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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) 131.8(5) 127.21(10) C(1A)-Br(2A)-Br(5)#1 Cu(1)-Br(5)-Br(4A)#5 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) 177.2(9) 3.296(12) C(1A)-Br(1A)-Br(6) Cu(2)-Br(6)-Br(3B)#5 111.0(3)Br(6)-Br(1B)111.0(3) 3.40(3) C(1B)-Br(1B)-Br(6) 171.8(14) Cu(2)-Br(6)-Br(3B)#5 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) C(1B)-Br(3B)-Br(6)#4 Br(6)-Br(3B)#5 3.384(15) 170.1(13) Cu(2)-Br(6)-Br(1B) 75.2(4) Network II^c 3.3807(10) C(1)-Br(1)-Br(5)#1 Br(5)-Br(1)#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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to c) Symmetry transformations used to generate equivalent atoms: #1 - x+3/2, -y+3/2, -z+1 = #4 x-1/2, y+1/2, z#5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z #10 -x+2,y,-z+1/2 Halogen-bonded assembly of hybrid inorganic/organic 3D-networks from tetrabromomethane and dibromocuprate salts Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; *E-mail: jkochi@uh.edu*

Table S1. Geometry of halogen bonding in compounds I and II^a

Table S1. Geometry of halogen bonding in compounds I and II^a

Distanses, Å

Angles, deg

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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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)	
		Netwo	rk 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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to generate equivalent atoms: #1 x+1,y-1,z #2 -x+1,-y+1,-z+1 #4 x+1,y,z #5 x-1,y,z #6 x-1,y+1,z c) Symmetry transformations used to generate equivalent atoms: #1 -x+3/2,-y+3/2,-z+1 #4 x-1/2,y+1/2,z #5 x y+1 z 7 -x+2 -y+1 -z+1 #8 x+1/2 y-1/2 z #9 x y-1 z = #10 -x+2 y -z+1/2						
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)	

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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) 131.8(5) Cu(1)-Br(5)-Br(4A)#5 127.21(10) C(1A)-Br(2A)-Br(5)#1 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) 177.2(9) 111.0(3) 3.296(12) C(1A)-Br(1A)-Br(6) Cu(2)-Br(6)-Br(3B)#5 Br(6)-Br(1B)3.40(3) 111.0(3) C(1B)-Br(1B)-Br(6) 171.8(14) Cu(2)-Br(6)-Br(3B)#5 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) C(1B)-Br(3B)-Br(6)#4 Br(6)-Br(3B)#5 3.384(15) 170.1(13) Cu(2)-Br(6)-Br(1B) 75.2(4) Network II^c 3.3807(10) C(1)-Br(1)-Br(5)#1 Br(5)-Br(1)#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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to c) Symmetry transformations used to generate equivalent atoms: #1 - x + 3/2 - y + 3/2 - z + 1 = #4 - x - 1/2 - y + 1/2 - z = 1#10 -x+2,y,-z+1/2 #5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z 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) 3.3662(10) C(1)-Br(2)-Br(5)#4 170.79(13) Cu(1)-Br(5)-Br(2)#8 94.41(3)

Table S1. Geometry of halogen bonding in compounds I and II^a

Br(5)-Br(2)#8 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)3.4458(10) C(1)-Br(4)-Br(5)#7 177.68(13) Cu(1)-Br(5)-Br(4)#7 99.06(3) Br(5)-Br(4)#7a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to generate equivalent atoms: #1 x+1,y-1,z #2 -x+1,-y+1,-z+1 #4 x+1,y,z #5 x-1,y,z #6 x-1,y+1,z c) Symmetry transformations used to generate equivalent atoms: #1 - x + 3/2, -y + 3/2, -z + 1 = #4 - x - 1/2, -y + 1/2, -z + 1#5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z #10 - x + 2, y, -z + 1/2

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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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 $99.06(3)$ a) See ORTEP diagrams in Figures S1 and S2 for atom labeling.b) Symmetry transformations used to generate equivalent atoms: $\#1 x+1,y-1,z \#2 -x+1,-y+1,-z+1 \#4 x+1,y,z \#5 x-1,y,z \#6 x-1,y+1,z$ $extrema x-1,y+1,z = x+3/2,-y+3/2,-z+1 \#4 x-1/2,y+1/2,z$ c) Symmetry transformations used to generate equivalent atoms: $\#1 - x+3/2,-y+3/2,-z+1 \#4 x-1/2,y+1/2,z$							

Table S1. Geometry of halogen bonding in compounds I and II^a

 $\#5 x, y+1, z \ 7 \ \textbf{-x+2, -y+1, -z+1} \quad \#8 \ x+1/2, y-1/2, z \quad \#9 \ x, y-1, z \quad \#10 \ \textbf{-x+2, y, -z+1/2}$



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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) 131.8(5) Cu(1)-Br(5)-Br(4A)#5 127.21(10) C(1A)-Br(2A)-Br(5)#1 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) 177.2(9) Cu(2)-Br(6)-Br(3B)#5 111.0(3) C(1A)-Br(1A)-Br(6) Br(6)-Br(1B)3.40(3) 111.0(3) C(1B)-Br(1B)-Br(6) 171.8(14) Cu(2)-Br(6)-Br(3B)#5 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) C(1B)-Br(3B)-Br(6)#4 Br(6)-Br(3B)#5 3.384(15) 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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to c) Symmetry transformations used to generate equivalent atoms: #1 - x+3/2, -y+3/2, -z+1 = #4 x-1/2, y+1/2, z#5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z #10 - x + 2, y, -z + 1/2Figure 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).

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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) 131.8(5) Cu(1)-Br(5)-Br(4A)#5 127.21(10) C(1A)-Br(2A)-Br(5)#1 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) 177.2(9) 111.0(3) C(1A)-Br(1A)-Br(6) Cu(2)-Br(6)-Br(3B)#5 Br(6)-Br(1B)3.40(3) 111.0(3) C(1B)-Br(1B)-Br(6) 171.8(14) Cu(2)-Br(6)-Br(3B)#5 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) C(1B)-Br(3B)-Br(6)#4 170.1(13) Br(6)-Br(3B)#5 3.384(15) 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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to c) Symmetry transformations used to generate equivalent atoms: #1 - x+3/2, -y+3/2, -z+1 = #4 x-1/2, y+1/2, z

Table S1. Geometry of halogen bonding in compounds I and II^a

#5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z #10 -x+2,y,-z+1/2



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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to generate equivalent atoms: #1 x+1,y-1,z #2 -x+1,-y+1,-z+1 #4 x+1,y,z #5 x-1,y,z #6 x-1,y+1,z c) Symmetry transformations used to generate equivalent atoms: #1 -x+3/2,-y+3/2,-z+1 #4 x-1/2,y+1/2,z #5 x y+1 z 7 -x+2 -y+1 -z+1 #8 x+1/2 y-1/2 z #9 x y-1 z #10 -x+2 y -z+1/2							
Figure 2. ORTEP diagram of II with ellipsoids drawn with 50% probability							
(symmetry code: #1 -x+2,y,-z+1/2).							

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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to generate equivalent atoms: $\#1 x+1,y-1,z \ \#2 \ -x+1,-y+1,-z+1 \ \#4 \ x+1,y,z \ \#5 \ x-1,y,z \ \#6 \ x-1,y+1,z$ c) Symmetry transformations used to generate equivalent atoms: $\#1 \ -x+3/2,-y+3/2,-z+1 \ \#4 \ x-1/2,y+1/2,z$							

Table S1. Geometry of halogen bonding in compounds I and II^a

c) Symmetry transformations used to generate equivalent atoms: #1 -x+3/2,-y+3/2,-z #5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z #10 -x+2,y,-z+1/2



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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) 177.2(9) Cu(2)-Br(6)-Br(3B)#5 111.0(3) C(1A)-Br(1A)-Br(6) Br(6)-Br(1B)3.40(3) 111.0(3) C(1B)-Br(1B)-Br(6) 171.8(14) Cu(2)-Br(6)-Br(3B)#5 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 C(1B)-Br(3B)-Br(6)#4 170.1(13) 3.384(15) 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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to c) Symmetry transformations used to generate equivalent atoms: #1 - x+3/2, -y+3/2, -z+1 = #4 x-1/2, y+1/2, z#5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z #10 - x + 2, y, -z + 1/2

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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to generate equivalent atoms: $\#1 x+1,y-1,z \#2 -x+1,-y+1,-z+1 \#4 x+1,y,z \#5 x-1,y,z \#6 x-1,y+1,z$ c) Symmetry transformations used to generate equivalent atoms: $\#1 -x+3/2 -y+3/2 -z+1 = \#4 x-1/2 y+1/2 z$							

Table S1. Geometry of halogen bonding in compounds I and II^a

#5 x,y+1,z 7 -x+2,-y+1,-z+1 #8 x+1/2,y-1/2,z #9 x,y-1,z #10 -x+2,y,-z+1/2



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

Sergiy V. Rosokha, Jianjiang Lu, Tetyana Y. Rosokha and Jay K. Kochi, Department of Chemistry, University of Houston, Houston TX 77204 USA Fax: 713-743-2709; Tel: 713-743-3293; E-mail: jkochi@uh.edu

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) 131.8(5) Cu(1)-Br(5)-Br(4A)#5 127.21(10) C(1A)-Br(2A)-Br(5)#1 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) 177.2(9) 111.0(3) 3.296(12) C(1A)-Br(1A)-Br(6) Cu(2)-Br(6)-Br(3B)#5 Br(6)-Br(1B)3.40(3) 111.0(3) C(1B)-Br(1B)-Br(6) 171.8(14) Cu(2)-Br(6)-Br(3B)#5 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) C(1B)-Br(3B)-Br(6)#4 Br(6)-Br(3B)#5 3.384(15) 170.1(13) Cu(2)-Br(6)-Br(1B) 75.2(4) Network II^c 3.3807(10) C(1)-Br(1)-Br(5)#1 Br(5)-Br(1)#1 170.88(14) Cu(1)-Br(5)-Br(1)#1 138.45(3) 94.41(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 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)

Table S1. Geometry of halogen bonding in compounds I and II^a

a) See ORTEP diagrams in Figures S1 and S2 for atom labeling. b) Symmetry transformations used to generate equivalent atoms: $\#1 x+1,y-1,z \ \#2 \ -x+1,-y+1,-z+1 \ \#4 \ x+1,y,z \ \#5 \ x-1,y,z \ \#6 \ x-1,y+1,z \ c)$ Symmetry transformations used to generate equivalent atoms: $\#1 \ -x+3/2,-y+3/2,-z+1 \ \#4 \ x-1/2,y+1/2,z \ \#5 \ x,y+1,z \ 7 \ -x+2,-y+1,-z+1 \ \#8 \ x+1/2,y-1/2,z \ \#9 \ x,y-1,z \ \#10 \ -x+2,y,-z+1/2$

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 Me₄N⁺CuBr₂⁻ and CBr₄ in CH₂Cl₂ (compare: S. Andersson and S. Jagner, Acta Chem. Scand. A, 1986, 40, 177.)