

Stacks of DMANH⁺ – scaffolding for ribbon shaped Cl⁻ bridged oxonium ions

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Table 1S. Geometry of hydrogen bonds formed in the structures studied.

1	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
	O1-H1OA...Cl2#1	0.826(14)	2.129(14)	2.9533(5)	176.6(13)
	O1-H1OB...Cl1	0.811(15)	2.160(15)	2.9697(5)	176.2(13)
	O2-H2OA...Cl1	0.792(16)	2.224(16)	3.0129(6)	173.6(15)
	O2-H2OB...Cl1#1	0.818(14)	2.171(14)	2.9855(6)	173.8(14)
	O2-H3O...O2	1.202(18)	1.230(18)	2.4297(9)	175.5(18)
	N2-H2N...N1	1.117(13)	1.542(13)	2.6027(6)	155.9(11)
	Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, y-1/2, -z+3/2				
	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
	O1-H1OA...Cl1	0.790(14)	2.179(14)	2.9682(5)	179.3(13)
2	O1-H1OB...Cl2	0.827(13)	2.145(13)	2.9717(5)	177.4(13)
	O2-H2OA...Cl2	0.811(13)	2.166(13)	2.9768(5)	178.0(12)
	O2-H2OB...Cl1#1	0.783(15)	2.185(15)	2.9654(5)	174.2(14)
	O1-H3O1...O1#2	1.21	1.21	2.4267(9)	180.00(4)
	O2-H3O2...O2#3	1.22	1.22	2.4324(10)	180.00(4)
	N2-H2N...N1	1.163(12)	1.475(12)	2.5910(5)	158.2(11)
	Symmetry transformations used to generate equivalent atoms: #1 x+1, y, z; #2 -x+1, -y, -z; #3 -x+2, -y, -z				
	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
	O2-H2OA...O1	0.849(13)	1.860(14)	2.7003(13)	170.0(12)
	O3-H3OA...O2	0.952(19)	1.620(19)	2.5608(11)	168.8(16)
3	O4A-H7O...O3	1.22(2)	1.27(2)	2.3764(16)	144.6(16)
	O4A-H8O...O5A	1.20(3)	1.35(3)	2.528(3)	166(2)
	O5B-H8O...O4B	1.29(3)	1.31(3)	2.496(4)	148(2)
	O5A-H5OA...O6	0.843(18)	1.853(18)	2.669(3)	162.6(18)
	O5B-H5OA...O6	0.936(18)	1.853(18)	2.733(4)	155.6(17)
	O1-H1OA...Cl1#1	0.838(16)	2.313(17)	3.1491(10)	175.2(14)
	O1-H1OB...Cl2#1	0.838(17)	2.385(18)	3.2205(10)	175.1(14)
	O4A-H4O...Cl2#1	1.09(2)	1.98(2)	2.9913(13)	152.0(16)
	O5B-H5OB...Cl3#1	0.82(3)	2.20(3)	3.003(4)	166(3)
	O2-H2OB...Cl1	0.839(17)	2.228(17)	3.0635(9)	73.6(14)
4	O6-H6OA...Cl2	0.893(16)	2.340(16)	3.2086(9)	164.2(13)
	O6-H6OB...Cl3	0.853(19)	2.32(2)	3.1681(9)	172.4(17)
	N2A-H2NA...N1A	1.113(15)	1.521(15)	2.5872(10)	158.1(13)
	N2B-H2NB...N1B	1.033(14)	1.617(14)	2.5905(11)	155.2(12)
	Symmetry transformations used to generate equivalent atoms: #1 x, -y+1/2, z-1/2				
	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
	O2...O1				2.6776(0.0065)
	O3...O2				2.5915(0.0056)
	O4A...O3				2.3291(0.0102)
	O4A...O5A				2.5556(0.0132)
	O5B...O4B				2.4675(0.0196)
	O5A...O6				2.6289(0.0141)
	O5B...O6				2.7648(0.0174)
	O1...Cl1#1				3.1722(0.0044)
	O1...Cl2#1				3.1883(0.0043)
	O4A...Cl2#1				2.9581(0.0073)
	O5B...Cl3#1				2.9092(0.0166)
	O2...Cl1				3.0274(0.0042)
	O6...Cl2				3.1596(0.0040)
	O6...Cl3				3.1651(0.0041)
	N2A-H2NA...N1A	0.81	1.84	2.586(5)	154.2
	N2B-H2NB...N1B	1.07	1.61	2.590(4)	150.3
	Symmetry transformations used to generate equivalent atoms: #1 x-1/2, -y+1/2, z				