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Table 1. Experimental details of the structure determinations

Solvate	**1**	**2**	**3**
Chemical formula	$C_{22}H_{40}N_{14}S_4$	$C_8H_{16}N_4OS$	$C_{19}H_{34}N_{14}S_4$
M_r	628.92	216.31	586.84
Crystal system, space group	triclinic, $P\bar{1}$	triclinic, $P\bar{1}$	triclinic, $P\bar{1}$
Temperature (K)	100	170	100
a (Å)	7.9939(2)	8.3895(3)	7.7966(5)
b (Å)	9.0331(4)	9.1961(3)	9.0094(5)
c (Å)	11.1337(5)	15.9849(6)	10.8792(7)
α (°)	89.976(4)	103.892(3)	89.053(5)
β (°)	83.248(3)	97.021(3)	85.454(5)
γ (°)	85.245(3)	90.970(3)	83.906(5)
V(Å^3)	795.60	1186.83	757.45
d_{calc} (g/cm^{-3})	1.313	1.211	1.284
Z	1	4	1
Radiation, wavelength	Mo $K\alpha$, λ = 0.71073 Å	Cu $K\alpha$, λ = 1.54184 Å	Mo $K\alpha$, λ = 0.71073 Å
F(000)	334	464	310
μ (mm^{-1})	0.34	2.26	0.35
Crystal size (mm)	0.20 × 0.18 × 0.07	0.25 × 0.25 × 0.10	0.5 × 0.4 × 0.3
Transmissions	0.96–1.00	0.30–1.00	0.97–1.00
$2\theta_{max}$ (°)	62	152.5	60
No. of measured and independent reflections	60506, 4780	49484, 4970	41367, 4364
Completeness	98.9% to 2θ 60°	99.9% to 2θ 150°	98.6%
R_{int}	0.049	0.044	0.036
$wR(F^2)$ all refl., $R1$ [$F > 4\sigma(F)$], $S(F^2)$	0.086, 0.038, 1.05	0.099, 0.034, 1.04	0.079, 0.032, 1.05
No. of parameters	216	300	206
$\Delta\rho_{max,min}$ (e Å^{-3})	0.45, –0.25	0.27, –0.24	0.31, –0.22

Table 2. Details of hydrogen bonding [Å and °] for **2** [a]

	D–H⋯A	d(D–H)	d(H⋯A)	d(D⋯A)	<(DHA)	Angle between D–H vector and molecular plane containing A
1	N1–H01⋯N41	0.86(2)	2.14(2)	2.9971(15)	169.2(18)	
2	N1–H02⋯S2^{i}	0.900(18)	2.473(18)	3.3623(11)	169.7(15)	10.0
3	N3–H04⋯S2	0.89(2)	2.52(2)	3.4008(12)	173.7(16)	7.7
4	N3–H03⋯N31	0.91(2)	2.41(2)	3.2516(16)	155.0(17)	
5	N4–H05⋯O2	0.89(2)	1.97(2)	2.8159(15)	159.1(18)	
6	N4–H06⋯S1	0.93(2)	2.44(2)	3.3649(12)	172.2(15)	12.4
7	N6–H08⋯S1^{ii}	0.87(2)	2.54(2)	3.4048(11)	174.2(17)	4.8
8	N6–H07⋯O1	0.864(18)	2.298(17)	2.9708(15)	134.8(14)	
9	N6–H07⋯O2	0.864(18)	2.484(17)	3.1663(15)	136.3(14)	
10	O1–H09⋯N11	0.84(2)	1.99(2)	2.8350(15)	175(2)	
11	O2–H10⋯N21	0.85(2)	1.98(2)	2.8233(15)	175(2)	

[a] Symmetry transformations used to generate equivalent atoms: (i) x+1, y, z; (ii) x+1, y, z.

Table 3. Details of hydrogen bonding [Å and °] for **1** [a]

	D–H⋯A	d(D–H)	d(H⋯A)	d(D⋯A)	<(DHA)	Angle between D–H vector and molecular plane containing A
1	N1–H01⋯S2	0.85(2)	2.51(2)	3.3267(13)	162.1(17)	77.2
2	N1–H02⋯S1^{i}	0.847(19)	2.583(19)	3.4121(13)	166.5(16)	1.4
3	N3–H03⋯S2	0.85(2)	2.83(2)	3.5831(13)	150.0(16)	79.3
4	N3–H04⋯N14	0.85(2)	2.30(2)	3.1280(17)	165.9(17)	
5	N4–H05⋯S1^{ii}	0.855(19)	2.709(19)	3.4937(13)	153.1(15)	74.8
6	N4–H06⋯S2^{iii}	0.847(19)	2.539(19)	3.3819(13)	173.8(17)	7.0
7	N6–H07⋯S1^{ii}	0.877(19)	2.56(2)	3.3915(13)	157.8(16)	66.6
8	N6–H08⋯N21	0.89(2)	2.06(2)	2.9385(16)	151.9	
9	C23–H23⋯N11	0.95	2.62	3.4862(15)	171.4(18)	
10	C24–H24B⋯N11	0.98	2.59	3.5050(18)	155.5	

[a] Symmetry transformation used to generate equivalent atoms: (i) –x+1, –y+2, –z; (ii) x–1, y, z; (iii) –x, –y+2, –z+1.