

Supplementary Material (ESI) for *CrystEngComm*

Electronic Supplementary Information to the paper:

Solvent-bridged frameworks of hydrogen bonds in crystals of

9-aminoacridinium halides

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Supplementary Material (ESI) for *CrystEngComm*

Table S1. π - π interactions (distances in Å and angles in degrees) in **1**.

CgI ^a	CgJ ^a	Cg \cdots Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ^v	4.052(1)	0.0(1)	3.428(1)	2.160(1)
1	2 ^{vi}	3.709(1)	0.9(1)	3.431(1)	1.409(1)
1	3 ^v	3.816(1)	1.1(1)	3.451(1)	1.629(1)
2	2 ^{vi}	3.577(1)	0.0(1)	3.410(1)	1.080(1)
3	2 ^v	4.007(1)	1.1(1)	3.470(1)	2.109(1)

Symmetry code: (v) 1-x, 1-y, 1-z; (vi) 1-x, -y, 1-z.

^aCg represents the centre of gravity of the rings as follows (Figure S1): Cg1 ring C9/C11/C12/N10/C14/C13, Cg2 ring C1-C4/C12/C11, Cg3 ring C5-C8/C13/C14.

^bCg \cdots Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

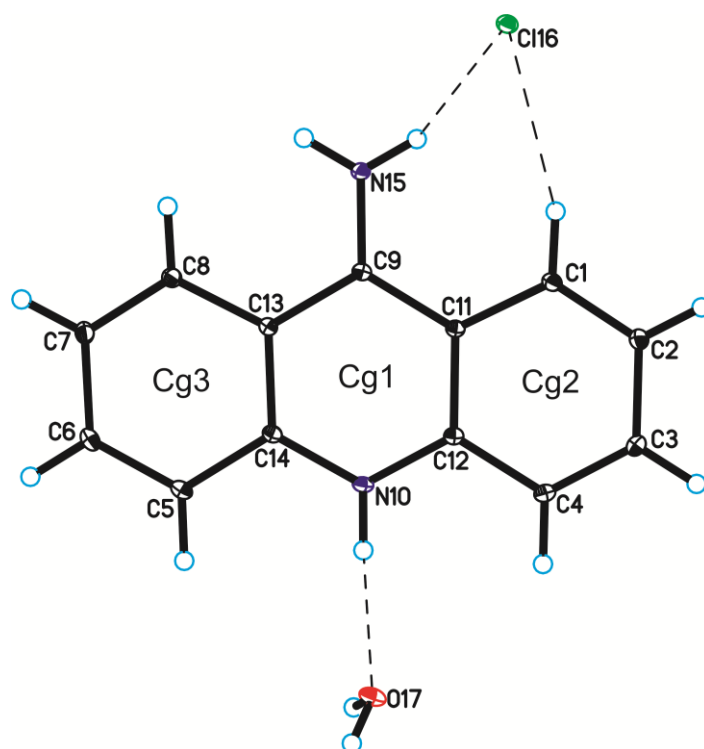


Figure S1. Molecular structure of compound **1** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.

Supplementary Material (ESI) for *CrystEngComm*

Table S2. π - π interactions (distances in Å and angles in degrees) in **2**.

CgI ^a	CgJ ^a	Cg \cdots Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ^v	4.150(2)	0.0(2)	3.460(2)	2.291(2)
1	2 ^{vi}	3.871(2)	0.8(2)	3.445(2)	1.765(2)
1	3 ^v	3.838(2)	0.6(2)	3.468(2)	1.644(2)
2	2 ^{vi}	3.560(2)	0.0(2)	3.450(2)	0.878(2)
3	2 ^v	4.095(2)	0.9(2)	3.475(2)	2.166(2)

Symmetry code: (v) 1-x, 1-y, 1-z; (vi) 1-x, 2-y, 1-z.

^aCg represents the centre of gravity of the rings (Figure S2).

^bCg \cdots Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

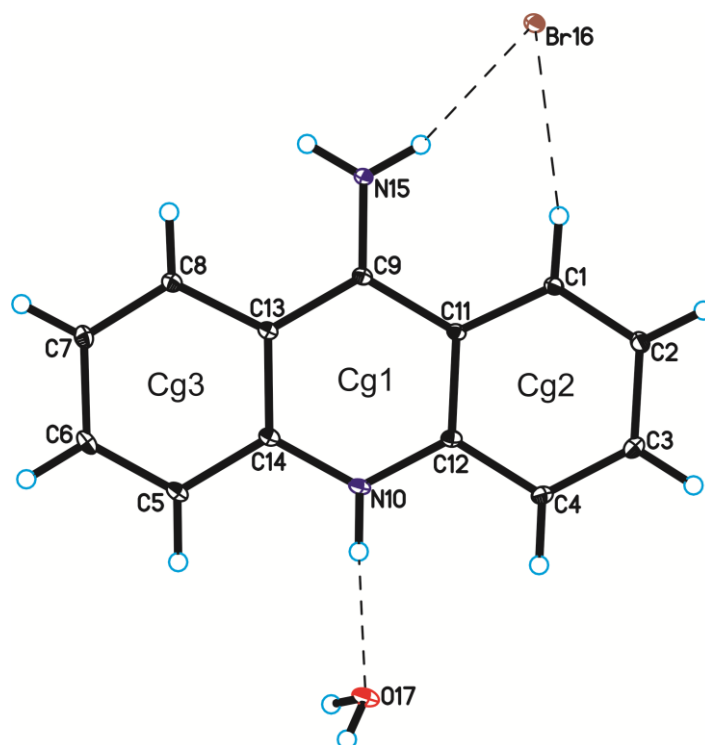


Figure S2. Molecular structure of compound **2** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.

Supplementary Material (ESI) for *CrystEngComm*

Table S3. π - π interactions (distances in Å and angles in degrees) in **3**.

CgI ^a	CgJ ^a	Cg \cdots Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ^{iv}	3.655(3)	0.0(2)	3.391(2)	1.364(2)
1	3 ^{iv}	3.579(3)	2.3(2)	3.392(2)	1.327(2)
2	1 ^{iv}	3.733(3)	3.0(2)	3.429(2)	1.142(2)
3	3 ^{iv}	4.093(3)	0.0(2)	3.345(2)	2.358(2)

Symmetry code: (iv) $x, 1/2-y, 1/2+z$.

^aCg represents the centre of gravity of the rings (Figure S3).

^bCg \cdots Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

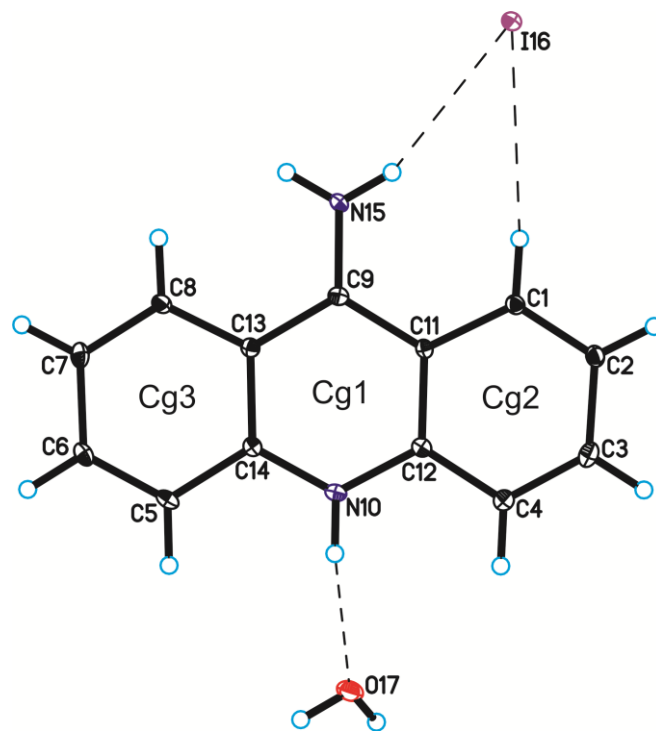


Figure S3. Molecular structure of compound **3** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.

Supplementary Material (ESI) for *CrystEngComm*

Table S4. π - π interactions (distances in Å and angles in degrees) in **4**.

CgI ^a	CgJ ^a	Cg...Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ⁱⁱⁱ	4.183(1)	0.0(1)	3.465(1)	2.343(1)
1	1 ^{iv}	3.670(1)	0.0(1)	3.403(1)	1.374(1)
1	3 ⁱⁱⁱ	3.636(1)	0.5(1)	3.448(1)	1.154(1)
1	3 ^{iv}	3.635(1)	0.5(1)	3.407(1)	1.267(1)
2	3 ⁱⁱⁱ	4.107(1)	2.7(1)	3.404(1)	2.298(1)
2	3 ^{iv}	3.730(1)	2.7(1)	3.451(1)	1.415(1)

Symmetry code: (iii) $-x, 2-y, 1-z$; (iv) $1-x, 2-y, 1-z$.

^aCg represents the centre of gravity of the rings (Figure S4).

^bCg...Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

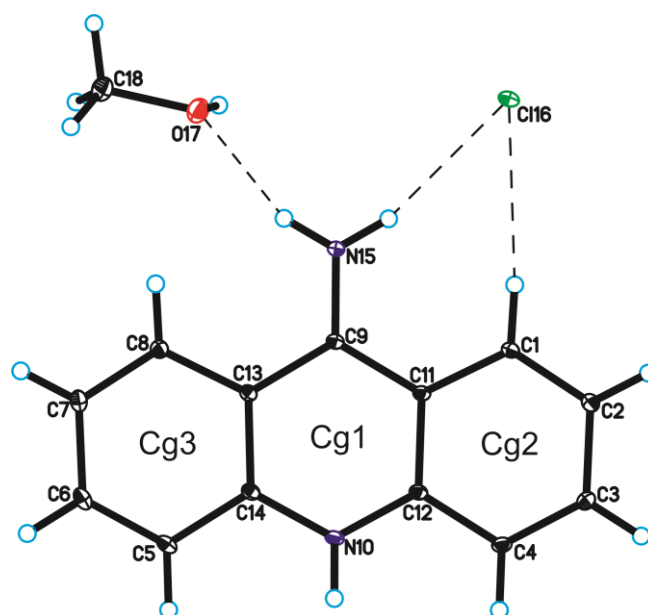


Figure S4. Molecular structure of compound **4** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.

Supplementary Material (ESI) for *CrystEngComm*

Table S5. π - π interactions (distances in Å and angles in degrees) in **5**.

CgI ^a	CgJ ^a	Cg...Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ⁱⁱⁱ	3.686(3)	0.0(2)	3.460(2)	1.271(2)
1	1 ^{iv}	4.165(3)	0.0(2)	3.460(2)	2.319(2)
1	3 ⁱⁱⁱ	3.662(3)	0.7(2)	3.445(2)	1.242(2)
1	3 ^{iv}	3.671(3)	0.7(2)	3.445(2)	1.268(2)
2	3 ⁱⁱⁱ	3.756(3)	2.6(2)	3.468(2)	1.442(2)
2	3 ^{iv}	4.083(3)	2.6(2)	3.468(2)	2.155(2)

Symmetry code: (iii) 1-x, 1-y, 1-z ; (iv) 2-x, 1-y, 1-z.

^aCg represents the centre of gravity of the rings (Figure S5).

^bCg...Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

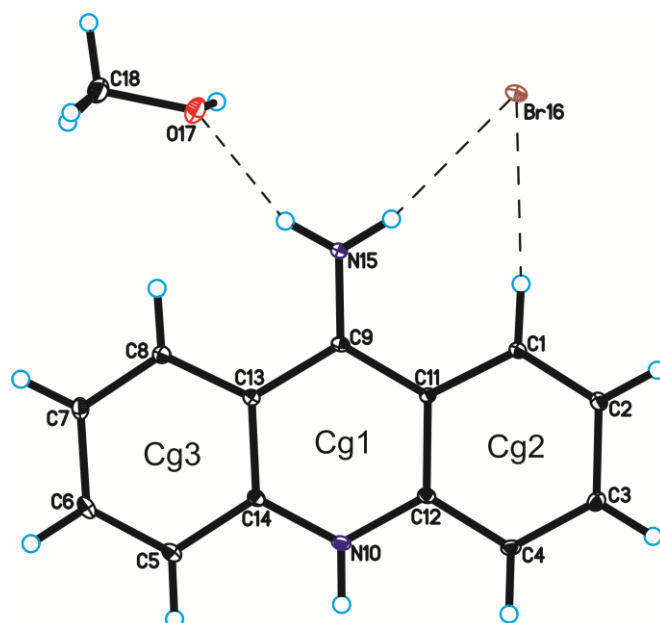


Figure S5. Molecular structure of compound **5** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.

Supplementary Material (ESI) for *CrystEngComm*

Table S6. π - π interactions (distances in Å and angles in degrees) in **6**.

CgI ^a	CgJ ^a	Cg \cdots Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ⁱⁱ	3.713(4)	0.0(3)	3.465(2)	1.334(2)
1	3 ⁱⁱ	3.890(4)	1.9(3)	3.452(2)	1.793(2)
2	1 ⁱⁱ	3.656(4)	0.3(3)	3.448(2)	1.216(2)
2	2 ⁱⁱ	3.939(4)	0.0(3)	3.464(2)	1.875(2)

Symmetry code: (ii) $x, 1/2-y, -1/2+z$.

^aCg represents the centre of gravity of the rings (Figure S6).

^bCg \cdots Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

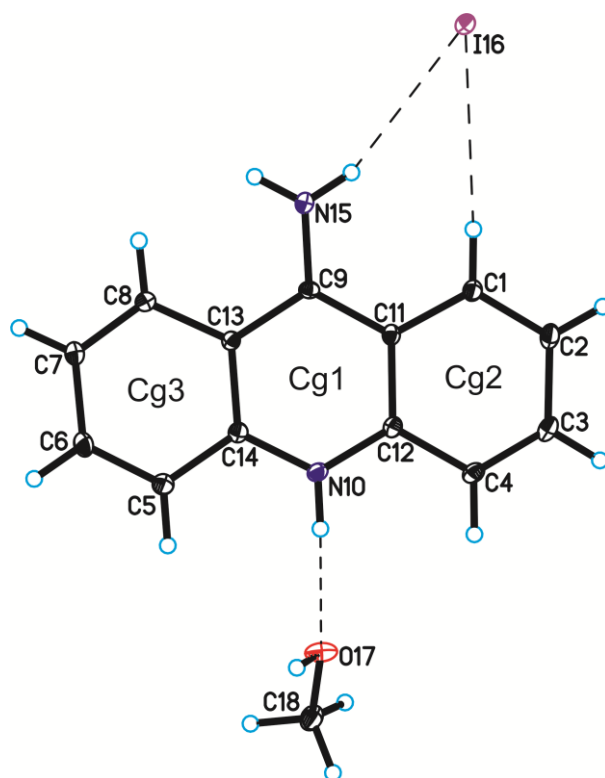


Figure S6. Molecular structure of compound **6** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.

Supplementary Material (ESI) for *CrystEngComm*

Table S 7. π - π interactions (distances in Å and angles in degrees) in **7**.

CgI ^a	CgJ ^a	Cg \cdots Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ⁱⁱⁱ	3.794(1)	0.0(1)	3.409(1)	1.596(2)
1	2 ⁱⁱⁱ	3.572(1)	0.9(1)	3.415(1)	1.047(2)
2	2 ⁱⁱⁱ	3.814(1)	0.0(1)	3.433(1)	1.662(2)

Symmetry code: (iii) $x, 1-y, 1/2+z$.

^aCg represents the centre of gravity of the rings (Figure S7).

^bCg \cdots Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

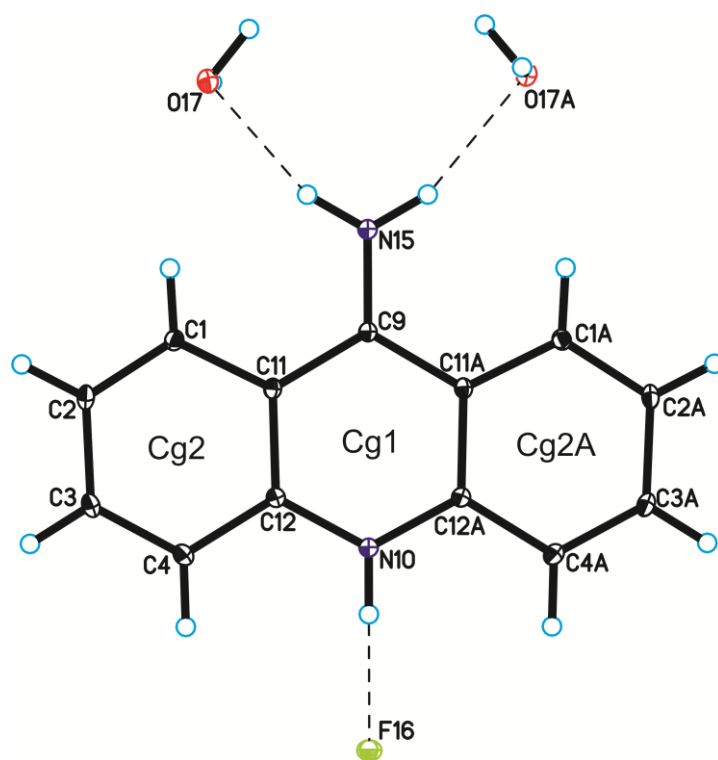


Figure S7. Molecular structure of compound **7** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.

Supplementary Material (ESI) for *CrystEngComm*

Table S8. π - π interactions (distances in Å and angles in degrees) in **8**.

CgI ^a	CgJ ^a	Cg \cdots Cg ^b	Dihedral angle ^c	Interplanar distance ^d	Offset ^e
1	1 ^v	3.523(3)	0.0(2)	3.421(2)	0.842(2)
1	3 ^v	3.820(3)	3.3(2)	3.422(2)	1.698(2)
2	1 ^v	3.888(3)	3.7(2)	3.500(2)	1.693(2)
2	2 ^v	4.181(3)	0.0(2)	3.502(2)	2.284(2)
3	3 ^v	3.979(3)	0.0(2)	3.373(2)	2.111(2)

Symmetry code: (v) $1/2-x, 1/2+y, z$.

^aCg represents the centre of gravity of the rings as follows (Figure S8).

^bCg \cdots Cg is the distance between ring centroids.

^cThe dihedral angle is that between the mean planes of CgI and CgJ.

^dThe interplanar distance is the perpendicular distance from CgI to ring J.

^eThe offset is the perpendicular distance from ring I to ring J.

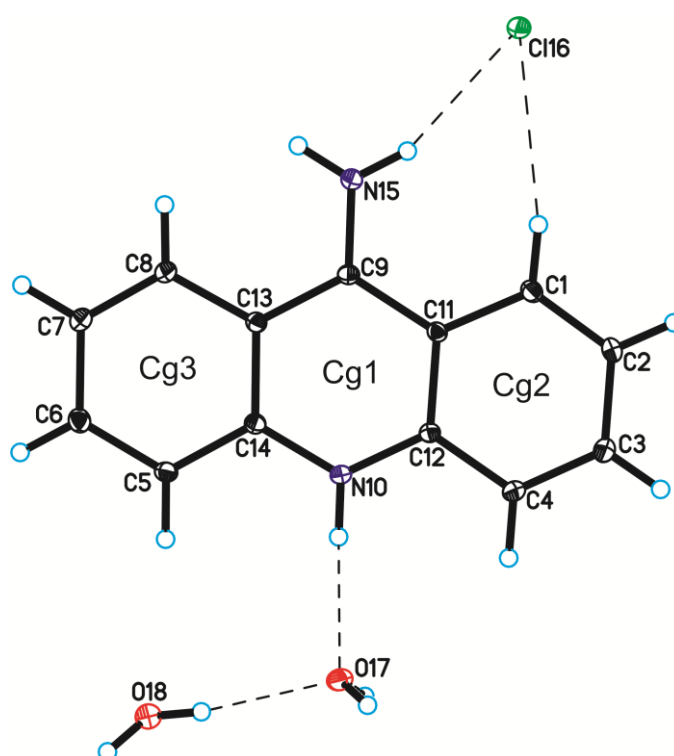


Figure S8. Molecular structure of compound **8** in the crystal showing the atom labelling scheme and 25% probability displacement ellipsoids (H atoms are spheres of arbitrary size). Cg1, Cg2 and Cg3 denote the ring centroids.