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Supporting information for article:

Salt formation, hydrogen-bonding patterns and supramolecular architectures of acridine with different acid molecules

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Computing details

Program(s) used to refine structure: *SHELXL97* (Sheldrick,1997); molecular graphics: *ORTEP* for Windows (Farrugia,2012); software used to prepare material for publication: *WinGX* publication routines (Farrugia,2012).

(S1) *Acridine – 4-amino salicylic acid*

Crystal data	$F(000) = 696$
$C_{20}H_{16}N_2O_3$	$D_x = 1.263 \text{ Mg m}^{-3}$
$M_r = 332.35$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, $P2_12_12_1$	Cell parameters from 6906 reflections
$a = 7.1209 (5) \text{ \AA}$	$\theta = 2.6\text{--}28.3^\circ$
$b = 12.1988(12) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 20.1202 (18) \text{ \AA}$	$T = 293 \text{ K}$
$V = 1747.8 (3) \text{ \AA}^3$	Block
$Z = 4$	$0.88 \times 0.50 \times 0.23 \text{ mm}$
<i>Data collected</i>	
Bruker D8 Quest eco diffractometer	$R_{\text{int}} = 0.023$
20496 measured reflections	$\theta_{\max} = 25.9^\circ, \theta_{\min} = 2.7^\circ$
4274 independent reflections	$h = -9 \rightarrow 6$
3934 reflections with $I > 2s(I)$	$k = -16 \rightarrow 16$
<i>Refinement</i>	
Refinement on F^2	$l = -26 \rightarrow 26$
Least-squares matrix: full	1 restraints
$R[F^2 > 2\sigma(F^2)] = 0.037$	Primary atom site location: structure-invariant direct methods
$wR(F^2) = 0.112$	Secondary atom site location: difference Fourier map
$S = 1.07$	Hydrogen site location: mixed
4274 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0765P)^2 + 0.0658P]$ where $P = (F_o^2 + 2F_c^2)/3$
290 parameters	
H atoms treated by a mixture of independent and constrained refinement	$\Delta\rho_{\max} = 0.19 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.16 \text{ e \AA}^{-3}$

Special details

Geometry: Allesds(expect the esd in the dihedral angle between two l.s planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

(S2)Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

Atom	x	y	z	U_{iso}^*/U_{eq}
O3	0.62266 (13)	0.74164 (9)	0.29886 (6)	0.0559 (3)
O2	0.51812 (15)	0.57511 (9)	0.36654 (5)	0.0552 (3)
O1	0.22130 (16)	0.51923 (8)	0.36038 (6)	0.0590 (3)
N2	0.1561 (2)	0.96426 (10)	0.19765 (8)	0.0610 (3)
N1	0.26192 (16)	0.37488 (9)	0.45353 (5)	0.0442 (2)
C15	0.29836 (16)	0.69110 (9)	0.31332 (6)	0.0367 (2)
C14	0.34981 (18)	0.58939 (10)	0.34906 (6)	0.0421 (3)
C18	0.20294 (17)	0.87705 (9)	0.23705 (6)	0.0417 (2)
C16	0.43767 (16)	0.76183 (10)	0.28820 (6)	0.0395 (3)
C20	0.11121 (16)	0.71904 (10)	0.30111 (6)	0.0414 (3)
C19	0.06189 (17)	0.80983 (11)	0.26471 (7)	0.0437 (3)
C17	0.39049 (17)	0.85247 (10)	0.25015 (7)	0.0443 (3)
C7	0.2536 (2)	0.22836 (11)	0.55772 (6)	0.0501 (3)
C6	0.2548 (2)	0.18865 (10)	0.49289 (6)	0.0460 (3)
C1	0.25990 (17)	0.26626 (10)	0.43989 (6)	0.0425 (3)
C2	0.2618 (2)	0.22936 (13)	0.37333 (7)	0.0540 (3)
C8	0.25627 (19)	0.34026 (11)	0.57105 (6)	0.0465 (3)
C9	0.26015 (19)	0.41456 (11)	0.51636 (6)	0.0451 (3)
C5	0.2516 (3)	0.07505 (12)	0.47674 (9)	0.0615 (4)
C13	0.2540 (2)	0.38421 (15)	0.63666 (7)	0.0605 (4)
C3	0.2577 (3)	0.12005 (15)	0.36041 (8)	0.0660 (4)
C4	0.2527 (3)	0.04228 (15)	0.41247 (10)	0.0700 (4)
C10	0.2624 (3)	0.52876 (13)	0.52776 (8)	0.0624 (4)
C12	0.2562 (3)	0.49381 (18)	0.64618 (9)	0.0726 (5)
C11	0.2594 (3)	0.56670 (16)	0.59123 (10)	0.0753 (5)
H10	0.258 (3)	0.5774 (17)	0.4891 (10)	0.075 (6)*
H20	0.016 (3)	0.6723 (16)	0.3195 (9)	0.065 (5)*
H2B	0.245 (3)	0.9962 (16)	0.1749 (9)	0.063 (5)*
H1A	0.256 (3)	0.4329 (15)	0.4155 (9)	0.065 (5)*
H13	0.247 (3)	0.3311 (17)	0.6764 (11)	0.075 (6)*

H5	0.247 (3)	0.0230 (17)	0.5138 (9)	0.074 (6)*
H2	0.260 (3)	0.2835 (14)	0.3402 (9)	0.058 (5)*
H7	0.246 (3)	0.1771 (16)	0.5939 (10)	0.067 (5)*
H3	0.260 (3)	0.0930 (16)	0.3120 (10)	0.071 (6)*
H12	0.252 (4)	0.526 (2)	0.6973 (11)	0.094 (7)*
H2A	0.021 (3)	0.9765 (18)	0.1899 (10)	0.073 (6)*
H19	-0.073 (2)	0.8282 (13)	0.2554 (8)	0.049 (4)*
H17	0.493 (3)	0.8951 (15)	0.2308 (9)	0.059 (5)*
H16	0.615 (3)	0.685 (2)	0.3293 (11)	0.074 (6)*
H4	0.257 (4)	-0.0347 (19)	0.3991 (10)	0.087 (7)*
H11	0.272 (3)	0.648 (2)	0.5982 (12)	0.096 (7)*

(S3) *Atomic displacement parameters (\AA^2)*

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0332 (4)	0.0517 (5)	0.0828 (7)	-0.0016 (4)	-0.0030 (4)	0.0075 (5)
O2	0.0490 (5)	0.0532 (5)	0.0635 (6)	0.0071 (4)	-0.0071 (4)	0.0059 (4)
O1	0.0595 (6)	0.0517 (5)	0.0656 (6)	-0.0103 (5)	-0.0126 (5)	0.0221 (5)
N2	0.0501 (7)	0.0453 (6)	0.0874 (9)	0.0001 (5)	-0.0023 (6)	0.0227 (6)
N1	0.0458 (5)	0.0441 (5)	0.0425 (5)	-0.0008 (4)	-0.0020 (4)	0.0051 (4)
C15	0.0367 (5)	0.0345 (5)	0.0390 (5)	-0.0016 (4)	0.0014 (4)	-0.0034 (4)
C14	0.0461 (6)	0.0404 (6)	0.0397 (5)	0.0007 (5)	-0.0007 (4)	-0.0004 (4)
C18	0.0424 (6)	0.0312 (5)	0.0515 (6)	-0.0005 (4)	-0.0007 (5)	-0.0018 (4)
C16	0.0334 (5)	0.0369 (5)	0.0483 (6)	-0.0015 (4)	0.0000 (4)	-0.0052 (5)
C20	0.0347 (5)	0.0405 (6)	0.0489 (6)	-0.0026 (4)	0.0043 (5)	0.0008 (5)
C19	0.0332 (5)	0.0398 (6)	0.0580 (7)	0.0003 (4)	-0.0001 (5)	-0.0006 (5)
C17	0.0383 (6)	0.0358 (5)	0.0590 (7)	-0.0044 (4)	0.0030 (5)	0.0009 (5)
C7	0.0539 (7)	0.0509 (7)	0.0454 (6)	0.0012 (6)	-0.0018 (6)	0.0122 (5)
C6	0.0447 (6)	0.0431 (6)	0.0502 (6)	0.0005 (5)	-0.0015 (5)	0.0055 (5)
C1	0.0380 (5)	0.0459 (6)	0.0436 (6)	0.0002 (5)	-0.0013 (5)	0.0027 (5)
C2	0.0542 (8)	0.0633 (8)	0.0445 (6)	-0.0007 (7)	-0.0022 (6)	-0.0024 (6)
C8	0.0456 (6)	0.0537 (7)	0.0401 (5)	-0.0005 (5)	-0.0007 (5)	0.0024 (5)
C9	0.0449 (6)	0.0455 (6)	0.0448 (6)	-0.0005 (5)	0.0007 (5)	0.0024 (5)
C5	0.0677 (9)	0.0434 (7)	0.0733 (9)	0.0018 (7)	-0.0003 (8)	0.0034 (6)
C13	0.0621 (8)	0.0765 (10)	0.0430 (6)	-0.0068 (8)	0.0006 (6)	-0.0021 (6)
C3	0.0654 (9)	0.0726 (10)	0.0600 (8)	0.0002 (8)	-0.0016 (7)	-0.0194 (7)
C4	0.0734 (11)	0.0490 (8)	0.0875 (12)	0.0013 (8)	-0.0002 (9)	-0.0156 (7)

C10	0.0775 (11)	0.0462 (8)	0.0634 (9)	-0.0004 (7)	0.0029 (8)	-0.0020 (6)
C12	0.0763 (11)	0.0866 (12)	0.0549 (8)	-0.0103 (9)	0.0064 (8)	-0.0228 (8)
C11	0.0876 (13)	0.0608 (10)	0.0775 (11)	-0.0054 (9)	0.0055 (10)	-0.0201 (8)

(S4) Geometric parameters (\AA , °)

O3—C16	1.3571 (14)	C7—H7	0.96 (2)
O3—H16	0.93 (2)	C6—C5	1.424 (2)
O2—C14	1.2611 (17)	C6—C1	1.4265 (17)
O1—C14	1.2735 (16)	C1—C2	1.4130 (18)
N2—C18	1.3679 (17)	C2—C3	1.359 (2)
N2—H2B	0.87 (2)	C2—H2	0.939 (19)
N2—H2A	0.98 (2)	C8—C13	1.4250 (19)
N1—C1	1.3532 (17)	C8—C9	1.4258 (17)
N1—C9	1.3538 (16)	C9—C10	1.412 (2)
N1—H1A	1.043 (19)	C5—C4	1.354 (3)
C15—C20	1.3973 (16)	C5—H5	0.98 (2)
C15—C16	1.4086 (16)	C13—C12	1.351 (3)
C15—C14	1.4802 (16)	C13—H13	1.03 (2)
C18—C17	1.3939 (17)	C3—C4	1.414 (3)
C18—C19	1.4110 (18)	C3—H3	1.03 (2)
C16—C17	1.3862 (18)	C4—H4	0.98 (2)
C20—C19	1.3736 (19)	C10—C11	1.359 (2)
C20—H20	0.96 (2)	C10—H10	0.98 (2)
C19—H19	1.004 (17)	C12—C11	1.419 (3)
C17—H17	0.98 (2)	C12—H12	1.10 (2)
C7—C8	1.3912 (19)	C11—H11	1.01 (3)
C7—C6	1.3915 (19)		
C16—O3—H16	100.5 (14)	N1—C1—C2	120.26 (11)
C18—N2—H2B	118.4 (14)	N1—C1—C6	119.91 (11)
C18—N2—H2A	116.6 (12)	C2—C1—C6	119.83 (12)
H2B—N2—H2A	123.7 (18)	C3—C2—C1	119.59 (14)
C1—N1—C9	122.64 (10)	C3—C2—H2	123.6 (11)
C1—N1—H1A	121.1 (10)	C1—C2—H2	116.7 (11)

C9—N1—H1A	116.2 (10)	C7—C8—C13	123.20 (13)
C20—C15—C16	117.34 (11)	C7—C8—C9	118.38 (12)
C20—C15—C14	121.73 (10)	C13—C8—C9	118.42 (13)
C16—C15—C14	120.90 (11)	N1—C9—C10	120.29 (13)
O2—C14—O1	122.70 (12)	N1—C9—C8	119.57 (12)
O2—C14—C15	119.11 (11)	C10—C9—C8	120.14 (13)
O1—C14—C15	118.19 (11)	C4—C5—C6	120.37 (15)
N2—C18—C17	120.69 (12)	C4—C5—H5	122.4 (12)
N2—C18—C19	120.46 (12)	C6—C5—H5	117.2 (12)
C17—C18—C19	118.84 (12)	C12—C13—C8	120.24 (15)
O3—C16—C17	117.86 (11)	C12—C13—H13	120.9 (12)
O3—C16—C15	121.04 (11)	C8—C13—H13	118.9 (12)
C17—C16—C15	121.07 (11)	C2—C3—C4	121.15 (14)
C19—C20—C15	122.30 (11)	C2—C3—H3	119.7 (11)
C19—C20—H20	120.2 (12)	C4—C3—H3	119.1 (11)
C15—C20—H20	117.5 (12)	C5—C4—C3	120.65 (15)
C20—C19—C18	119.80 (11)	C5—C4—H4	123.2 (12)
C20—C19—H19	121.6 (10)	C3—C4—H4	116.1 (12)
C18—C19—H19	118.5 (9)	C11—C10—C9	119.25 (16)
C16—C17—C18	120.55 (11)	C11—C10—H10	122.7 (12)
C16—C17—H17	117.5 (11)	C9—C10—H10	118.0 (12)
C18—C17—H17	121.8 (11)	C13—C12—C11	120.67 (15)
C8—C7—C6	121.48 (11)	C13—C12—H12	118.9 (13)
C8—C7—H7	119.6 (12)	C11—C12—H12	120.5 (13)
C6—C7—H7	118.9 (12)	C10—C11—C12	121.28 (17)
C7—C6—C5	123.56 (13)	C10—C11—H11	117.7 (14)
C7—C6—C1	118.02 (12)	C12—C11—H11	120.7 (14)
C5—C6—C1	118.41 (13)		
C20—C15—C14—O2	-170.66 (12)	C5—C6—C1—C2	-0.07 (19)
C16—C15—C14—O2	11.57 (17)	N1—C1—C2—C3	-179.29 (14)
C20—C15—C14—O1	9.93 (17)	C6—C1—C2—C3	0.4 (2)
C16—C15—C14—O1	-167.84 (12)	C6—C7—C8—C13	179.61 (14)
C20—C15—C16—O3	178.85 (11)	C6—C7—C8—C9	0.1 (2)

C14—C15—C16—O3	-3.29 (18)	C1—N1—C9—C10	-179.98 (14)
C20—C15—C16—C17	-3.07 (17)	C1—N1—C9—C8	0.09 (19)
C14—C15—C16—C17	174.79 (11)	C7—C8—C9—N1	-0.3 (2)
C16—C15—C20—C19	1.69 (18)	C13—C8—C9—N1	-179.84 (13)
C14—C15—C20—C19	-176.15 (12)	C7—C8—C9—C10	179.79 (15)
C15—C20—C19—C18	1.4 (2)	C13—C8—C9—C10	0.2 (2)
N2—C18—C19—C20	176.39 (13)	C7—C6—C5—C4	179.90 (17)
C17—C18—C19—C20	-3.10 (19)	C1—C6—C5—C4	-0.2 (3)
O3—C16—C17—C18	179.53 (12)	C7—C8—C13—C12	-179.78 (17)
C15—C16—C17—C18	1.39 (19)	C9—C8—C13—C12	-0.2 (2)
N2—C18—C17—C16	-177.76 (13)	C1—C2—C3—C4	-0.4 (3)
C19—C18—C17—C16	1.74 (19)	C6—C5—C4—C3	0.2 (3)
C8—C7—C6—C5	-179.80 (15)	C2—C3—C4—C5	0.1 (3)
C8—C7—C6—C1	0.3 (2)	N1—C9—C10—C11	179.63 (17)
C9—N1—C1—C2	179.98 (12)	C8—C9—C10—C11	-0.5 (3)
C9—N1—C1—C6	0.31 (19)	C8—C13—C12—C11	0.5 (3)
C7—C6—C1—N1	-0.51 (19)	C9—C10—C11—C12	0.7 (3)
C5—C6—C1—N1	179.60 (14)	C13—C12—C11—C10	-0.7 (3)
C7—C6—C1—C2	179.82 (13)		

(S5) Acridine – 5-chloro salicylic acid*Crystal data* $C_{20}H_{14}NO_3Cl$ $M_r = 351.77$ Monoclinic, $P2_1/n$ $a = 11.4959 (7) \text{ \AA}$ $b = 8.3756 (9) \text{ \AA}$ $c = 17.4500 (16) \text{ \AA}$ $\alpha = 90^\circ$ $\beta = 102.255 (2)^\circ$ $\gamma = 90^\circ$ $V = 1641.9 (3) \text{ \AA}^3$ $Z = 4$ *Data collection*

Bruker D8 Quest Eco

Absorption correction: multi-scan

3797 measured reflections

3797 independent reflections

2710 reflections with $I > 2\sigma(I)$ *Refinement* $F(000) = 728$ $D_x = 1.423 \text{ Mg m}^{-3}$ Mo Ka radiation, $\lambda = 0.71076 \text{ \AA}$

Cell parameters from 3294 reflections

 $\theta = 3.1\text{--}28.3^\circ$ $\mu = 0.29 \text{ mm}^{-1}$ $T = 293 \text{ K}$

Needle

 $0.59 \times 0.18 \times 0.14 \text{ mm}$ $R_{\text{int}} = 0.028$ $\theta_{\max} = 28.0^\circ, \theta_{\min} = 2.7^\circ$ $h = -15 \rightarrow 15$ $k = -11 \rightarrow 11$ $l = -23 \rightarrow 23$

Refinement on F^2

Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.132$

$S = 1.13$
 3797 reflections

282 parameters

H atoms treated by a mixture of
 independent and constrained refinement $\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$

1 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference

Fourier map

Hydrogen site location: mixed

$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 0.2537P]$
 where $P = (F_o^2 + 2F_c^2)/3$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table (S6): Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

Atom	x	y	z	U_{iso}^*/U_{eq}
C1	-0.02038 (4)	0.33762 (8)	0.58099 (4)	0.0674 (2)
O3	0.47198 (12)	0.37110 (19)	0.75929 (9)	0.0570 (4)
H15	0.511583	0.432402	0.738517	0.086*
O1	0.38228 (12)	0.61637 (18)	0.55023 (9)	0.0585 (4)
O2	0.51752 (12)	0.56169 (19)	0.65882 (9)	0.0620 (4)
N1	0.51215 (12)	0.78413 (17)	0.47126 (8)	0.0359 (3)
H1A	0.480757	0.720522	0.499862	0.043*
C19	0.20871 (14)	0.4396 (2)	0.60411 (10)	0.0366 (4)
H19	0.184922	0.495817	0.557441	0.044*
C1	0.44264 (14)	0.84074 (19)	0.40423 (10)	0.0350 (4)
C15	0.36035 (15)	0.3636 (2)	0.71594 (10)	0.0387 (4)
C14	0.32583 (14)	0.44966 (18)	0.64566 (10)	0.0328 (3)
C13	0.62853 (14)	0.8226 (2)	0.49551 (10)	0.0357 (4)
C6	0.49201 (15)	0.9474 (2)	0.35612 (11)	0.0394 (4)
C2	0.32168 (15)	0.7957 (2)	0.38217 (12)	0.0434 (4)
H2	0.288785	0.726613	0.413534	0.052*

C20	0.41509 (15)	0.5503 (2)	0.61573 (11)	0.0408 (4)
C8	0.68087 (15)	0.9315 (2)	0.45005 (11)	0.0396 (4)
C18	0.12773 (15)	0.3467 (2)	0.63185 (11)	0.0412 (4)
C12	0.69649 (16)	0.7561 (2)	0.56482 (11)	0.0460 (4)
H12	0.662244	0.684450	0.594267	0.055*
C7	0.61122 (16)	0.9911 (2)	0.38130 (11)	0.0449 (4)
H7	0.644761	1.062136	0.351156	0.054*
C17	0.16219 (18)	0.2584 (2)	0.70030 (12)	0.0494 (5)
H17	0.107414	0.193770	0.717841	0.059*
C3	0.25381 (17)	0.8544 (2)	0.31448 (12)	0.0504 (5)
H3	0.174041	0.825428	0.300214	0.060*
C16	0.27762 (18)	0.2671 (2)	0.74186 (12)	0.0488 (5)
H16	0.300864	0.208228	0.787732	0.059*
C4	0.30187 (18)	0.9583 (2)	0.26544 (13)	0.0541 (5)
H4	0.253967	0.995803	0.219166	0.065*
C5	0.41750 (18)	1.0036 (3)	0.28557 (12)	0.0513 (5)
H5	0.448429	1.072122	0.252970	0.062*
C11	0.81339 (17)	0.7983 (3)	0.58818 (12)	0.0544 (5)
H11	0.859043	0.753461	0.633473	0.065*
C9	0.80272 (17)	0.9732 (3)	0.47799 (13)	0.0540 (5)
H9	0.838891	1.045529	0.449971	0.065*
C10	0.86605 (17)	0.9085 (3)	0.54484 (13)	0.0585 (6)
H10	0.945393	0.937105	0.562484	0.070*

Table (S7): Atomic displacement parameters (\AA^2)

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0345 (3)	0.0876 (4)	0.0776 (4)	-0.0152 (2)	0.0062 (2)	0.0076 (3)
O3	0.0451 (8)	0.0682 (10)	0.0506 (9)	0.0029 (7)	-0.0062 (6)	0.0089 (7)
O1	0.0437 (7)	0.0713 (9)	0.0586 (9)	-0.0188 (7)	0.0064 (6)	0.0233 (7)
O2	0.0360 (7)	0.0773 (10)	0.0673 (10)	-0.0178 (7)	-0.0011 (6)	0.0098 (8)
N1	0.0326 (7)	0.0365 (7)	0.0395 (8)	-0.0077 (6)	0.0099 (6)	-0.0001 (6)
C19	0.0367 (8)	0.0372 (8)	0.0358 (9)	-0.0023 (7)	0.0072 (7)	0.0023 (7)
C1	0.0336 (8)	0.0323 (8)	0.0398 (9)	-0.0007 (6)	0.0092 (7)	-0.0031 (7)
C15	0.0384 (9)	0.0390 (9)	0.0372 (9)	0.0040 (7)	0.0046 (7)	-0.0005 (7)
C14	0.0335 (8)	0.0309 (8)	0.0343 (8)	-0.0011 (6)	0.0079 (6)	-0.0024 (6)

C13	0.0314 (8)	0.0387 (9)	0.0380 (9)	-0.0069 (7)	0.0093 (7)	-0.0087 (7)
C6	0.0399 (9)	0.0378 (9)	0.0426 (10)	0.0000 (7)	0.0133 (7)	-0.0007 (7)
C2	0.0340 (9)	0.0420 (9)	0.0530 (11)	-0.0059 (7)	0.0065 (8)	0.0013 (8)
C20	0.0362 (9)	0.0387 (9)	0.0472 (11)	-0.0057 (7)	0.0084 (7)	-0.0012 (8)
C8	0.0343 (8)	0.0417 (9)	0.0459 (10)	-0.0083 (7)	0.0158 (7)	-0.0083 (8)
C18	0.0340 (8)	0.0445 (10)	0.0460 (10)	-0.0053 (7)	0.0103 (7)	-0.0012 (8)
C12	0.0397 (9)	0.0556 (11)	0.0424 (10)	-0.0113 (8)	0.0079 (8)	-0.0032 (9)
C7	0.0439 (10)	0.0441 (10)	0.0521 (11)	-0.0059 (8)	0.0222 (9)	0.0025 (8)
C17	0.0520 (11)	0.0455 (10)	0.0566 (12)	-0.0045 (9)	0.0247 (9)	0.0095 (9)
C3	0.0358 (9)	0.0490 (11)	0.0620 (13)	-0.0005 (8)	0.0006 (8)	0.0003 (9)
C16	0.0541 (11)	0.0503 (11)	0.0437 (11)	0.0051 (9)	0.0141 (9)	0.0148 (9)
C4	0.0522 (12)	0.0545 (12)	0.0511 (12)	0.0084 (9)	0.0010 (9)	0.0050 (9)
C5	0.0526 (11)	0.0537 (11)	0.0491 (11)	0.0017 (9)	0.0144 (9)	0.0113 (9)
C11	0.0404 (10)	0.0710 (13)	0.0477 (12)	-0.0086 (10)	0.0002 (8)	-0.0076 (10)
C9	0.0399 (10)	0.0634 (13)	0.0622 (13)	-0.0170 (9)	0.0185 (9)	-0.0078 (10)
C10	0.0337 (9)	0.0788 (15)	0.0616 (14)	-0.0163 (10)	0.0067 (9)	-0.0143 (11)

Table (S8): Geometric parameters (\AA , °)

C1—C18	1.7467 (18)	C2—C3	1.362 (3)
O3—H15	0.8200	C8—C7	1.386 (3)
O3—C15	1.346 (2)	C8—C9	1.425 (3)
O1—C20	1.254 (2)	C18—C17	1.389 (3)
O2—C20	1.259 (2)	C12—H12	0.9300
N1—H1A	0.8600	C12—C11	1.365 (3)
N1—C1	1.355 (2)	C7—H7	0.9300
N1—C13	1.354 (2)	C17—H17	0.9300
C19—H19	0.9300	C17—C16	1.372 (3)
C19—C14	1.390 (2)	C3—H3	0.9300
C19—C18	1.378 (2)	C3—C4	1.413 (3)
C1—C6	1.424 (2)	C16—H16	0.9300
C1—C2	1.413 (2)	C4—H4	0.9300
C15—C14	1.405 (2)	C4—C5	1.355 (3)
C15—C16	1.394 (3)	C5—H5	0.9300
C14—C20	1.505 (2)	C11—H11	0.9300
C13—C8	1.424 (2)	C11—C10	1.409 (3)
C13—C12	1.408 (3)	C9—H9	0.9300
C6—C7	1.396 (3)	C9—C10	1.350 (3)

C6—C5	1.423 (3)	C10—H10	0.9300
C2—H2	0.9300		
C15—O3—H15	109.5	C19—C18—C17	120.82 (17)
C1—N1—H1A	118.3	C17—C18—Cl	118.89 (14)
C13—N1—H1A	118.3	C13—C12—H12	120.5
C13—N1—C1	123.32 (15)	C11—C12—C13	119.05 (18)
C14—C19—H19	119.9	C11—C12—H12	120.5
C18—C19—H19	119.9	C6—C7—H7	119.1
C18—C19—C14	120.19 (16)	C8—C7—C6	121.72 (17)
N1—C1—C6	119.53 (15)	C8—C7—H7	119.1
N1—C1—C2	120.51 (16)	C18—C17—H17	120.2
C2—C1—C6	119.96 (16)	C16—C17—C18	119.55 (17)
O3—C15—C14	121.72 (16)	C16—C17—H17	120.2
O3—C15—C16	118.65 (16)	C2—C3—H3	119.3
C16—C15—C14	119.64 (16)	C2—C3—C4	121.48 (18)
C19—C14—C15	119.16 (15)	C4—C3—H3	119.3
C19—C14—C20	120.62 (15)	C15—C16—H16	119.7
C15—C14—C20	120.22 (15)	C17—C16—C15	120.60 (17)
N1—C13—C8	119.01 (16)	C17—C16—H16	119.7
N1—C13—C12	120.38 (16)	C3—C4—H4	119.9
C12—C13—C8	120.61 (16)	C5—C4—C3	120.24 (19)
C7—C6—C1	117.82 (17)	C5—C4—H4	119.9
C7—C6—C5	123.77 (17)	C6—C5—H5	119.7
C5—C6—C1	118.42 (16)	C4—C5—C6	120.60 (18)
C1—C2—H2	120.4	C4—C5—H5	119.7
C3—C2—C1	119.29 (18)	C12—C11—H11	119.4
C3—C2—H2	120.4	C12—C11—C10	121.1 (2)
O1—C20—O2	124.98 (17)	C10—C11—H11	119.4
O1—C20—C14	117.93 (15)	C8—C9—H9	119.7
O2—C20—C14	117.09 (16)	C10—C9—C8	120.50 (19)
C13—C8—C9	117.86 (18)	C10—C9—H9	119.7
C7—C8—C13	118.57 (16)	C11—C10—H10	119.6
C7—C8—C9	123.57 (17)	C9—C10—C11	120.82 (18)
C19—C18—Cl	120.29 (14)	C9—C10—H10	119.6
Cl—C18—C17—C16	-178.51 (15)	C13—N1—C1—C2	179.89 (16)
O3—C15—C14—C19	-178.79 (16)	C13—C8—C7—C6	0.2 (3)
O3—C15—C14—C20	1.6 (3)	C13—C8—C9—C10	1.1 (3)

O3—C15—C16—C17	178.71 (18)	C13—C12—C11—C10	1.0 (3)
N1—C1—C6—C7	-1.0 (2)	C6—C1—C2—C3	0.4 (3)
N1—C1—C6—C5	179.27 (16)	C2—C1—C6—C7	178.60 (16)
N1—C1—C2—C3	179.99 (17)	C2—C1—C6—C5	-1.2 (3)
N1—C13—C8—C7	-1.7 (2)	C2—C3—C4—C5	-0.8 (3)
N1—C13—C8—C9	178.38 (16)	C8—C13—C12—C11	0.4 (3)
N1—C13—C12—C11	-179.40 (17)	C8—C9—C10—C11	0.2 (3)
C19—C14—C20—O1	-4.2 (3)	C18—C19—C14—C15	0.2 (2)
C19—C14—C20—O2	175.69 (17)	C18—C19—C14—C20	179.75 (16)
C19—C18—C17—C16	1.7 (3)	C18—C17—C16—C15	-0.1 (3)
C1—N1—C13—C8	1.9 (2)	C12—C13—C8—C7	178.54 (17)
C1—N1—C13—C12	-178.32 (16)	C12—C13—C8—C9	-1.4 (3)
C1—C6—C7—C8	1.1 (3)	C12—C11—C10—C9	-1.3 (3)
C1—C6—C5—C4	0.9 (3)	C7—C6—C5—C4	-178.82 (19)
C1—C2—C3—C4	0.6 (3)	C7—C8—C9—C10	-178.8 (2)
C15—C14—C20—O1	175.32 (17)	C3—C4—C5—C6	0.0 (3)
C15—C14—C20—O2	-4.8 (2)	C16—C15—C14—C19	1.4 (2)
C14—C19—C18—Cl	178.45 (13)	C16—C15—C14—C20	-178.15 (16)
C14—C19—C18—C17	-1.8 (3)	C5—C6—C7—C8	-179.14 (18)
C14—C15—C16—C17	-1.5 (3)	C9—C8—C7—C6	-179.87 (18)
C13—N1—C1—C6	-0.6 (2)		

Table (S9) Acridinium hippurate mono hydrate

Crystal data	
C ₂₂ H ₂₀ N ₂ O ₄	<i>F</i> (000) = 792
<i>M_r</i> = 376.4	<i>D_x</i> = 1.329 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ /c	Mo <i>K</i> _a radiation, λ = 0.71076 Å
Hall symbol: -P 2ybc	Cell parameters from 20467 reflections
<i>a</i> = 7.3436 (13) Å	θ = 2.5–28.2°
<i>b</i> = 11.0761 (15) Å	μ = 0.09 mm ⁻¹
<i>c</i> = 23.123 (3) Å	<i>T</i> = 293 K
β = 90.835 (5)°	Block
<i>V</i> = 1880.6 (5) Å ³	0.32 × 0.25 × 0.13 mm
<i>Z</i> = 4	
Data collection	
Bruker D8 Quest eco	<i>R</i> _{int} = 0.041

diffractometer	
Absorption correction: multi-scan	$\theta_{\max} = 28.3^\circ, \theta_{\min} = 2.6^\circ$
$T_{\min} = 0.659, T_{\max} = 0.746$	$h = -9 \rightarrow 9$
20467 measured reflections	$k = -12 \rightarrow 14$
4682 independent reflections	$l = -30 \rightarrow 30$
3285 reflections with $I > 2\sigma(I)$	
<i>Refinement</i>	
Refinement on F^2	Primary atom site location: direct - structure invariant direct methods
Least-squares matrix: full	Secondary atom site location: direct - structure invariant direct methods
$R[F^2 > 2\sigma(F^2)] = 0.071$	Hydrogen site location: difference Fourier map
$wR(F^2) = 0.162$	All H-atom parameters refined
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0248P)^2 + 1.1669P]$ where $P = (F_o^2 + 2F_c^2)/3$
4682 reflections	$(\Delta/\sigma)_{\max} = 0.001$
333 parameters	$\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table (S10) Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.2694 (2)	0.63814 (15)	0.52712 (7)	0.0355 (4)
H1	0.282236	0.708897	0.541950	0.043*
N2	0.6465 (2)	0.94285 (17)	0.63485 (8)	0.0444 (4)
H2A	0.751120	0.939366	0.618678	0.053*
O1	0.4802 (2)	0.89391 (19)	0.71219 (8)	0.0659 (5)
O4	-0.1047 (3)	0.8844 (2)	0.54402 (8)	0.0670 (5)
H4A	-0.001197	0.917434	0.548952	0.100*
H4B	-0.150498	0.919898	0.514638	0.100*
C9	0.3180 (3)	0.54168 (18)	0.55938 (8)	0.0333 (4)

C19	0.7671 (3)	0.79872 (19)	0.70331 (8)	0.0385 (5)
C1	0.2021 (2)	0.62926 (18)	0.47302 (8)	0.0341 (4)
O2	0.2294 (3)	0.9986 (2)	0.55713 (11)	0.0939 (8)
C8	0.2979 (3)	0.42387 (18)	0.53591 (9)	0.0361 (4)
C20	0.6182 (3)	0.8822 (2)	0.68382 (9)	0.0419 (5)
C6	0.1810 (3)	0.51312 (19)	0.44740 (8)	0.0371 (4)
C7	0.2296 (3)	0.41231 (19)	0.47987 (9)	0.0397 (5)
H7	0.216179	0.335796	0.463798	0.048*
C10	0.3887 (3)	0.5582 (2)	0.61573 (9)	0.0428 (5)
H10	0.402901	0.635394	0.630907	0.051*
C18	0.9486 (3)	0.8185 (2)	0.69102 (10)	0.0440 (5)
H18	0.981695	0.884295	0.668521	0.053*
O3	0.3874 (3)	0.83296 (18)	0.57241 (11)	0.0996 (9)
C2	0.1533 (3)	0.7344 (2)	0.44199 (10)	0.0439 (5)
H2	0.166144	0.810198	0.458874	0.053*
C14	0.7208 (3)	0.6983 (2)	0.73600 (9)	0.0483 (6)
H14	0.599340	0.684361	0.744655	0.058*
C5	0.1114 (3)	0.5072 (2)	0.38990 (9)	0.0481 (6)
H5	0.096385	0.432633	0.372007	0.058*
C21	0.5035 (3)	1.0138 (2)	0.60906 (11)	0.0499 (6)
H21A	0.557218	1.071159	0.582611	0.060*
H21B	0.444513	1.059522	0.639264	0.060*
C13	0.3496 (3)	0.3241 (2)	0.57120 (10)	0.0487 (6)
H13	0.338126	0.245897	0.556952	0.058*
C11	0.4358 (3)	0.4597 (2)	0.64768 (10)	0.0502 (6)
H11	0.482360	0.470013	0.684973	0.060*
C17	1.0807 (3)	0.7406 (2)	0.71208 (11)	0.0529 (6)
H17	1.202841	0.755504	0.704776	0.063*
C15	0.8516 (4)	0.6195 (2)	0.75567 (10)	0.0568 (6)
H15	0.818530	0.551840	0.776893	0.068*
C16	1.0314 (4)	0.6408 (2)	0.74398 (10)	0.0564 (7)
H16	1.120347	0.587711	0.757578	0.068*
C12	0.4152 (3)	0.3424 (2)	0.62519 (11)	0.0530 (6)
H12	0.447476	0.276382	0.647979	0.064*
C22	0.3606 (3)	0.9421 (2)	0.57665 (11)	0.0533 (6)
C3	0.0874 (3)	0.7232 (3)	0.38734 (10)	0.0552 (6)

H3	0.055175	0.792238	0.366702	0.066*
C4	0.0666 (3)	0.6092 (3)	0.36098 (10)	0.0574 (7)
H4	0.021590	0.604185	0.323254	0.069*

Table (S11) Atomic displacement parameters (\AA^2)

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0393 (9)	0.0300 (8)	0.0370 (9)	-0.0031 (7)	-0.0013 (7)	-0.0034 (7)
N2	0.0354 (9)	0.0445 (10)	0.0531 (11)	0.0002 (8)	-0.0042 (8)	-0.0022 (9)
O1	0.0458 (10)	0.0932 (15)	0.0587 (11)	0.0131 (10)	0.0070 (8)	-0.0052 (10)
O4	0.0577 (11)	0.0835 (14)	0.0599 (11)	-0.0074 (10)	0.0028 (9)	0.0100 (10)
C9	0.0297 (9)	0.0368 (10)	0.0334 (10)	0.0000 (8)	0.0029 (8)	0.0002 (8)
C19	0.0400 (11)	0.0438 (12)	0.0315 (10)	-0.0013 (9)	-0.0044 (8)	-0.0110 (9)
C1	0.0274 (9)	0.0400 (11)	0.0349 (10)	-0.0026 (8)	0.0021 (8)	-0.0001 (8)
O2	0.0671 (13)	0.0868 (15)	0.126 (2)	-0.0089 (12)	-0.0494 (13)	0.0332 (14)
C8	0.0350 (10)	0.0347 (10)	0.0387 (11)	0.0001 (8)	0.0060 (8)	-0.0012 (8)
C20	0.0380 (11)	0.0469 (12)	0.0405 (11)	-0.0013 (10)	-0.0040 (9)	-0.0123 (10)
C6	0.0350 (10)	0.0428 (11)	0.0337 (10)	-0.0029 (9)	0.0034 (8)	-0.0050 (9)
C7	0.0412 (11)	0.0356 (11)	0.0426 (11)	-0.0027 (9)	0.0059 (9)	-0.0105 (9)
C10	0.0439 (12)	0.0468 (12)	0.0377 (11)	-0.0008 (10)	-0.0010 (9)	-0.0043 (9)
C18	0.0427 (12)	0.0436 (12)	0.0456 (12)	-0.0044 (10)	-0.0058 (9)	-0.0071 (10)
O3	0.126 (2)	0.0430 (11)	0.128 (2)	-0.0118 (12)	-0.0673 (16)	-0.0174 (12)
C2	0.0421 (12)	0.0415 (12)	0.0480 (12)	-0.0004 (10)	0.0000 (10)	0.0054 (10)
C14	0.0501 (13)	0.0581 (14)	0.0367 (11)	-0.0053 (11)	0.0016 (10)	-0.0031 (10)
C5	0.0463 (12)	0.0590 (14)	0.0389 (11)	-0.0023 (11)	-0.0010 (9)	-0.0113 (11)
C21	0.0497 (13)	0.0311 (11)	0.0685 (15)	-0.0014 (10)	-0.0104 (11)	0.0010 (10)
C13	0.0541 (14)	0.0368 (12)	0.0552 (14)	0.0058 (10)	0.0047 (11)	0.0047 (10)
C11	0.0512 (13)	0.0634 (15)	0.0358 (11)	0.0031 (12)	-0.0036 (10)	0.0052 (11)
C17	0.0387 (12)	0.0608 (15)	0.0587 (14)	0.0034 (11)	-0.0070 (10)	-0.0147 (12)
C15	0.0702 (17)	0.0552 (15)	0.0450 (13)	0.0034 (13)	-0.0011 (12)	0.0026 (11)
C16	0.0646 (16)	0.0551 (15)	0.0492 (14)	0.0164 (13)	-0.0119 (12)	-0.0082 (12)
C12	0.0569 (15)	0.0516 (14)	0.0507 (14)	0.0098 (12)	0.0034 (11)	0.0166 (11)
C22	0.0585 (15)	0.0469 (14)	0.0541 (14)	-0.0105 (11)	-0.0193 (12)	0.0113 (11)
C3	0.0557 (14)	0.0634 (16)	0.0463 (13)	0.0039 (12)	-0.0045 (11)	0.0161 (12)
C4	0.0565 (15)	0.0812 (19)	0.0342 (12)	0.0012 (14)	-0.0078 (10)	0.0008 (12)

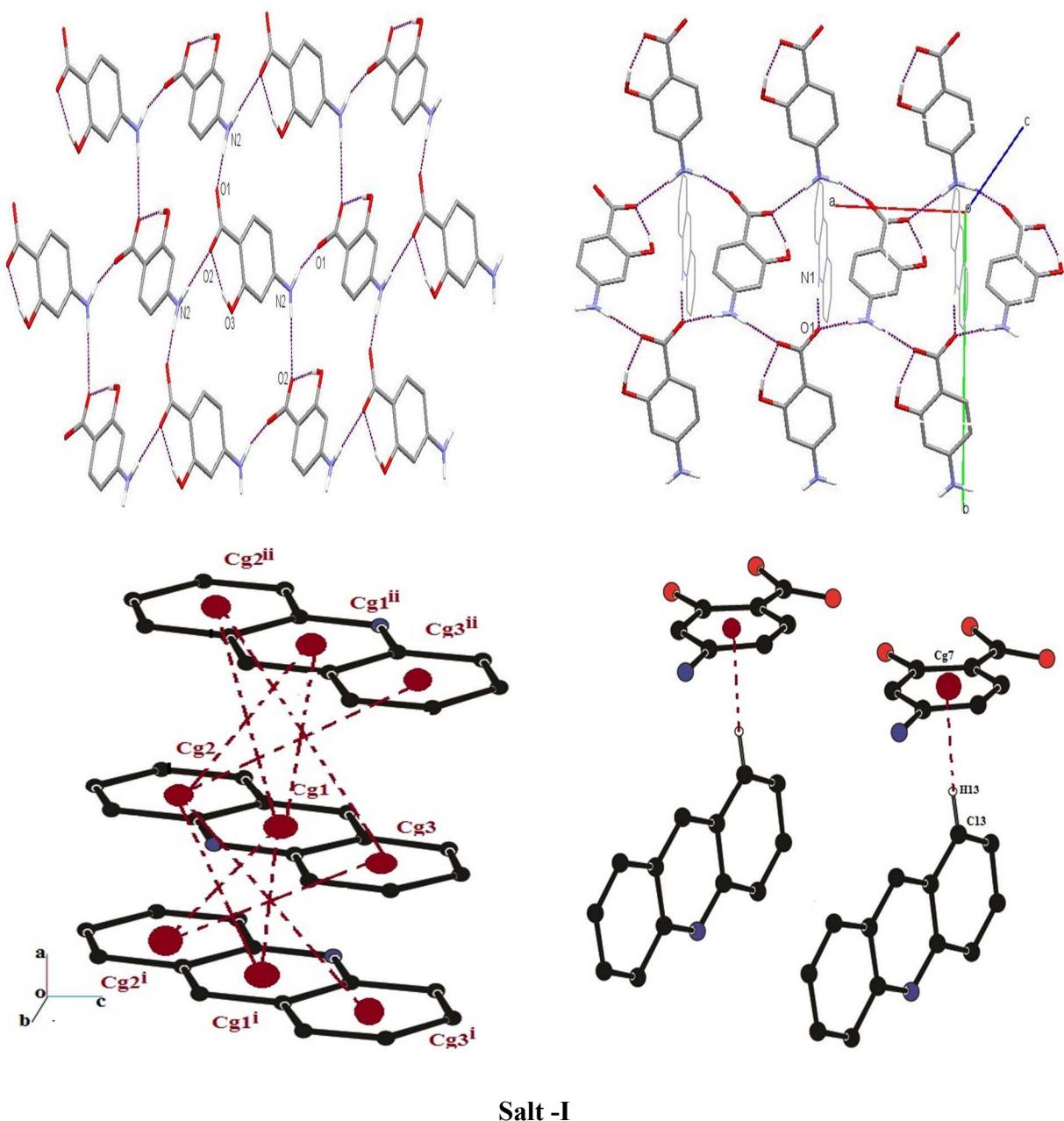
Table (S12) Geometric parameters (\AA , $^\circ$)

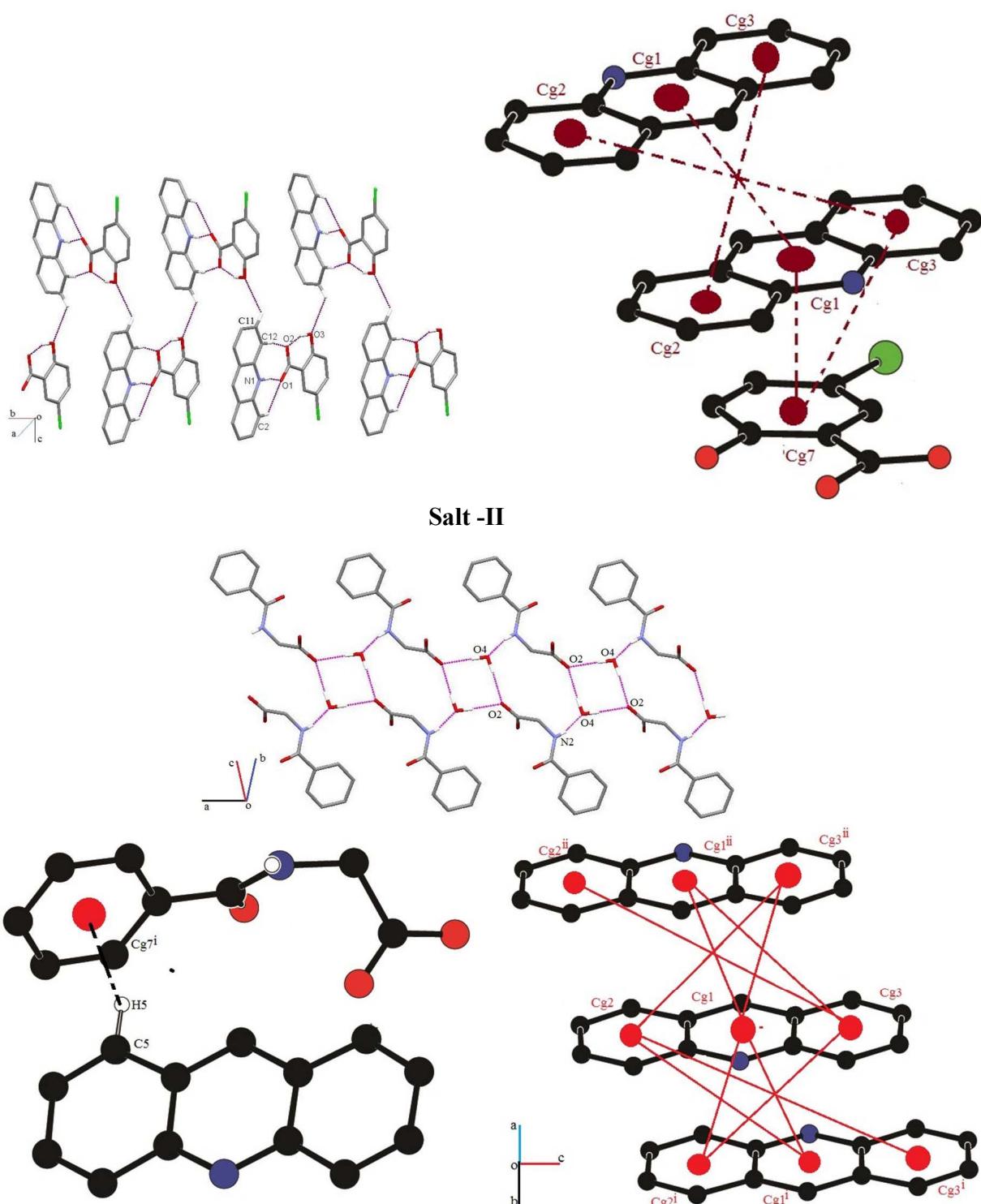
N1—H1	0.8600	C18—C17	1.381 (3)
N1—C9	1.348 (2)	O3—C22	1.229 (3)
N1—C1	1.342 (2)	C2—H2	0.9300
N2—H2A	0.8600	C2—C3	1.352 (3)
N2—C20	1.336 (3)	C14—H14	0.9300
N2—C21	1.435 (3)	C14—C15	1.370 (3)
O1—C20	1.222 (3)	C5—H5	0.9300
O4—H4A	0.8501	C5—C4	1.351 (4)
O4—H4B	0.8502	C21—H21A	0.9700
C9—C8	1.420 (3)	C21—H21B	0.9700
C9—C10	1.407 (3)	C21—C22	1.506 (3)
C19—C20	1.497 (3)	C13—H13	0.9300
C19—C18	1.384 (3)	C13—C12	1.347 (3)
C19—C14	1.390 (3)	C11—H11	0.9300
C1—C6	1.424 (3)	C11—C12	1.407 (4)
C1—C2	1.412 (3)	C17—H17	0.9300
O2—C22	1.230 (3)	C17—C16	1.381 (4)
C8—C7	1.389 (3)	C15—H15	0.9300
C8—C13	1.422 (3)	C15—C16	1.372 (4)
C6—C7	1.389 (3)	C16—H16	0.9300
C6—C5	1.419 (3)	C12—H12	0.9300
C7—H7	0.9300	C3—H3	0.9300
C10—H10	0.9300	C3—C4	1.409 (4)
C10—C11	1.359 (3)	C4—H4	0.9300
C18—H18	0.9300		
C9—N1—H1	118.4	C15—C14—C19	121.0 (2)
C1—N1—H1	118.4	C15—C14—H14	119.5
C1—N1—C9	123.27 (17)	C6—C5—H5	119.8
C20—N2—H2A	119.8	C4—C5—C6	120.5 (2)
C20—N2—C21	120.4 (2)	C4—C5—H5	119.8
C21—N2—H2A	119.8	N2—C21—H21A	108.6
H4A—O4—H4B	104.5	N2—C21—H21B	108.6
N1—C9—C8	119.45 (17)	N2—C21—C22	114.75 (19)
N1—C9—C10	120.03 (18)	H21A—C21—H21B	107.6
C10—C9—C8	120.52 (18)	C22—C21—H21A	108.6
C18—C19—C20	122.8 (2)	C22—C21—H21B	108.6
C18—C19—C14	118.8 (2)	C8—C13—H13	119.9
C14—C19—C20	118.4 (2)	C12—C13—C8	120.2 (2)

N1—C1—C6	119.37 (18)	C12—C13—H13	119.9
N1—C1—C2	120.05 (19)	C10—C11—H11	119.5
C2—C1—C6	120.58 (18)	C10—C11—C12	121.0 (2)
C9—C8—C13	117.99 (19)	C12—C11—H11	119.5
C7—C8—C9	118.39 (18)	C18—C17—H17	120.0
C7—C8—C13	123.6 (2)	C18—C17—C16	120.0 (2)
N2—C20—C19	116.35 (19)	C16—C17—H17	120.0
O1—C20—N2	122.9 (2)	C14—C15—H15	120.1
O1—C20—C19	120.8 (2)	C14—C15—C16	119.8 (2)
C7—C6—C1	118.42 (18)	C16—C15—H15	120.1
C7—C6—C5	123.8 (2)	C17—C16—H16	119.9
C5—C6—C1	117.8 (2)	C15—C16—C17	120.2 (2)
C8—C7—C6	121.10 (19)	C15—C16—H16	119.9
C8—C7—H7	119.5	C13—C12—C11	121.1 (2)
C6—C7—H7	119.5	C13—C12—H12	119.4
C9—C10—H10	120.4	C11—C12—H12	119.4
C11—C10—C9	119.1 (2)	O2—C22—C21	116.8 (2)
C11—C10—H10	120.4	O3—C22—O2	126.7 (2)
C19—C18—H18	119.9	O3—C22—C21	116.5 (2)
C17—C18—C19	120.1 (2)	C2—C3—H3	119.3
C17—C18—H18	119.9	C2—C3—C4	121.4 (2)
C1—C2—H2	120.5	C4—C3—H3	119.3
C3—C2—C1	119.0 (2)	C5—C4—C3	120.7 (2)
C3—C2—H2	120.5	C5—C4—H4	119.6
C19—C14—H14	119.5	C3—C4—H4	119.6
N1—C9—C8—C7	0.5 (3)	C20—C19—C14—C15	-179.2 (2)
N1—C9—C8—C13	-179.72 (19)	C6—C1—C2—C3	-0.5 (3)
N1—C9—C10—C11	179.6 (2)	C6—C5—C4—C3	-0.3 (4)
N1—C1—C6—C7	0.7 (3)	C7—C8—C13—C12	179.8 (2)
N1—C1—C6—C5	-179.31 (18)	C7—C6—C5—C4	179.9 (2)
N1—C1—C2—C3	179.3 (2)	C10—C9—C8—C7	-179.22 (19)
N2—C21—C22—O2	175.4 (2)	C10—C9—C8—C13	0.5 (3)
N2—C21—C22—O3	-4.7 (4)	C10—C11—C12—C13	0.5 (4)
C9—N1—C1—C6	-0.5 (3)	C18—C19—C20—N2	29.3 (3)
C9—N1—C1—C2	179.65 (18)	C18—C19—C20—O1	-149.9 (2)
C9—C8—C7—C6	-0.3 (3)	C18—C19—C14—C15	-0.3 (3)
C9—C8—C13—C12	0.1 (3)	C18—C17—C16—C15	-1.1 (4)
C9—C10—C11—C12	0.1 (3)	C2—C1—C6—C7	-179.46 (19)

C19—C18—C17—C16	2.0 (3)	C2—C1—C6—C5	0.5 (3)
C19—C14—C15—C16	1.2 (4)	C2—C3—C4—C5	0.3 (4)
C1—N1—C9—C8	-0.1 (3)	C14—C19—C20—N2	-151.83 (19)
C1—N1—C9—C10	179.64 (19)	C14—C19—C20—O1	29.0 (3)
C1—C6—C7—C8	-0.3 (3)	C14—C19—C18—C17	-1.3 (3)
C1—C6—C5—C4	-0.1 (3)	C14—C15—C16—C17	-0.5 (4)
C1—C2—C3—C4	0.1 (4)	C5—C6—C7—C8	179.7 (2)
C8—C9—C10—C11	-0.6 (3)	C21—N2—C20—O1	-8.3 (3)
C8—C13—C12—C11	-0.6 (4)	C21—N2—C20—C19	172.53 (18)
C20—N2—C21—C22	-77.4 (3)	C13—C8—C7—C6	179.9 (2)
C20—C19—C18—C17	177.5 (2)		

Fig S13: Intermolecular interaction packing view of salt (I,II & III)





Cg(1)-Cg(1) ⁱ	3.7141(13)	1-x,1-y,-z
Cg(1)-Cg(1) ⁱⁱ	3.7307(13)	2-x,1-y,-z
Cg(1)-Cg(3) ⁱⁱ	3.6297(14)	2-x,1-y,-z
Cg(2)-Cg(1) ⁱ	3.7493(14)	1-x,1-y,-z
Cg(2)-Cg(3) ⁱ	3.7447(14)	1-x,1-y,-z

Cg(2)–Cg(3) ⁱⁱ	3.7350(14)	2-x,1-y,-z
Cg(3)–Cg(1) ⁱ	3.6297(14)	1-x,1-y,-z
Cg(3)–Cg(2) ⁱ	3.7446(14)	1-x,1-y,z
Cg(3)–g(2) ⁱⁱ	3.7350(14)	2-x,1-y,-z

Salt -III**S14 Energy Frame work****Salt- I**

Interaction Energies (kJ/mol)

R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
0	-	6.73	B3LYP/6-31G(d,p)	-68.9	-15.8	-16.4	121.5	-23.7
0	-	10.08	B3LYP/6-31G(d,p)	1.8	-0.1	-0.4	0.0	1.5
0	x+1/2, -y+1/2, -z	11.43	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.6	0.0	-0.8
0	-	6.78	B3LYP/6-31G(d,p)	1.1	-2.0	-11.7	5.4	-7.2
0	-	7.28	B3LYP/6-31G(d,p)	8.7	-2.7	-10.8	6.1	1.5
0	-	13.18	B3LYP/6-31G(d,p)	-1.0	-0.0	-0.1	0.0	-1.1
0	-	13.45	B3LYP/6-31G(d,p)	-0.5	-0.0	-0.1	0.0	-0.7
0	-x+1/2, -y, z+1/2	11.13	B3LYP/6-31G(d,p)	0.4	-0.1	-1.1	0.0	-0.6
0	x, y, z	12.20	B3LYP/6-31G(d,p)	0.2	-0.0	-0.5	0.0	-0.3
0	-	9.51	B3LYP/6-31G(d,p)	0.0	-0.4	-0.6	0.0	-0.8
0	x+1/2, -y+1/2, -z	3.80	B3LYP/6-31G(d,p)	2.6	-3.1	-57.3	29.2	-31.4
0	-	7.64	B3LYP/6-31G(d,p)	-3.3	-1.0	-11.4	7.7	-9.4
0	-	5.89	B3LYP/6-31G(d,p)	-5.9	-2.2	-27.1	25.0	-16.1
0	-	8.15	B3LYP/6-31G(d,p)	-0.3	-0.5	-11.0	5.1	-7.1
0	-	7.99	B3LYP/6-31G(d,p)	-0.5	-1.4	-9.8	5.6	-6.6
0	-x, y+1/2, -z+1/2	12.43	B3LYP/6-31G(d,p)	0.0	-0.0	-0.3	0.0	-0.3
0	-x+1/2, -y, z+1/2	13.16	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.4
0	-x, y+1/2, -z+1/2	12.38	B3LYP/6-31G(d,p)	0.0	-0.0	-0.3	0.0	-0.3
0	-	8.35	B3LYP/6-31G(d,p)	0.2	-2.2	-3.2	0.7	-3.8

0	x, y, z	7.12	B3LYP/6-31G(d,p)	1.4	-0.1	-2.0	0.0	-0.3
0	-	8.85	B3LYP/6-31G(d,p)	-0.3	-0.2	-0.8	0.0	-1.2
0	-	8.68	B3LYP/6-31G(d,p)	2.6	-0.9	-1.6	0.0	0.7
0	-x+1/2, -y, z+1/2	12.51	B3LYP/6-31G(d,p)	0.1	-0.0	-0.4	0.0	-0.2
0	-x+1/2, -y, z+1/2	13.27	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.3
0	-x, y+1/2, -z+1/2	12.21	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.4	0.0	-0.4
0	-	13.12	B3LYP/6-31G(d,p)	0.7	-0.2	-0.4	0.0	0.2
0	-x+1/2, -y, z+1/2	19.72	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	0.0
0	-	9.62	B3LYP/6-31G(d,p)	-0.9	-0.3	-0.7	0.0	-1.7
0	-x, y+1/2, -z+1/2	12.15	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.4	0.0	-0.4
0	-	16.37	B3LYP/6-31G(d,p)	-0.3	-0.0	-0.0	0.0	-0.3
0	x, y, z	14.13	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.1	0.0	-0.1
0	-	11.85	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.1	0.0	-0.2
0	-	10.56	B3LYP/6-31G(d,p)	0.3	-0.1	-0.5	0.0	-0.2
0	-	11.08	B3LYP/6-31G(d,p)	0.1	-0.1	-0.4	0.0	-0.3
0	x, y, z	14.13	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.1	0.0	-0.1
0	-	14.29	B3LYP/6-31G(d,p)	-0.7	-0.0	-0.1	0.0	-0.8
0	-	16.10	B3LYP/6-31G(d,p)	0.4	-0.0	-0.0	0.0	0.4
0	x+1/2, -y+1/2, -z	15.24	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.0	0.0	-0.2
0	-	12.71	B3LYP/6-31G(d,p)	0.1	-0.1	-0.1	0.0	-0.0
0	-	17.01	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	0.0
0	-x+1/2, -y, z+1/2	21.00	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	0.0
0	-	19.16	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.0	0.0	-0.3
0	-	17.94	B3LYP/6-31G(d,p)	-0.3	-0.0	-0.0	0.0	-0.4
0	-x, y+1/2, -z+1/2	21.27	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
0	-	15.39	B3LYP/6-31G(d,p)	0.3	-0.0	-0.0	0.0	0.2
0	-	15.16	B3LYP/6-31G(d,p)	-0.0	-0.1	-0.1	0.0	-0.1
0	-	12.41	B3LYP/6-31G(d,p)	-0.3	-0.0	-0.1	0.0	-0.4
0	-	14.93	B3LYP/6-31G(d,p)	-0.1	-0.1	-0.1	0.0	-0.3
0	-	14.69	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.3

0	-x+1/2, -y, z+1/2	20.93	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	0.0
0	-	17.46	B3LYP/6-31G(d,p)	0.4	-0.0	-0.0	0.0	0.4
0	-x, y+1/2, -z+1/2	16.05	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.1
0	-	19.45	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.0	0.0	-0.1
0	-x, y+1/2, -z+1/2	21.23	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
0	-	14.69	B3LYP/6-31G(d,p)	-0.2	-0.1	-0.1	0.0	-0.4
0	-	13.07	B3LYP/6-31G(d,p)	-0.7	-0.0	-0.1	0.0	-0.8
0	-	17.30	B3LYP/6-31G(d,p)	0.2	-0.0	-0.0	0.0	0.2
0	-	18.48	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	0.0
0	-	18.71	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
0	-	18.56	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.0	0.0	-0.1
0	-	19.98	B3LYP/6-31G(d,p)	0.1	-0.0	-0.0	0.0	0.1
1	-	6.73	B3LYP/6-31G(d,p)	-68.9	-15.8	-16.4	121.5	-23.7

Scale factors for benchmarked energy models

See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Salt -II

Interaction Energies (kJ/mol)

R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	-	3.60	B3LYP/6-31G(d,p)	-13.3	-3.7	-51.0	29.2	-43.2
0	-	6.89	B3LYP/6-31G(d,p)	-65.6	-14.4	-15.9	111.8	-24.9

0	-	9.07	B3LYP/6-31G(d,p)	0.3	-0.1	-3.0	0.4	-2.2
0	-	6.12	B3LYP/6-31G(d,p)	-1.4	-0.9	-15.2	10.3	-9.1
0	-	9.57	B3LYP/6-31G(d,p)	-2.1	-0.4	-6.6	6.5	-4.3
0	x+1/2, -y+1/2, z+1/2	9.63	B3LYP/6-31G(d,p)	-1.2	-0.3	-8.7	4.9	-6.1
0	-x, -y, -z	10.10	B3LYP/6-31G(d,p)	-1.0	-0.1	-8.7	6.3	-4.8
0	-	9.60	B3LYP/6-31G(d,p)	-2.2	-1.3	-7.9	5.3	-6.9
0	-x+1/2, y+1/2, -z+1/2	9.38	B3LYP/6-31G(d,p)	-1.3	-0.4	-10.7	8.3	-5.8
0	-x, -y, -z	7.12	B3LYP/6-31G(d,p)	-0.8	-0.8	-6.2	0.3	-6.6
0	-x, -y, -z	3.69	B3LYP/6-31G(d,p)	-2.5	-3.7	-60.0	33.3	-37.0
0	-	8.85	B3LYP/6-31G(d,p)	-1.4	-0.2	-0.9	0.0	-2.4
0	-x+1/2, y+1/2, -z+1/2	9.32	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.8	0.0	-0.8
0	-	9.28	B3LYP/6-31G(d,p)	-0.7	-0.2	-5.6	3.1	-4.0
0	-	9.91	B3LYP/6-31G(d,p)	-0.6	-0.1	-0.8	0.0	-1.5
0	x+1/2, -y+1/2, z+1/2	11.22	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.7	0.0	-0.7
0	x, y, z	8.38	B3LYP/6-31G(d,p)	-0.4	-0.1	-1.2	0.0	-1.6
0	-	7.16	B3LYP/6-31G(d,p)	1.6	-0.2	-1.6	0.0	0.2
0	-	6.50	B3LYP/6-31G(d,p)	6.3	-2.2	-9.6	2.4	-1.8
0	-	8.98	B3LYP/6-31G(d,p)	2.4	-0.2	-1.0	0.0	1.5
0	-x, -y, -z	11.79	B3LYP/6-31G(d,p)	0.0	-0.0	-0.4	0.0	-0.3
0	-x+1/2, y+1/2, -z+1/2	11.93	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.4	0.0	-0.4
0	x+1/2, -y+1/2, z+1/2	11.63	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.2	0.0	-0.3
0	-	11.54	B3LYP/6-31G(d,p)	0.4	-0.0	-0.3	0.0	0.1
0	-	12.37	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.3
0	x, y, z	11.50	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.6	0.0	-0.8
0	-	9.57	B3LYP/6-31G(d,p)	0.2	-0.3	-6.2	4.2	-2.8
0	-	12.57	B3LYP/6-31G(d,p)	-0.7	-0.0	-0.2	0.0	-0.9
0	-	11.14	B3LYP/6-31G(d,p)	-0.6	-0.0	-0.2	0.0	-0.8
0	-	12.83	B3LYP/6-31G(d,p)	0.0	-0.0	-0.1	0.0	-0.1
0	-	15.10	B3LYP/6-31G(d,p)	0.1	-0.0	-0.1	0.0	0.0
0	-	12.12	B3LYP/6-31G(d,p)	0.2	-0.0	-0.1	0.0	0.1

0	x+1/2, -y+1/2, z+1/2	14.14	B3LYP/6-31G(d,p)	0.1	-0.0	-0.1	0.0	0.0
0	x, y, z	14.22	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.1	0.0	-0.1
0	-	16.15	B3LYP/6-31G(d,p)	0.3	-0.0	-0.0	0.0	0.3
0	-	16.66	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	-0.0
0	-	16.32	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
0	-	10.99	B3LYP/6-31G(d,p)	-0.5	-0.0	-0.3	0.0	-0.8
0	-x+1/2, y+1/2, -z+1/2	17.90	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
0	x+1/2, -y+1/2, z+1/2	17.73	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	-0.0
0	x+1/2, -y+1/2, z+1/2	15.57	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.0	0.0	-0.2
0	x, y, z	14.22	B3LYP/6-31G(d,p)	0.1	-0.0	-0.1	0.0	0.0
0	-	14.10	B3LYP/6-31G(d,p)	0.2	-0.0	-0.1	0.0	0.2
0	-	18.49	B3LYP/6-31G(d,p)	0.1	-0.0	-0.0	0.0	0.1
0	-x, -y, -z	17.63	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
0	-	13.92	B3LYP/6-31G(d,p)	0.0	-0.0	-0.1	0.0	-0.0
0	x+1/2, -y+1/2, z+1/2	18.64	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
0	-	19.16	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	-0.0
0	-x, -y, -z	16.03	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	0.0
0	-	18.92	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.0	0.0	-0.1
0	x, y, z	18.75	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	-0.0
0	-	18.38	B3LYP/6-31G(d,p)	0.1	-0.0	-0.0	0.0	0.1
0	-x, -y, -z	18.65	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0

Scale factors for benchmarked energy models

See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Salt-III

Interaction Energies (kJ/mol)

R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

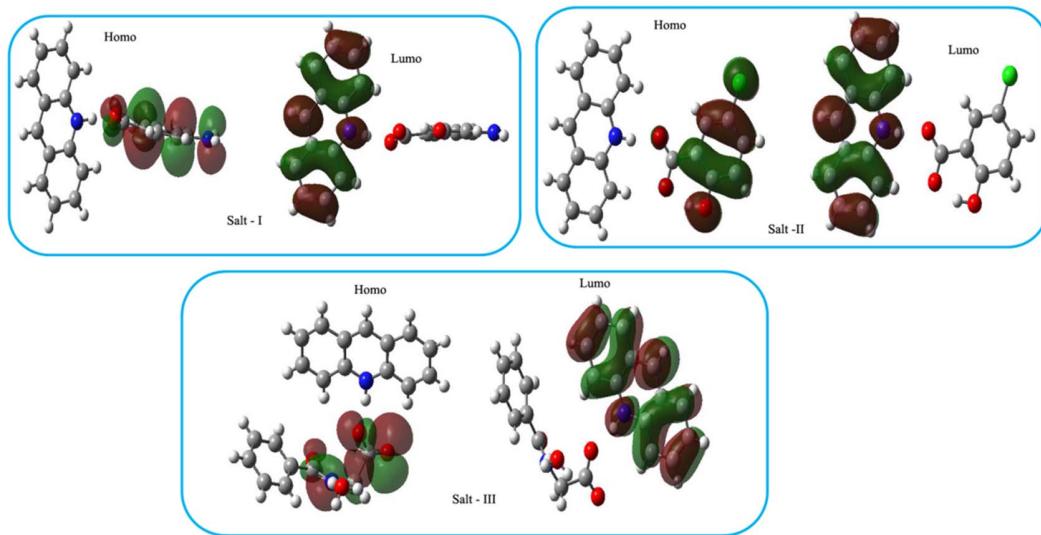
N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	-	5.80	B3LYP/6-31G(d,p)	-69.0	-13.7	-22.2	130.3	-22.0
1	-	5.72	B3LYP/6-31G(d,p)	-0.2	-1.1	-20.4	11.9	-11.4
1	-	8.67	B3LYP/6-31G(d,p)	0.9	-0.4	-1.4	0.0	-0.6
1	-x, -y, -z	8.69	B3LYP/6-31G(d,p)	-13.3	-1.4	-5.1	0.3	-19.3
1	-x, -y, -z	10.90	B3LYP/6-31G(d,p)	-0.8	-0.1	-0.2	0.0	-1.0
2	x, y, z	11.08	B3LYP/6-31G(d,p)	1.2	-0.0	-0.3	0.0	1.0
2	-x, y+1/2, -z+1/2	7.15	B3LYP/6-31G(d,p)	-6.9	-1.4	-8.5	4.0	-13.4
2	x, -y+1/2, z+1/2	13.75	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.1	0.0	-0.3
1	-	7.95	B3LYP/6-31G(d,p)	-4.5	-1.6	-12.5	11.6	-9.6
2	x, y, z	7.34	B3LYP/6-31G(d,p)	-10.8	-2.3	-10.4	7.9	-17.3
1	-	9.00	B3LYP/6-31G(d,p)	-2.4	-1.1	-12.2	10.2	-7.7
1	-	8.05	B3LYP/6-31G(d,p)	1.4	-1.5	-8.3	3.6	-4.8
1	-	9.07	B3LYP/6-31G(d,p)	-1.9	-0.3	-13.3	9.3	-8.0
1	-	6.73	B3LYP/6-31G(d,p)	3.9	-0.8	-9.2	3.8	-2.1
1	-	11.39	B3LYP/6-31G(d,p)	-0.4	-0.1	-0.2	0.0	-0.6
1	-x, -y, -z	14.26	B3LYP/6-31G(d,p)	0.9	-0.0	-0.0	0.0	0.9
2	x, -y+1/2, z+1/2	11.73	B3LYP/6-31G(d,p)	1.7	-0.0	-0.2	0.0	1.6
1	-	18.99	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.0	0.0	-0.0
2	-x, y+1/2, -z+1/2	8.48	B3LYP/6-31G(d,p)	0.9	-1.2	-11.4	5.0	-6.8
1	-	16.89	B3LYP/6-31G(d,p)	0.1	-0.0	-0.0	0.0	0.0
1	-	8.55	B3LYP/6-31G(d,p)	1.1	-0.3	-1.9	0.0	-0.6
1	-	11.23	B3LYP/6-31G(d,p)	0.5	-0.1	-1.5	0.0	-0.7
1	x, y, z	13.29	B3LYP/6-31G(d,p)	-0.3	-0.0	-0.1	0.0	-0.3
1	-	15.22	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.0	0.0	-0.2

1	-x, -y, -z	12.66	B3LYP/6-31G(d,p)	4.2	-0.3	-0.5	0.0	3.8
1	-	10.36	B3LYP/6-31G(d,p)	-2.3	-0.4	-2.5	0.2	-4.9
1	-	9.62	B3LYP/6-31G(d,p)	-0.6	-0.2	-0.8	0.0	-1.4
1	-	11.77	B3LYP/6-31G(d,p)	0.6	-0.1	-0.4	0.0	0.2
2	-x, y+1/2, -z+1/2	11.76	B3LYP/6-31G(d,p)	0.3	-0.0	-0.1	0.0	0.2
1	-	15.57	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.1	0.0	-0.1
1	-x, -y, -z	9.94	B3LYP/6-31G(d,p)	0.8	-0.2	-0.4	0.0	0.4
1	-	18.25	B3LYP/6-31G(d,p)	0.1	-0.0	-0.0	0.0	0.0
1	-x, -y, -z	11.92	B3LYP/6-31G(d,p)	-1.2	-0.0	-0.1	0.0	-1.4
1	x, -y+1/2, z+1/2	17.42	B3LYP/6-31G(d,p)	0.4	-0.0	-0.0	0.0	0.4
1	-	12.79	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.1	0.0	-0.3
1	x, -y+1/2, z+1/2	18.66	B3LYP/6-31G(d,p)	-0.5	-0.0	-0.0	0.0	-0.6
1	-	10.40	B3LYP/6-31G(d,p)	0.4	-0.1	-0.3	0.0	0.1
2	x, y, z	14.69	B3LYP/6-31G(d,p)	-1.4	-0.0	-0.1	0.0	-1.6
1	-	11.42	B3LYP/6-31G(d,p)	0.1	-0.1	-0.2	0.0	-0.1
1	-	9.91	B3LYP/6-31G(d,p)	-0.6	-0.1	-0.6	0.0	-1.3
1	-	14.11	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.2	0.0	-0.2
1	-	15.69	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	-0.0
1	x, y, z	13.29	B3LYP/6-31G(d,p)	0.6	-0.0	-0.1	0.0	0.5
1	-	13.15	B3LYP/6-31G(d,p)	-0.0	-0.0	-0.2	0.0	-0.2
1	-	20.66	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	0.0
2	x, -y+1/2, z+1/2	14.73	B3LYP/6-31G(d,p)	0.6	-0.0	-0.0	0.0	0.6
1	-	13.31	B3LYP/6-31G(d,p)	0.3	-0.0	-0.2	0.0	0.1
1	-x, y+1/2, -z+1/2	17.22	B3LYP/6-31G(d,p)	-0.4	-0.0	-0.0	0.0	-0.4
1	-	18.34	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.0	0.0	-0.2
1	-	15.27	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.0	0.0	-0.1
1	-x, -y, -z	16.66	B3LYP/6-31G(d,p)	-0.7	-0.0	-0.0	0.0	-0.7
1	-x, -y, -z	16.64	B3LYP/6-31G(d,p)	-0.3	-0.0	-0.0	0.0	-0.3
1	-	15.09	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.0	0.0	-0.2
2	x, -y+1/2, z+1/2	16.38	B3LYP/6-31G(d,p)	0.3	-0.0	-0.0	0.0	0.3

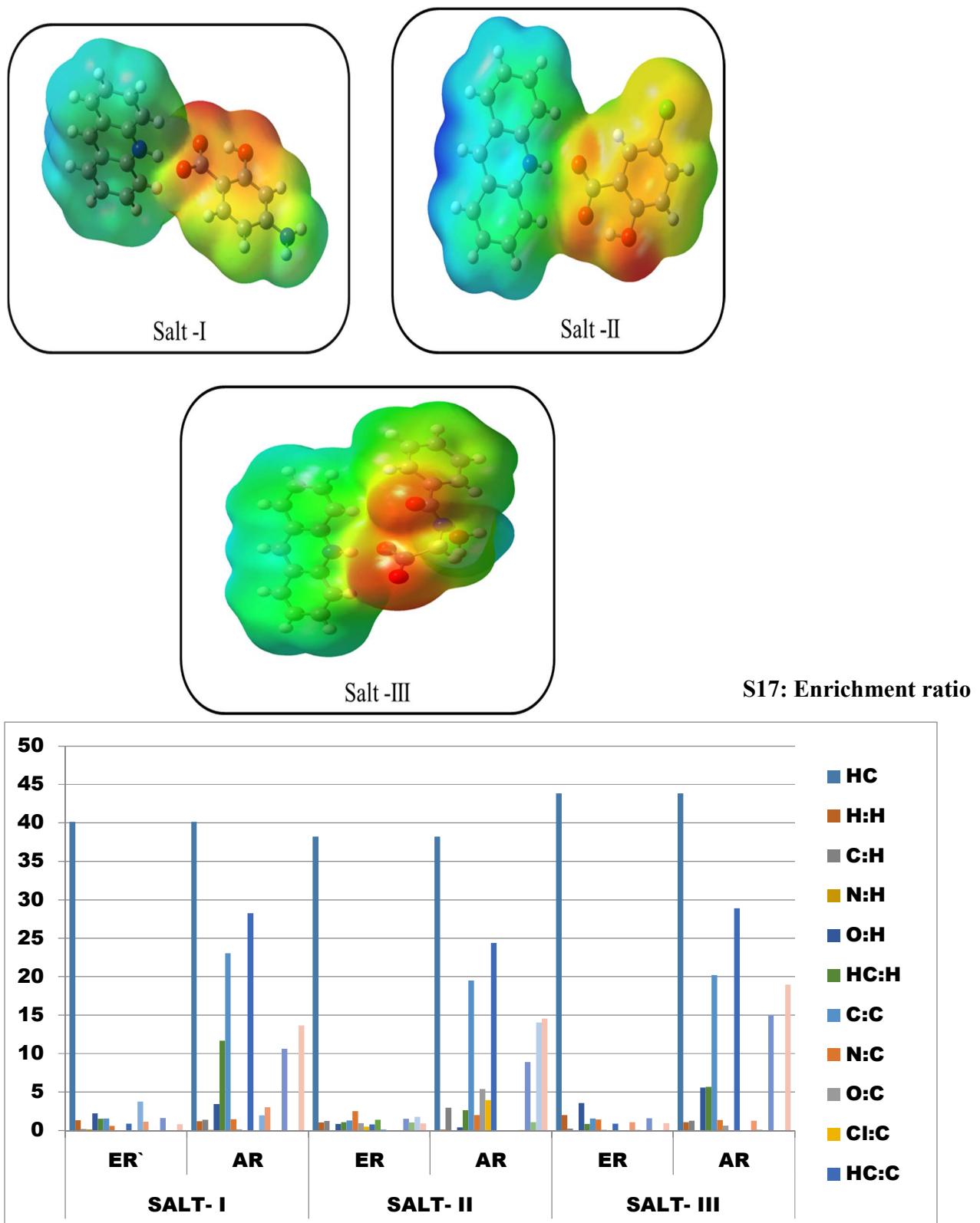
Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

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CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

S15: Frontier Molecular Orbital



S16: Electrostatic Potential Map



calculation:

