(3)Cu(2)N(5)	C(36)			2.8(5)
Cu(2)N(6)	C(23)	C(24)		-169.3(7)	Cl(3)Cu(2)N(6)	C(23)			111.2(6)
Cu(2)N(6)	C(27)	C(26)		170.0(7)	Cl(3)Cu(2)N(6)	C(27)			-59.8(7)
Cu(2)N(6)	C(27)	C(28)		-9(1)	Cl(3)Cu(2)N(7)	C(30)			-119.3(5)
Cu(2)N(7)	C(30)	C(29)		-7.2(9)	Cl(3)Cu(2)N(7)	C(34)			59.7(7)
Cu(2)N(7)	C(30)	C(31)		176.8(7)	N(1) Cu(1)N(2)	C(2)			16.3(6)
Cu(2)N(7)	C(34)	C(33)		-177.6(6)	N(1) Cu(1)N(2)	C(6)			-164.9(8)
Cu(2)N(7)	C(34)	C(35)		2(1)	N(1) Cu(1)N(3)	C(9)			-11.3(6)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

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Table of torsion or conformation angles for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4
(cont.)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
N(1)	Cu(1)	N(3)	C(13)	166.0(9)	N(3)	C(13)	C(12)	C(11)	0(2)
N(1)	Cu(1)	N(4)	C(16)	-2.9(6)	N(4)	Cu(1)	N(1)	C(1)	-126.1(5)
N(1)	Cu(1)	N(4)	C(20)	-174.0(9)	N(4)	Cu(1)	N(1)	C(8)	115.8(6)
N(1)	C(1)	C(2)	N(2)	-34(1)	N(4)	Cu(1)	N(1)	C(15)	-5.9(6)
N(1)	C(1)	C(2)	C(3)	150.3(8)	N(4)	Cu(1)	N(2)	C(2)	99.7(6)
N(1)	C(8)	C(9)	N(3)	28(1)	N(4)	Cu(1)	N(2)	C(6)	-81.5(8)
N(1)	C(8)	C(9)	C(10)	-156.6(8)	N(4)	Cu(1)	N(3)	C(9)	-95.2(6)
N(1)	C(15)	C(16)	N(4)	-18(1)	N(4)	Cu(1)	N(3)	C(13)	82.1(8)
N(1)	C(15)	C(16)	C(17)	164.8(9)	N(4)	C(16)	C(17)	C(18)	-1(2)
N(2)	Cu(1)	N(1)	C(1)	-32.6(5)	N(4)	C(20)	C(19)	C(18)	1(2)
N(2)	Cu(1)	N(1)	C(8)	-150.7(6)	N(5)	Cu(2)	N(6)	C(23)	6.5(6)
N(2)	Cu(1)	N(1)	C(15)	87.5(6)	N(5)	Cu(2)	N(6)	C(27)	-164.5(7)
N(2)	Cu(1)	N(3)	C(9)	1(1)	N(5)	Cu(2)	N(7)	C(30)	-14.5(5)
N(2)	Cu(1)	N(3)	C(13)	178.4(8)	N(5)	Cu(2)	N(7)	C(34)	164.5(7)
N(2)	Cu(1)	N(4)	C(16)	-83.1(6)	N(5)	C(22)	C(23)	N(6)	-38.8(9)
N(2)	Cu(1)	N(4)	C(20)	105.8(9)	N(5)	C(22)	C(23)	C(24)	145.7(8)
N(2)	C(2)	C(3)	C(4)	-2(1)	N(5)	C(29)	C(30)	N(7)	37.3(9)
N(2)	C(6)	C(5)	C(4)	2(1)	N(5)	C(29)	C(30)	C(31)	-146.8(8)
N(3)	Cu(1)	N(1)	C(1)	143.3(5)	N(5)	C(36)	C(37)	N(8)	92.2(9)
N(3)	Cu(1)	N(1)	C(8)	25.2(5)	N(5)	C(36)	C(37)	C(38)	-88.1(9)
N(3)	Cu(1)	N(1)	C(15)	-96.6(6)	N(6)	Cu(2)	N(5)	C(22)	-26.1(5)
N(3)	Cu(1)	N(2)	C(2)	4(1)	N(6)	Cu(2)	N(5)	C(29)	-145.3(5)
N(3)	Cu(1)	N(2)	C(6)	-177.3(8)	N(6)	Cu(2)	N(5)	C(36)	94.5(5)
N(3)	Cu(1)	N(4)	C(16)	78.0(6)	N(6)	Cu(2)	N(7)	C(30)	-4(1)
N(3)	Cu(1)	N(4)	C(20)	-93.1(9)	N(6)	Cu(2)	N(7)	C(34)	175.4(8)
N(3)	C(9)	C(10)	C(11)	-2(2)	N(6)	C(23)	C(24)	C(25)	-2(2)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

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Table of torsion or conformation angles for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4
(cont.)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
N(6)	C(27)	C(26)	C(25)	-1(2)	C(9)	N(3)	C(13)	C(14)	177.3(9)
N(7)	Cu(2)	N(5)	C(22)	150.8(5)	C(9)	C(8)	N(1)	C(15)	83.4(9)
N(7)	Cu(2)	N(5)	C(29)	31.5(5)	C(9)	C(10)	C(11)	C(12)	2(2)
N(7)	Cu(2)	N(5)	C(36)	-88.7(5)	C(10)	C(9)	N(3)	C(13)	2(1)
N(7)	Cu(2)	N(6)	C(23)	-4(1)	C(10)	C(11)	C(12)	C(13)	-1(2)
N(7)	Cu(2)	N(6)	C(27)	-175.5(8)	C(11)	C(12)	C(13)	C(14)	-178(1)
N(7)	C(30)	C(31)	C(32)	2(1)	C(15)	C(16)	N(4)	C(20)	-175.8(8)
N(7)	C(34)	C(33)	C(32)	0(1)	C(15)	C(16)	C(17)	C(18)	175.9(9)
N(8)	C(37)	C(38)	C(39)	0(1)	C(16)	N(4)	C(20)	C(19)	-1(1)
N(8)	C(41)	C(40)	C(39)	1(1)	C(16)	N(4)	C(20)	C(21)	178.8(9)
C(1)	N(1)	C(8)	C(9)	-148.6(7)	C(16)	C(17)	C(18)	C(19)	1(2)
C(1)	N(1)	C(15)	C(16)	128.9(8)	C(17)	C(16)	N(4)	C(20)	1(1)
C(1)	C(2)	N(2)	C(6)	-174.2(8)	C(17)	C(18)	C(19)	C(20)	-1(2)
C(1)	C(2)	C(3)	C(4)	173.9(9)	C(18)	C(19)	C(20)	C(21)	-179(1)
C(2)	N(2)	C(6)	C(5)	-2(1)	C(22)	N(5)	C(29)	C(30)	-155.9(6)
C(2)	N(2)	C(6)	C(7)	-179.5(8)	C(22)	N(5)	C(36)	C(37)	-66.6(8)
C(2)	C(1)	N(1)	C(8)	158.9(7)	C(22)	C(23)	N(6)	C(27)	-172.4(7)
C(2)	C(1)	N(1)	C(15)	-72.9(8)	C(22)	C(23)	C(24)	C(25)	172.6(9)
C(2)	C(3)	C(4)	C(5)	1(1)	C(23)	N(6)	C(27)	C(26)	-1(1)
C(3)	C(2)	N(2)	C(6)	2(1)	C(23)	N(6)	C(27)	C(28)	179.6(7)
C(3)	C(4)	C(5)	C(6)	-1(2)	C(23)	C(22)	N(5)	C(29)	149.7(6)
C(4)	C(5)	C(6)	C(7)	179.4(9)	C(23)	C(22)	N(5)	C(36)	-80.0(8)
C(8)	N(1)	C(15)	C(16)	-103.9(9)	C(23)	C(24)	C(25)	C(26)	0(2)
C(8)	C(9)	N(3)	C(13)	176.5(8)	C(24)	C(23)	N(6)	C(27)	3(1)
C(8)	C(9)	C(10)	C(11)	-176.9(9)	C(24)	C(25)	C(26)	C(27)	2(2)
C(9)	N(3)	C(13)	C(12)	-1(2)	C(25)	C(26)	C(27)	C(28)	178.0(9)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

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Table of torsion or conformation angles for [CuCl(Me3tpa)][CuCl2(Me3tpa)]ClO4
(cont.)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C(29)	N(5)	C(36)	C(37)	64.4(9)					
C(29)	C(30)	N(7)	C(34)	173.7(7)					
C(29)	C(30)	C(31)	C(32)	-174.0(9)					
C(30)	N(7)	C(34)	C(33)	1(1)					
C(30)	N(7)	C(34)	C(35)	-178.8(7)					
C(30)	C(29)	N(5)	C(36)	74.7(8)					
C(30)	C(31)	C(32)	C(33)	0(2)					
C(31)	C(30)	N(7)	C(34)	-2(1)					
C(31)	C(32)	C(33)	C(34)	-1(2)					
C(32)	C(33)	C(34)	C(35)	-179.6(9)					
C(36)	C(37)	N(8)	C(41)	-179.6(7)					
C(36)	C(37)	C(38)	C(39)	-179.6(7)					
C(37)	N(8)	C(41)	C(40)	-1(1)					
C(37)	N(8)	C(41)	C(42)	178.4(9)					
C(37)	C(38)	C(39)	C(40)	-1(1)					
C(38)	C(37)	N(8)	C(41)	1(1)					
C(38)	C(39)	C(40)	C(41)	0(1)					
C(39)	C(40)	C(41)	C(42)	-178.8(9)					

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Table of Least-Squares Planes

----- Plane number 1 -----

Atoms Defining Plane	Distance	esd
Cl(1)	0.0372	0.0023
N(1)	0.3879	0.0063
N(2)	-0.3742	0.0069
N(3)	-0.3893	0.0071

Additional Atoms	Distance
Cu(1)	-0.6001

Mean deviation from plane is 0.2971 angstroms
Chi-squared: 10031.3

----- Plane number 2 -----

Atoms Defining Plane	Distance	esd
N(1)	0.0000	
N(2)	0.0000	
N(3)	0.0000	

Additional Atoms	Distance
Cu(1)	-0.0846
Cl(1)	1.4252

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
2	1	25.86

