Supplementary information for Chemical Communication
Paper

Halogen-bonded assembly of hybrid inorganic/organic 3D-networks from tetrabromomethane and dibromocuprate salts

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Table S1. Geometry of halogen bonding in compounds **I** and **II**[a]

Distanses, Å		Angles, deg			
		Network **I**			
Br(5)-Br(2A)#2	3.583(7)	C(1A)-Br(4A)-Br(5)#4	165.5(7)	Cu(1)-Br(5)-Br(2A)#2	63.72(12)
Br(5)-Br(2B)#2	3.782(19)	C(1B)-Br(4B)-Br(5)#4	159.2(13)	Cu(1)-Br(5)-Br(2B)#2	59.8(4)
Br(5)-Br(4A)#5	3.342(6)	C(1A)-Br(2A)-Br(5)#1	131.8(5)	Cu(1)-Br(5)-Br(4A)#5	127.21(10)
Br(5)-Br(4B)#5	3.441(14)	C(1B)-Br(2B)-Br(5)#1	135.6(12)	Cu(1)-Br(5)-Br(4B)#5	127.29(19)
Br(6)-Br(1A)	3.296(12)	C(1A)-Br(1A)-Br(6)	177.2(9)	Cu(2)-Br(6)-Br(3B)#5	111.0(3)
Br(6)-Br(1B)	3.40(3)	C(1B)-Br(1B)-Br(6)	171.8(14)	Cu(2)-Br(6)-Br(3B)#5	111.0(3)
Br(6)-Br(3A)#5	3.326(9)	C(1A)-Br(3A)-Br(6)#4	171.8(6)	Cu(2)-Br(6)-Br(1A)	77.1(2)
Br(6)-Br(3B)#5	3.384(15)	C(1B)-Br(3B)-Br(6)#4	170.1(13)	Cu(2)-Br(6)-Br(1B)	75.2(4)
		Network **II**[c]			
Br(5)-Br(1)#1	3.3807(10)	C(1)-Br(1)-Br(5)#1	170.88(14)	Cu(1)-Br(5)-Br(1)#1	138.45(3)
Br(5)-Br(2)#8	3.3662(10)	C(1)-Br(2)-Br(5)#4	170.79(13)	Cu(1)-Br(5)-Br(2)#8	94.41(3)
Br(5)-Br(3)#9	3.3786(10)	C(1)-Br(3)-Br(5)#5	174.84(13)	Cu(1)-Br(5)-Br(3)#9	142.05(3)
Br(5)-Br(4)#7	3.4458(10)	C(1)-Br(4)-Br(5)#7	177.68(13)	Cu(1)-Br(5)-Br(4)#7	99.06(3)

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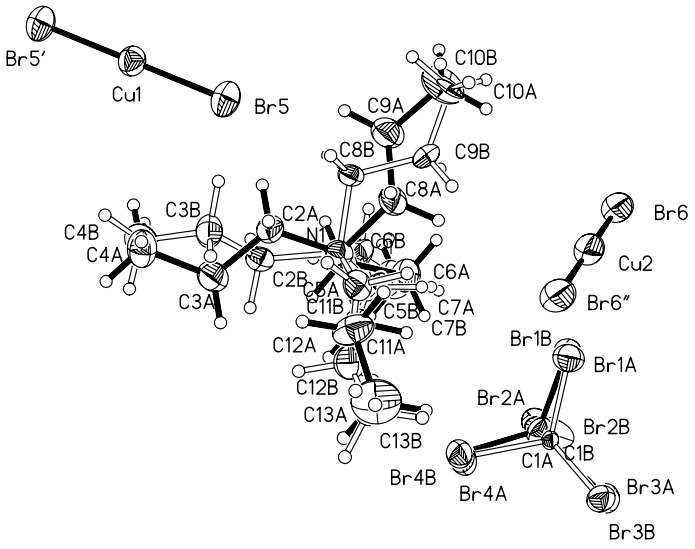

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Figure S1. ORTEP diagram of **I** with ellipsoids drawn with 50% probability (symmetry code: #1 -x,-y+2,-z+1 #2 -x+1,-y+1,-z).

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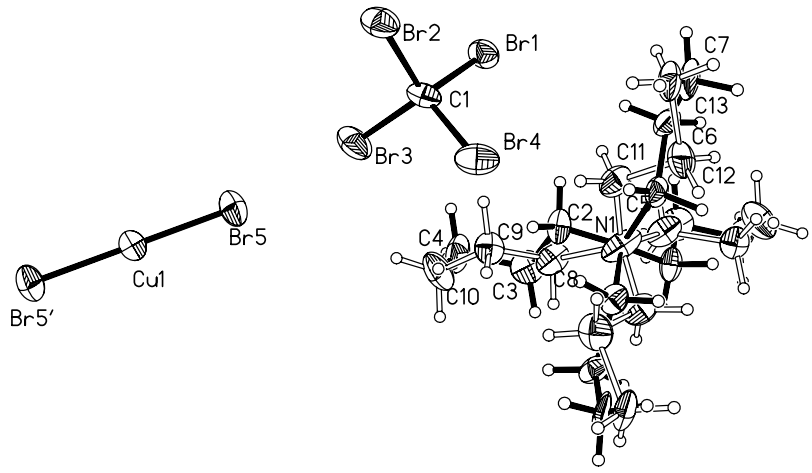

Supplementary information for Chemical Communication
Paper

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Table S1. Geometry of halogen bonding in compounds **I** and **II**[a]

Distanses, Å		Angles, deg			
		Network **I**			
Br(5)-Br(2A)#2	3.583(7)	C(1A)-Br(4A)-Br(5)#4	165.5(7)	Cu(1)-Br(5)-Br(2A)#2	63.72(12)
Br(5)-Br(2B)#2	3.782(19)	C(1B)-Br(4B)-Br(5)#4	159.2(13)	Cu(1)-Br(5)-Br(2B)#2	59.8(4)
Br(5)-Br(4A)#5	3.342(6)	C(1A)-Br(2A)-Br(5)#1	131.8(5)	Cu(1)-Br(5)-Br(4A)#5	127.21(10)
Br(5)-Br(4B)#5	3.441(14)	C(1B)-Br(2B)-Br(5)#1	135.6(12)	Cu(1)-Br(5)-Br(4B)#5	127.29(19)
Br(6)-Br(1A)	3.296(12)	C(1A)-Br(1A)-Br(6)	177.2(9)	Cu(2)-Br(6)-Br(3B)#5	111.0(3)
Br(6)-Br(1B)	3.40(3)	C(1B)-Br(1B)-Br(6)	171.8(14)	Cu(2)-Br(6)-Br(3B)#5	111.0(3)
Br(6)-Br(3A)#5	3.326(9)	C(1A)-Br(3A)-Br(6)#4	171.8(6)	Cu(2)-Br(6)-Br(1A)	77.1(2)
Br(6)-Br(3B)#5	3.384(15)	C(1B)-Br(3B)-Br(6)#4	170.1(13)	Cu(2)-Br(6)-Br(1B)	75.2(4)
		Network **II**[c]			
Br(5)-Br(1)#1	3.3807(10)	C(1)-Br(1)-Br(5)#1	170.88(14)	Cu(1)-Br(5)-Br(1)#1	138.45(3)
Br(5)-Br(2)#8	3.3662(10)	C(1)-Br(2)-Br(5)#4	170.79(13)	Cu(1)-Br(5)-Br(2)#8	94.41(3)
Br(5)-Br(3)#9	3.3786(10)	C(1)-Br(3)-Br(5)#5	174.84(13)	Cu(1)-Br(5)-Br(3)#9	142.05(3)
Br(5)-Br(4)#7	3.4458(10)	C(1)-Br(4)-Br(5)#7	177.68(13)	Cu(1)-Br(5)-Br(4)#7	99.06(3)

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Figure 2. ORTEP diagram of **II** with ellipsoids drawn with 50% probability (symmetry code: #1 -x+2,y,-z+1/2).

A)

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		Network **II**[c]			
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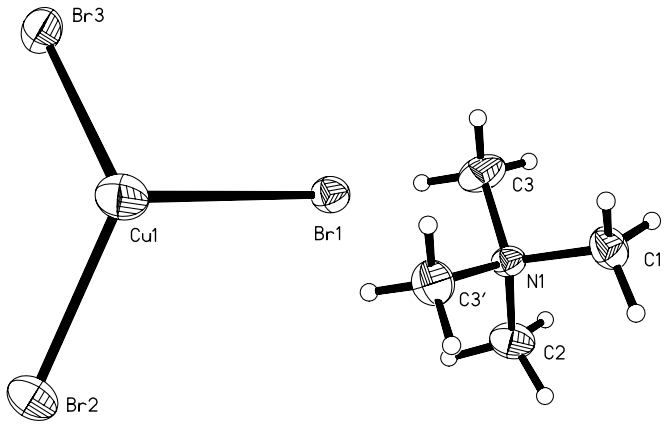

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Br(6)-Br(3A)#5	3.326(9)	C(1A)-Br(3A)-Br(6)#4	171.8(6)	Cu(2)-Br(6)-Br(1A)	77.1(2)
Br(6)-Br(3B)#5	3.384(15)	C(1B)-Br(3B)-Br(6)#4	170.1(13)	Cu(2)-Br(6)-Br(1B)	75.2(4)
		Network **II**[c]			
Br(5)-Br(1)#1	3.3807(10)	C(1)-Br(1)-Br(5)#1	170.88(14)	Cu(1)-Br(5)-Br(1)#1	138.45(3)
Br(5)-Br(2)#8	3.3662(10)	C(1)-Br(2)-Br(5)#4	170.79(13)	Cu(1)-Br(5)-Br(2)#8	94.41(3)
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B)

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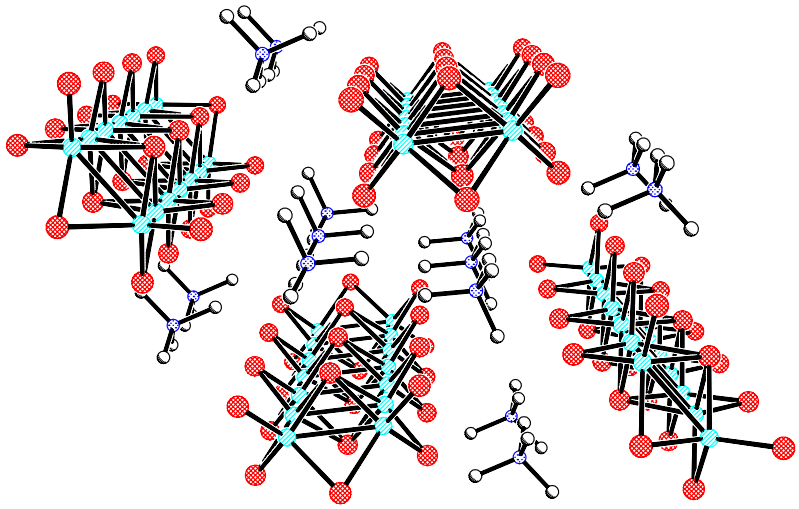

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Figure S3. (A) ORTEP diagram (ellipsoids drawn with 50% probability, symmetry code: #1 -x+1,-y+1,-z) and (B) fragment of crystal lattice of tetramethylammonium catena-(μ_4-bromo)-bis(μ_2-bromo) -di-copper(I)) resulted from crystallization from mixture of $Me_4N^+CuBr_2^-$ and CBr_4 in CH_2Cl_2 (compare: S. Andersson and S. Jagner, Acta Chem. Scand. A, 1986, 40, 177.)