Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information

Synthesis, Crystal Structure, Thermal and Luminescence Properties of CuX(2,3-dimethylpyrazine) (X = Cl, Br, I) Coordination Polymers

Inke Jeß, Petr Taborsky, Jiří Pospíšil and Christian Näther

Figure S1: Experimental (top) and calculated (bottom) X-ray powder pattern of compound **1**.

Figure S2: Experimental (top) and calculated (bottom) X-ray powder pattern of compound **2**.

Figure S3: Experimental (top) and calculated (bottom) X-ray powder pattern of compound **3**.

Figure S4: Experimental X-ray powder pattern of the residue obtained in the thermal decomposition reaction of compound **2** (top) and calculated pattern for compound **3** (bottom).

Details on the structure determination of form **I** (solvent-free).

Details on the structure determination of form **II** (solvent-free).

Details on the structure determination of form **III** (hydrate).

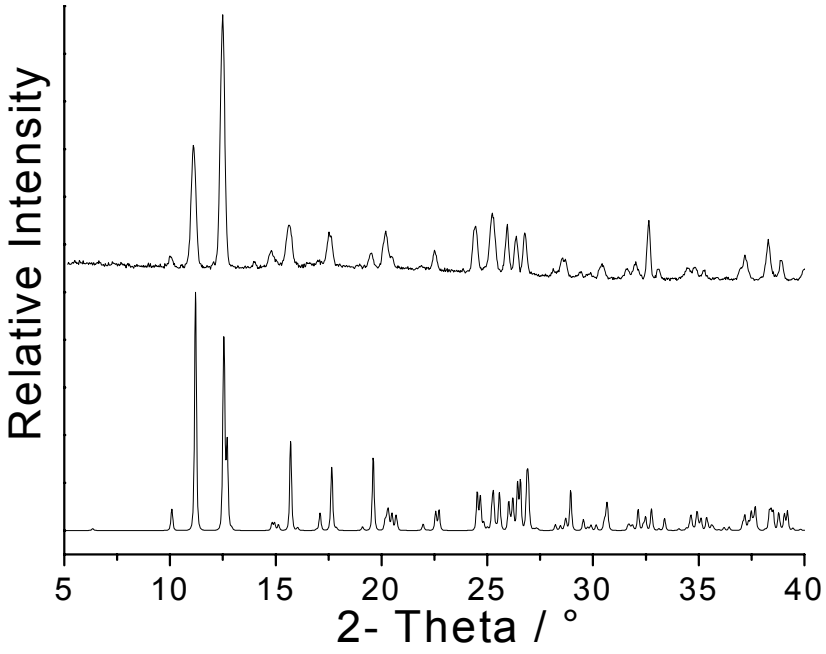

Figure S1: Experimental (top) and calculated (bottom) X-ray powder pattern of compound **1**.

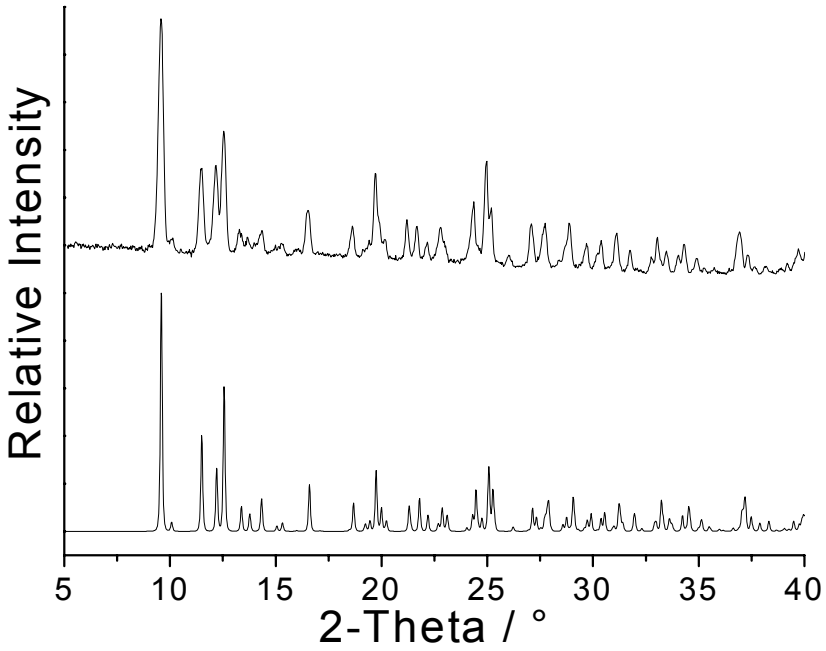

Figure S2: Experimental (top) and calculated (bottom) X-ray powder pattern of compound **2**.

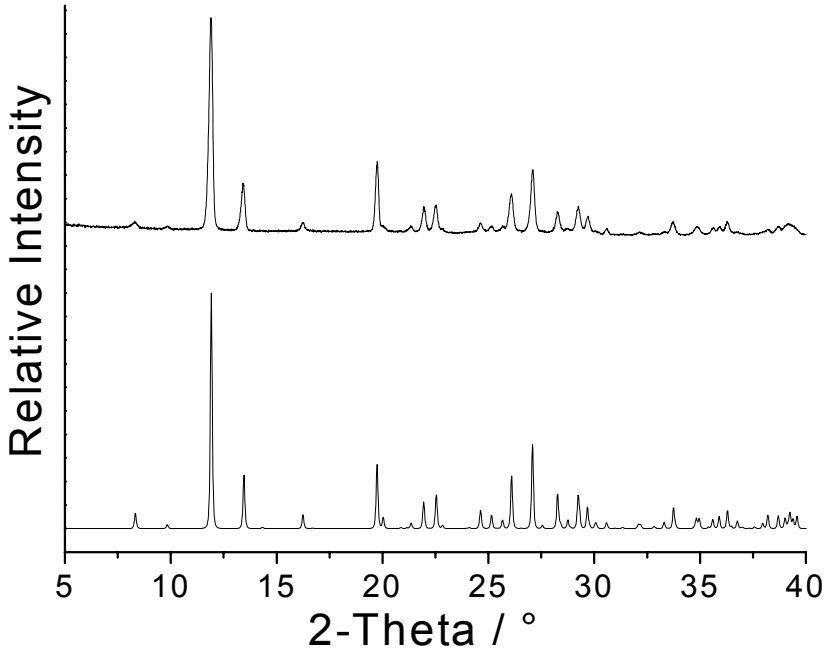

Figure S3: Experimental (top) and calculated (bottom) X-ray powder pattern of compound **3**.

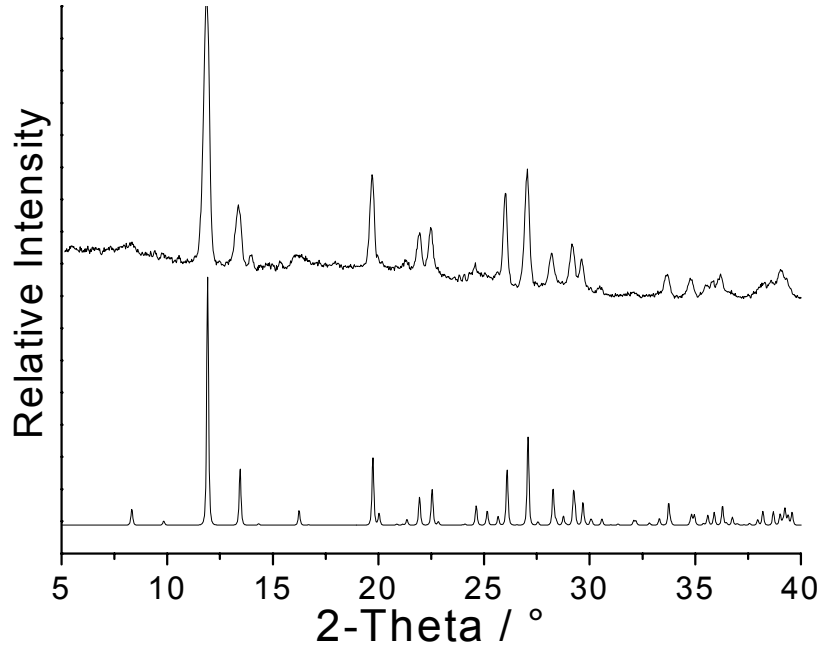

Figure S4: Experimental X-ray powder pattern of the residue obtained in the thermal decomposition reaction of compound **2** (top) and calculated pattern for compound **3** (bottom).

Table 1. Crystal data and structure refinement for di-(μ_2-iodo)-bis(2,3-dimethylpyrazine-N)-(μ_2-2,3-dimethylpyrazine)-di-copper(I) (Compound **1**)

Identification code	d120	
Empirical formula	$C_{18}H_{24}Cu_2I_2N_6$	
Formula weight	705.31	
Temperature	220(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.2001(12) Å	α= 90°.
	b = 11.2746(6) Å	β= 101.345(9)°.
	c = 14.3556(10) Å	γ = 90°.
Volume	2253.4(3) Å^3	
Z	4	
Density (calculated)	2.079 Mg/m^3	
Absorption coefficient	4.644 mm^{-1}	
F(000)	1352	
Crystal size	0.2 x 0.15 x 0.12 mm^3	
Theta range for data collection	2.31 to 27.10°.	
Index ranges	-18<=h<=17, -14<=k<=12, -18<=l<=18	
Reflections collected	11218	
Independent reflections	5042 [R(int) = 0.0477]	
Completeness to theta = 27.10°	98.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5042 / 0 / 260	
Goodness-of-fit on F^2	0.951	
Final R indices [I>2sigma(I)]	R1 = 0.0376, wR2 = 0.0853	
R indices (all data)	R1 = 0.0547, wR2 = 0.0913	
Largest diff. peak and hole	1.251 and -1.097 e.Å^{-3}	

Comments:

All non-hydrogen atoms were refined anisotropic. The hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and refined using a riding model.

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)
Cu(1)	745(1)	9248(1)	5435(1)	23(1)
I(1)	-930(1)	9253(1)	5959(1)	24(1)
Cu(2)	4541(1)	9300(1)	9247(1)	24(1)
I(2)	5963(1)	10788(1)	9084(1)	26(1)
N(1)	1933(2)	9539(3)	6518(2)	17(1)
C(1)	2047(3)	10432(4)	7146(3)	17(1)
C(2)	2835(3)	10450(4)	7919(3)	17(1)
N(2)	3476(3)	9561(3)	8045(2)	19(1)
C(3)	3380(3)	8709(4)	7380(3)	19(1)
C(4)	2617(3)	8711(4)	6624(3)	20(1)
C(5)	1316(3)	11389(4)	7016(3)	27(1)
C(6)	2987(4)	11429(5)	8626(4)	31(1)
N(11)	954(2)	7484(3)	4956(2)	18(1)
C(11)	1039(3)	6489(4)	5466(3)	18(1)
C(12)	1175(3)	5379(4)	5055(3)	22(1)
N(12)	1150(3)	5278(4)	4119(3)	28(1)
C(13)	1033(4)	6285(4)	3615(3)	30(1)
C(14)	959(3)	7373(4)	4017(3)	22(1)
C(15)	984(4)	6561(4)	6500(3)	30(1)
C(16)	1345(4)	4259(4)	5626(4)	32(1)
N(21)	5014(3)	7536(3)	9072(2)	22(1)
C(21)	4494(4)	6543(4)	8968(3)	24(1)
C(22)	4932(4)	5432(4)	8882(3)	31(1)
N(22)	5887(4)	5340(4)	9030(3)	36(1)
C(23)	6397(4)	6329(5)	9175(4)	36(1)
C(24)	5973(3)	7432(4)	9155(3)	26(1)
C(25)	3441(4)	6622(5)	8952(4)	35(1)
C(26)	4367(5)	4330(5)	8633(4)	46(2)

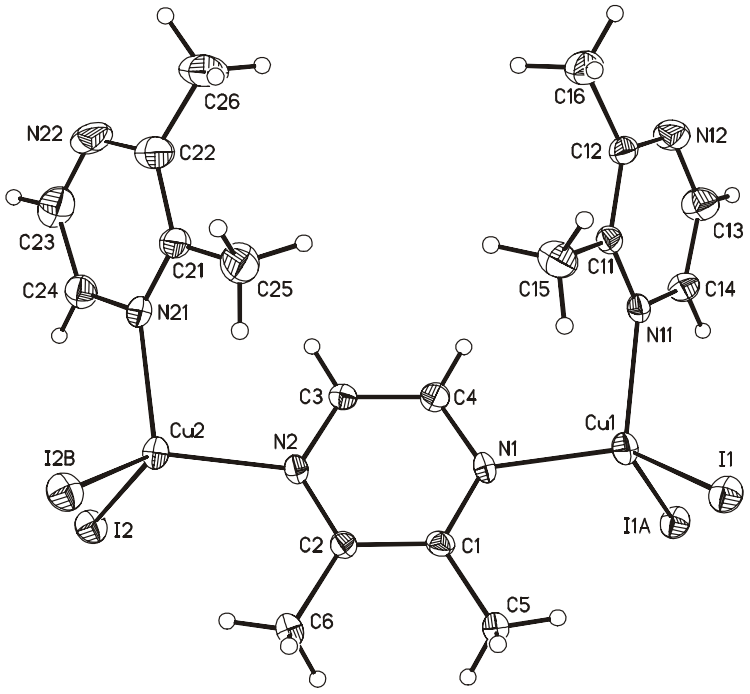

Table 3. Bond lengths [Å] and angles [°] for d120.

Cu(1)-N(1)	2.083(4)	Cu(2)-N(2)	2.080(4
Cu(1)-N(11)	2.143(3)	Cu(2)-N(21)	2.131(4
Cu(1)-I(1)	2.6307(6)	Cu(2)-I(2B)	2.6336
Cu(1)-I(1A)	2.6716(6)	Cu(2)-I(2)	2.6712
Cu(1)-Cu(1A)	2.8055(11)	Cu(2)-Cu(2B)	2.7843
I(1)-Cu(1A)	2.6716(6)	I(2)-Cu(2B)	2.6336
N(1)-Cu(1)-N(11)	104.02(14)	N(2)-Cu(2)-N(21)	103.21(14
N(1)-Cu(1)-I(1)	115.54(9)	N(2)-Cu(2)-I(2B)	118.51(10
N(11)-Cu(1)-I(1)	106.50(9)	N(21)-Cu(2)-I(2B)	102.72(9)
N(1)-Cu(1)-I(1A)	105.94(10)	N(2)-Cu(2)-I(2)	106.10(10
N(11)-Cu(1)-I(1A)	107.85(9)	N(21)-Cu(2)-I(2)	108.34(10
I(1)-Cu(1)-I(1A)	116.12(2)	I(2B)-Cu(2)-I(2)	116.69(2)
N(1)-Cu(1)-Cu(1A)	131.75(11)	N(2)-Cu(2)-Cu(2B)	135.84(11
N(11)-Cu(1)-Cu(1A)	123.93(10)	N(21)-Cu(2)-Cu(2B)	120.67(11
I(1)-Cu(1)-Cu(1A)	58.77(2)	I(2B)-Cu(2)-Cu(2B)	59.00(2)
I(1A)-Cu(1)-Cu(1A)	57.35(2)	I(2)-Cu(2)-Cu(2B)	57.69(2)
Cu(1)-I(1)-Cu(1A)	63.88(2)	Cu(2B)-I(2)-Cu(2)	63.31(2)
N(1)-C(4)	1.334(6)	C(2)-N(2)	1.343(6
N(1)-C(1)	1.340(5)	C(2)-C(6)	1.487(6
C(1)-C(2)	1.413(6)	N(2)-C(3)	1.342(6
C(1)-C(5)	1.483(6)	C(3)-C(4)	1.374(6
C(4)-N(1)-C(1)	117.4(4)	N(2)-C(2)-C(6)	117.3(4)
N(1)-C(1)-C(2)	120.8(4)	C(1)-C(2)-C(6)	122.3(4)
N(1)-C(1)-C(5)	118.3(4)	C(3)-N(2)-C(2)	117.8(4)
C(2)-C(1)-C(5)	121.0(4)	N(2)-C(3)-C(4)	121.0(4)
N(2)-C(2)-C(1)	120.4(4)	N(1)-C(4)-C(3)	122.3(4)
N(11)-C(11)	1.333(5)	C(12)-N(12)	1.342(6
N(11)-C(14)	1.356(5)	C(12)-C(16)	1.498(6
C(11)-C(12)	1.413(6)	N(12)-C(13)	1.340(6
C(11)-C(15)	1.503(6)	C(13)-C(14)	1.369(7
C(11)-N(11)-C(14)	116.8(4)	N(12)-C(12)-C(16)	116.5(4)
N(11)-C(11)-C(12)	121.4(4)	C(11)-C(12)-C(16)	122.6(4)
N(11)-C(11)-C(15)	118.7(4)	C(13)-N(12)-C(12)	116.4(4)
C(12)-C(11)-C(15)	119.9(4)	N(12)-C(13)-C(14)	122.9(4)
N(12)-C(12)-C(11)	121.0(4)	N(11)-C(14)-C(13)	121.2(4)
N(21)-C(21)	1.333(6)	C(22)-N(22)	1.335(7
N(21)-C(24)	1.349(6)	C(22)-C(26)	1.483(8
C(21)-C(22)	1.414(7)	N(22)-C(23)	1.323(8
C(21)-C(25)	1.494(7)	C(23)-C(24)	1.380(7
C(21)-N(21)-C(24)	117.7(4)	N(22)-C(22)-C(26)	117.3(5)
N(21)-C(21)-C(22)	120.7(5)	C(21)-C(22)-C(26)	122.4(5)
N(21)-C(21)-C(25)	118.8(4)	C(23)-N(22)-C(22)	117.9(4)
C(22)-C(21)-C(25)	120.5(5)	N(22)-C(23)-C(24)	122.2(5)
N(22)-C(22)-C(21)	120.3(5)	N(21)-C(24)-C(23)	120.6(5)

Symmetry transformations used to generate equivalent atoms: A: -x,-y+2,-z+1 ; B : -x+1,-y+2,-z+2

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu(1)	23(1)	25(1)	18(1)	-1(1)	-2(1)	-1(1)
I(1)	22(1)	24(1)	24(1)	6(1)	4(1)	-1(1)
Cu(2)	20(1)	25(1)	23(1)	-1(1)	-4(1)	2(1)
I(2)	26(1)	26(1)	26(1)	0(1)	6(1)	-6(1)
N(1)	16(2)	22(2)	13(2)	-2(1)	-1(1)	-3(1)
C(1)	21(2)	13(2)	17(2)	0(2)	3(2)	-1(2)
C(2)	18(2)	16(2)	17(2)	0(2)	1(2)	-1(2)
N(2)	18(2)	19(2)	18(2)	-1(1)	-3(1)	-2(1)
C(3)	19(2)	17(2)	20(2)	-3(2)	3(2)	1(2)
C(4)	21(2)	22(2)	17(2)	-2(2)	5(2)	2(2)
C(5)	25(2)	23(2)	26(2)	-5(2)	-8(2)	4(2)
C(6)	28(2)	28(3)	30(2)	-9(2)	-9(2)	2(2)
N(11)	17(2)	20(2)	15(2)	-1(1)	-2(1)	-1(1)
C(11)	17(2)	17(2)	19(2)	1(2)	1(2)	-2(2)
C(12)	16(2)	18(2)	30(2)	3(2)	2(2)	0(2)
N(12)	33(2)	24(2)	27(2)	-6(2)	8(2)	4(2)
C(13)	37(3)	29(3)	24(2)	-3(2)	10(2)	4(2)
C(14)	23(2)	21(2)	23(2)	1(2)	6(2)	3(2)
C(15)	45(3)	26(3)	19(2)	2(2)	4(2)	-6(2)
C(16)	31(3)	25(2)	39(3)	4(2)	6(2)	-1(2)
N(21)	24(2)	22(2)	17(2)	1(1)	-3(2)	3(2)
C(21)	35(3)	20(2)	16(2)	1(2)	1(2)	2(2)
C(22)	53(3)	23(2)	17(2)	1(2)	10(2)	3(2)
N(22)	53(3)	27(2)	29(2)	-1(2)	12(2)	18(2)
C(23)	34(3)	46(3)	28(2)	-2(2)	10(2)	15(3)
C(24)	26(2)	30(3)	23(2)	-4(2)	6(2)	4(2)
C(25)	30(3)	32(3)	39(3)	4(2)	2(2)	-7(2)
C(26)	83(5)	22(3)	32(3)	0(2)	9(3)	-1(3)

Table 5. Hydrogen coordinates ($x 10^4$) and isotropic displacement parameters ($Å^2 x 10^3$).

	x	y	z	U(eq)
H(3)	3841	8103	7432	23
H(4)	2576	8107	6166	24
H(5A)	1635	12154	7102	40
H(5B)	909	11298	7480	40
H(5C)	927	11342	6381	40
H(6A)	2552	11333	9064	46
H(6B)	2864	12184	8300	46
H(6C)	3645	11410	8977	46
H(13)	1002	6243	2956	35
H(14)	910	8056	3634	26
H(15A)	1615	6420	6886	45
H(15B)	538	5968	6642	45
H(15C)	762	7344	6638	45
H(16A)	1255	3581	5202	48
H(16B)	895	4215	6053	48
H(16C)	1997	4257	5993	48
H(23)	7071	6278	9295	43
H(24)	6357	8118	9200	31
H(25A)	3279	7426	9103	52
H(25B)	3272	6080	9418	52
H(25C)	3087	6412	8325	52
H(26A)	4140	4296	7951	69
H(26B)	3821	4329	8948	69
H(26C)	4769	3647	8839	69

Table 1. Crystal data and structure refinement for CuI(2,3-dimethylpyrazine) (Compound **2**).

Identification code	d117	
Empirical formula	$C_6H_8CuIN_2$	
Formula weight	298.58	
Temperature	220(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.8505(5) Å	α= 90°.
	b = 12.8482(7) Å	β= 103.152(6)°.
	c = 13.5837(8) Å	γ = 90°.
Volume	1674.08(16) $Å^3$	
Z	8	
Density (calculated)	2.369 Mg/m^3	
Absorption coefficient	6.223 mm^{-1}	
F(000)	1120	
Crystal size	0.18 x 0.15 x 0.12 mm^3	
Theta range for data collection	2.32 to 28.04°.	
Index ranges	-12<=h<=12, -16<=k<=16, -17<=l<=11	
Reflections collected	10181	
Independent reflections	3972 [R(int) = 0.0530]	
Completeness to theta = 28.04°	98.2 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3972 / 0 / 186	
Goodness-of-fit on F^2	0.976	
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.0738	
R indices (all data)	R1 = 0.0645, wR2 = 0.0821	
Extinction coefficient	0.0020(2)	
Largest diff. peak and hole	0.766 and -0.965 $e.Å^{-3}$	

Comments:

All non-hydrogen atoms were refined anisotropic. The hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and refined using a riding model.

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)
Cu(1)	7842(1)	1936(1)	5840(1)	27(1)
Cu(2)	8877(1)	-164(1)	5522(1)	29(1)
I(1)	8879(1)	1380(1)	4206(1)	23(1)
I(2)	8974(1)	690(1)	7347(1)	27(1)
N(1)	8649(5)	3404(3)	6133(4)	23(1)
C(1)	8104(6)	4265(4)	5619(5)	26(1)
C(2)	8786(6)	5228(4)	5819(5)	26(1)
N(2)	10013(6)	5315(4)	6474(5)	34(1)
C(3)	10539(7)	4440(5)	6970(5)	34(1)
C(4)	9863(6)	3514(5)	6814(5)	26(1)
C(5)	6774(8)	4164(6)	4844(7)	48(2)
C(6)	8172(8)	6208(5)	5307(6)	43(2)
N(11)	5719(5)	1699(4)	5406(4)	21(1)
C(11)	4856(5)	1853(4)	6034(4)	19(1)
C(12)	3478(5)	1473(4)	5768(5)	21(1)
N(12)	2980(4)	995(4)	4876(4)	20(1)
C(13)	3825(6)	928(5)	4237(5)	24(1)
C(14)	5185(6)	1262(5)	4503(4)	24(1)
C(15)	5411(6)	2429(5)	7010(5)	33(1)
C(16)	2515(6)	1604(5)	6481(5)	28(1)

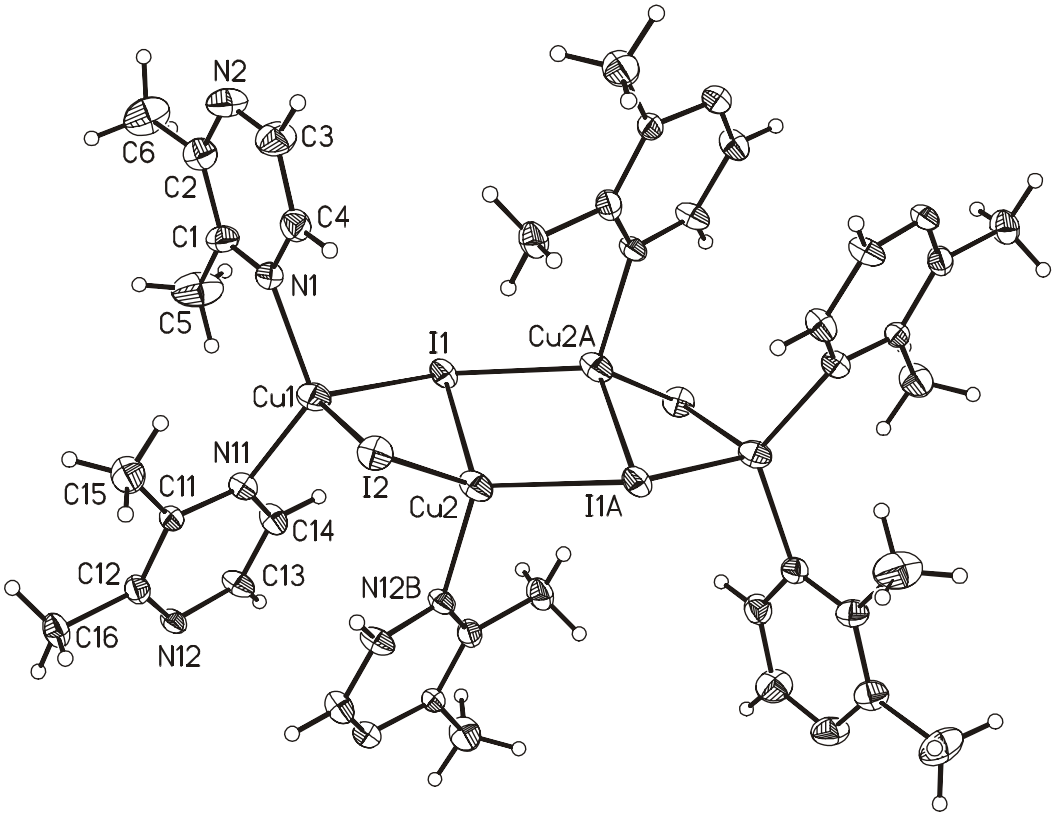

Table 3. Bond lengths [Å] and angles [°].

Cu(1)-N(1)	2.050(5)	Cu(2)-N(12B)	2.080(4
Cu(1)-N(11)	2.063(5)	Cu(2)-I(1A)	2.6632
Cu(1)-I(2)	2.6369(9)	Cu(2)-I(1)	2.6703
Cu(1)-I(1)	2.7403(9)	Cu(2)-I(2)	2.6921
Cu(1)-Cu(2)	2.9506(11)	Cu(2)-Cu(2A)	2.9175
N(1)-Cu(1)-N(11)	120.95(18)	N(12B)-Cu(2)-I(1A)	112.85(1
N(1)-Cu(1)-I(2)	109.34(15)	N(12B)-Cu(2)-I(1)	109.97(1
N(11)-Cu(1)-I(2)	110.76(14)	I(1A)-Cu(2)-I(1)	113.68(3
N(1)-Cu(1)-I(1)	101.40(14)	N(12B)-Cu(2)-I(2)	107.05(1
N(11)-Cu(1)-I(1)	105.70(14)	I(1A)-Cu(2)-I(2)	104.90(3
I(2)-Cu(1)-I(1)	107.49(3)	I(1)-Cu(2)-I(2)	107.94(3
N(1)-Cu(1)-Cu(2)	137.58(13)	N(12B)-Cu(2)-Cu(2A)	131.85(1
N(11)-Cu(1)-Cu(2)	100.65(13)	I(1A)-Cu(2)-Cu(2A)	56.95(3
I(2)-Cu(1)-Cu(2)	57.28(2)	I(1)-Cu(2)-Cu(2A)	56.72(3
I(1)-Cu(1)-Cu(2)	55.82(2)	I(2)-Cu(2)-Cu(2A)	121.10(4
Cu(1)-I(2)-Cu(2)	67.23(3)	N(12B)-Cu(2)-Cu(1)	101.21(1
Cu(2A)-I(1)-Cu(2)	66.32(3)	I(1A)-Cu(2)-Cu(1)	145.05(3
Cu(2A)-I(1)-Cu(1)	119.42(3)	I(1)-Cu(2)-Cu(1)	58.10(2
Cu(2)-I(1)-Cu(1)	66.08(2)	I(2)-Cu(2)-Cu(1)	55.49(2
		Cu(2A)-Cu(2)-Cu(1)	105.34(4
N(1)-C(4)	1.343(8)	N(11)-C(14)	1.343(8
N(1)-C(1)	1.353(8)	N(11)-C(11)	1.349(7
C(1)-C(2)	1.405(8)	C(11)-C(12)	1.410(7
C(1)-C(5)	1.488(9)	C(11)-C(15)	1.508(9
C(2)-N(2)	1.332(8)	C(12)-N(12)	1.348(8
C(2)-C(6)	1.498(9)	C(12)-C(16)	1.512(7
N(2)-C(3)	1.352(9)	N(12)-C(13)	1.335(7
C(3)-C(4)	1.357(8)	N(12)-Cu(2B)	2.080(4
C(4)-N(1)-C(1)	117.1(5)	C(13)-C(14)	1.374(7
N(1)-C(1)-C(2)	120.3(5)	C(14)-N(11)-C(11)	117.8(5)
N(1)-C(1)-C(5)	118.4(5)	N(11)-C(11)-C(12)	119.7(5)
C(2)-C(1)-C(5)	121.3(6)	N(11)-C(11)-C(15)	118.3(5)
N(2)-C(2)-C(1)	121.6(5)	C(12)-C(11)-C(15)	122.0(5)
N(2)-C(2)-C(6)	116.7(5)	N(12)-C(12)-C(11)	121.3(5)
C(1)-C(2)-C(6)	121.7(6)	N(12)-C(12)-C(16)	118.3(5)
C(2)-N(2)-C(3)	116.7(5)	C(11)-C(12)-C(16)	120.4(5)
N(2)-C(3)-C(4)	122.2(6)	C(13)-N(12)-C(12)	117.4(5)
N(1)-C(4)-C(3)	121.9(6)	N(12)-C(13)-C(14)	121.6(6)
		N(11)-C(14)-C(13)	121.8(5)

Symmetry transformations used to generate equivalent atoms: A: -x+2,-y,-z+1; B: -x+1,-y,-z+1

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu(1)	21(1)	30(1)	28(1)	-2(1)	2(1)	-6(1)
Cu(2)	20(1)	35(1)	31(1)	-1(1)	6(1)	-5(1)
I(1)	19(1)	29(1)	23(1)	3(1)	8(1)	0(1)
I(2)	27(1)	30(1)	21(1)	-1(1)	3(1)	-2(1)
N(1)	20(2)	21(2)	27(3)	-4(2)	7(2)	-2(2)
C(1)	25(3)	23(3)	29(3)	-3(3)	4(2)	-6(2)
C(2)	32(3)	28(3)	20(3)	4(2)	8(2)	-2(2)
N(2)	33(3)	28(3)	37(3)	-1(2)	2(2)	-10(2)
C(3)	32(3)	34(3)	32(4)	-6(3)	-2(3)	-5(3)
C(4)	20(2)	28(3)	28(3)	-2(2)	4(2)	1(2)
C(5)	40(4)	42(4)	48(5)	11(4)	-19(3)	-10(3)
C(6)	56(4)	29(3)	39(4)	15(3)	0(3)	2(3)
N(11)	19(2)	24(2)	20(3)	1(2)	5(2)	-2(2)
C(11)	19(2)	18(2)	23(3)	1(2)	9(2)	0(2)
C(12)	19(2)	23(3)	24(3)	3(2)	8(2)	3(2)
N(12)	14(2)	24(2)	21(2)	-2(2)	5(2)	-4(2)
C(13)	19(2)	35(3)	19(3)	-1(2)	4(2)	-8(2)
C(14)	18(2)	35(3)	18(3)	-4(2)	4(2)	-1(2)
C(15)	28(3)	40(3)	30(3)	-13(3)	5(3)	-4(3)
C(16)	27(3)	34(3)	27(3)	-1(3)	15(3)	2(2)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$).

	x	y	z	U(eq)
H(3)	11403	4475	7438	41
H(4)	10256	2932	7194	31
H(5A)	6946	4282	4178	72
H(5B)	6110	4674	4975	72
H(5C)	6398	3470	4874	72
H(6A)	8841	6770	5479	65
H(6B)	7332	6383	5530	65
H(6C)	7944	6105	4581	65
H(13)	3482	646	3590	29
H(14)	5757	1183	4041	28
H(15A)	4825	3028	7046	49
H(15B)	6356	2659	7036	49
H(15C)	5408	1970	7577	49
H(16A)	2832	1167	7071	42
H(16B)	1576	1402	6140	42
H(16C)	2517	2326	6690	42

Table 1. Crystal data and structure refinement for jg368a (Compound **3**)

Identification code	jg368a	
Empirical formula	$C_6H_8Cu_2I_2N_2$	
Formula weight	489.02	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 4.3210(9) Å	α= 90°.
	b = 17.974(3) Å	β= 92.63(3)°.
	c = 13.1672(16) Å	γ = 90°.
Volume	1021.5(3) $Å^3$	
Z	4	
Density (calculated)	3.180 Mg/m^3	
Absorption coefficient	10.154 mm^{-1}	
F(000)	888	
Crystal size	0.08 x 0.08 x 0.07 mm^3	
Theta range for data collection	2.75 to 27.01°.	
Index ranges	0<=h<=5, -22<=k<=2, -16<=l<=16	
Reflections collected	2859	
Independent reflections	2238 [R(int) = 0.0371]	
Completeness to theta = 27.01°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2238 / 0 / 111	
Goodness-of-fit on F^2	0.996	
Final R indices [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0723	
R indices (all data)	R1 = 0.0700, wR2 = 0.0800	
Largest diff. peak and hole	1.171 and -0.857 $e.Å^{-3}$	

Comments:

All non-hydrogen atoms were refined anisotropic. The hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and refined using a riding model.

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)
Cu(1)	1258(2)	4429(1)	7078(1)	37(1)
Cu(2)	4908(2)	3247(1)	7665(1)	35(1)
I(1)	145(1)	3637(1)	8754(1)	29(1)
I(2)	5927(1)	4028(1)	5992(1)	28(1)
N(1)	1095(14)	5566(3)	7235(4)	28(1)
C(1)	2606(15)	5944(4)	7983(5)	27(1)
C(2)	2280(16)	6731(4)	8048(5)	26(1)
N(2)	462(14)	7106(3)	7370(4)	27(1)
C(3)	-964(19)	6707(4)	6622(6)	36(2)
C(4)	-638(17)	5951(4)	6550(6)	34(2)
C(5)	4553(17)	5523(4)	8755(6)	36(2)
C(6)	3889(17)	7167(4)	8875(6)	33(2)

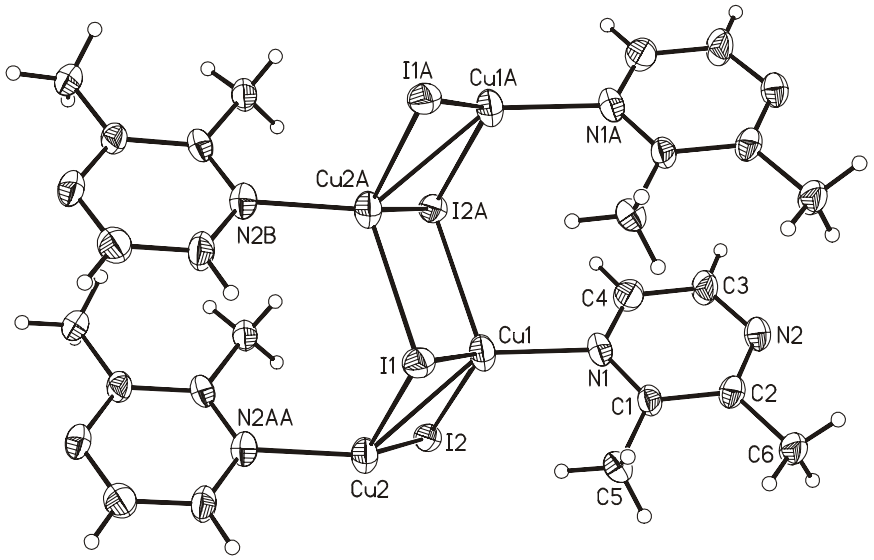

Table 3. Bond lengths [Å] and angles [°].

Cu(1)-N(1)	2.056(6)	Cu(2)-I(1)	2.6556(13)
Cu(1)-I(2)	2.6271(13)	Cu(2)-I(2)	2.6663(11)
Cu(1)-I(1)	2.6887(12)	Cu(2)-I(1)#3	2.7146(13)
Cu(1)-Cu(2)	2.7358(14)	I(1)-Cu(2)#1	2.7146(13)
Cu(1)-I(2)#1	2.7515(13)	I(2)-Cu(1)#3	2.7515(14)
Cu(2)-N(2)#2	2.058(6)		
N(1)-Cu(1)-I(2)	110.99(17)	N(2)#2-Cu(2)-I(1)	102.34(16)
N(1)-Cu(1)-I(1)	115.86(17)	N(2)#2-Cu(2)-I(2)	121.42(16)
I(2)-Cu(1)-I(1)	118.20(4)	I(1)-Cu(2)-I(2)	117.98(4)
N(1)-Cu(1)-Cu(2)	139.95(18)	N(2)#2-Cu(2)-I(1)#3	109.33(17)
I(2)-Cu(1)-Cu(2)	59.59(3)	I(1)-Cu(2)-I(1)#3	107.14(4)
I(1)-Cu(1)-Cu(2)	58.61(3)	I(2)-Cu(2)-I(1)#3	97.80(4)
N(1)-Cu(1)-I(2)#1	106.31(17)	N(2)#2-Cu(2)-Cu(1)	136.41(18)
I(2)-Cu(1)-I(2)#1	106.88(4)	I(1)-Cu(2)-Cu(1)	59.81(3)
I(1)-Cu(1)-I(2)#1	96.38(4)	I(2)-Cu(2)-Cu(1)	58.18(3)
Cu(2)-Cu(1)-I(2)#1	113.68(4)	I(1)#3-Cu(2)-Cu(1)	113.89(4)
Cu(2)-I(1)-Cu(1)	61.58(3)	Cu(1)-I(2)-Cu(2)	62.23(4)
Cu(2)-I(1)-Cu(2)#1	107.14(4)	Cu(1)-I(2)-Cu(1)#3	106.88(4)
Cu(1)-I(1)-Cu(2)#1	83.06(4)	Cu(2)-I(2)-Cu(1)#3	82.77(4)

Table 3. Bond lengths [Å] and angles [°].

N(1)-C(4)	1.337(9)	C(2)-C(6)	1.489(9)
N(1)-C(1)	1.342(9)	N(2)-C(3)	1.344(9)
C(1)-C(2)	1.424(9)	N(2)-Cu(2)#4	2.058(5)
C(1)-C(5)	1.495(10)	C(3)-C(4)	1.371(10)
C(2)-N(2)	1.342(9)		
C(4)-N(1)-C(1)	118.2(6)	N(2)-C(2)-C(1)	121.0(6)
C(4)-N(1)-Cu(1)	117.8(5)	N(2)-C(2)-C(6)	117.5(6)
C(1)-N(1)-Cu(1)	124.0(5)	C(1)-C(2)-C(6)	121.5(6)
N(1)-C(1)-C(2)	120.0(6)	C(2)-N(2)-C(3)	117.0(6)
N(1)-C(1)-C(5)	118.8(6)	C(2)-N(2)-Cu(2)#4	123.9(5)
C(2)-C(1)-C(5)	121.1(6)	N(2)-C(3)-C(4)	122.3(7)
C(3)-N(2)-Cu(2)#4	118.8(5)	N(1)-C(4)-C(3)	121.4(7)

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z #2 -x+1/2,y-1/2,-z+3/2 #3 x+1,y,z #4 -x+1/2,y+1/2,-z+3/2

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu(1)	41(1)	22(1)	48(1)	-2(1)	4(1)	3(1)
Cu(2)	39(1)	21(1)	45(1)	0(1)	3(1)	0(1)
I(1)	24(1)	30(1)	31(1)	1(1)	2(1)	-1(1)
I(2)	26(1)	27(1)	31(1)	2(1)	1(1)	-1(1)
N(1)	33(3)	20(3)	32(3)	-1(2)	6(3)	5(3)
C(1)	26(3)	20(3)	34(4)	-5(3)	6(3)	2(3)
C(2)	31(3)	19(3)	29(4)	2(3)	4(3)	-6(3)
N(2)	35(3)	21(3)	26(3)	2(2)	6(2)	0(2)
C(3)	46(4)	18(3)	41(4)	5(3)	-11(4)	1(3)
C(4)	34(4)	31(4)	36(4)	-2(3)	1(3)	-3(3)
C(5)	31(4)	24(3)	51(5)	1(3)	-7(4)	5(3)
C(6)	36(4)	20(3)	41(4)	2(3)	-9(3)	-2(3)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$).

	x	y	z	U(eq)
H(3)	-2215	6954	6137	43
H(4)	-1645	5699	6013	40
H(5B)	3491	5493	9379	54
H(5C)	6494	5775	8876	54
H(5A)	4923	5030	8507	54
H(6C)	5530	7453	8600	49
H(6C)	4739	6833	9385	49
H(6A)	2438	7496	9175	49