Crystal Structure Report for Inter-molecular Compound 3.

A specimen of $C_{18}H_{14}N_3S_2$, approximate dimensions 0.078 mm x 0.165 mm x 0.466 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

Table 1: Data collection details.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temp/K
Omega	59.424	-10.00	350.00	0.00	54.74	-0.50	360	1.00	0.71073	50	1.4	100
Omega	59.424	-10.00	350.00	90.00	54.74	-0.50	240	1.00	0.71073	50	1.4	100
Omega	59.424	-10.00	350.00	180.00	54.74	-0.50	120	1.00	0.71073	50	1.4	100
Phi	59.424	0.00	0.00	0.00	54.74	3.00	60	1.00	0.71073	50	1.4	100
Omega	39.961	30.00	312.00	0.00	54.74	0.50	12	1.00	0.71073	50	1.4	100
Omega	39.961	30.00	312.00	120.00	54.74	0.50	12	1.00	0.71073	50	1.4	100
Omega	39.961	30.00	312.00	240.00	54.74	0.50	12	1.00	0.71073	50	1.4	100

A total of 816 frames were collected. The total exposure time was 0.23 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 12835 reflections to a maximum θ angle of 26.03° (0.81 Å resolution), of which 3078 were independent (average redundancy 4.170, completeness = 98.2%, R_{int} = 7.06%, R_{sig} = 7.67%) and 2452 (79.66%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.1528(4) Å, b = 10.1416(4) Å, c = 14.4342(6) Å, β = 103.1180(10)°, volume = 1590.01(11) $Å^3$, are based upon the refinement of the XYZ-centroids of 7263 reflections above 20 σ(I) with 4.953° < 2θ < 59.91°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.880. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8590 and 0.9740.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{18}H_{14}N_3S_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 220 variables converged at R1 = 7.99%, for the observed data and wR2 = 15.69% for all data. The goodness-of-fit was 1.154. The largest peak in the final difference electron density synthesis was 0.496 $e^-/Å^3$ and the largest hole was -0.519 $e^-/Å^3$ with an RMS deviation of 0.126 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.405 g/cm^3 and F(000), 700 e^-.

Table 2. Sample and crystal data.

Identification code	**Inter-molecular compound 3**	
Chemical formula	$C_{18}H_{14}N_3S_2$	
Formula weight	336.44 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.078 x 0.165 x 0.466 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 11.1528(4) Å	α = 90°
	b = 10.1416(4) Å	ß = 103.1180(10)°
	c = 14.4342(6) Å	γ = 90°
Volume	1590.01(11) $Å^3$	
Z	4	
Density (calculated)	1.405 g/cm^3	
Absorption coefficient	0.337 mm^{-1}	
F(000)	700	

Table 3. Data collection and structure refinement.

Theta range for data collection	2.48 to 26.03°
Index ranges	-13<=h<=13, -12<=k<=9, -17<=l<=17
Reflections collected	12835
Independent reflections	3078 [R(int) = 0.0706]
Coverage of independent reflections	98.2%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9740 and 0.8590
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$

Data / restraints / parameters	3078 / 24 / 220	
Goodness-of-fit on F^2	1.154	
Final R indices	2452 data; I>2σ(I)	R1 = 0.0799, wR2 = 0.1377
	all data	R1 = 0.1051, wR2 = 0.1569
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0129P)^2+9.1521P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.496 and -0.519 eÅ^{-3}	
R.M.S. deviation from mean	0.126 eÅ^{-3}	

Table 4. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²).

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
S1	0.14129(10)	0.84983(12)	0.55216(8)	0.0133(3)
N1	0.3607(3)	0.8354(4)	0.6715(3)	0.0107(8)
C1	0.2601(4)	0.7738(4)	0.6185(3)	0.0104(9)
S2	0.58399(10)	0.79235(12)	0.78980(8)	0.0144(3)
N2	0.4043(3)	0.6281(4)	0.6998(3)	0.0122(8)
C2	0.4508(4)	0.7478(5)	0.7215(3)	0.0124(10)
C3	0.2810(4)	0.6282(4)	0.6366(3)	0.0095(8)
N3	0.3795(4)	0.9720(4)	0.6803(3)	0.0139(9)
C4	0.1824(4)	0.5645(4)	0.6809(3)	0.0100(9)
C5	0.1487(4)	0.5996(4)	0.7639(3)	0.0119(9)
C6	0.0584(4)	0.5254(4)	0.7924(3)	0.0130(10)
C8	0.0357(4)	0.3867(5)	0.6530(3)	0.0172(10)
C7	0.0035(4)	0.4198(5)	0.7381(3)	0.0186(11)
C9	0.1256(4)	0.4596(4)	0.6245(3)	0.0120(9)
C10	0.1799(4)	0.4493(4)	0.5406(3)	0.0106(9)
C11	0.1556(4)	0.3608(5)	0.4654(3)	0.0163(10)
C12	0.2242(4)	0.3693(5)	0.3961(3)	0.0159(10)
C13	0.3166(4)	0.4635(4)	0.4037(3)	0.0149(10)

	x/a	y/b	z/c	U(eq)
C14	0.3415(4)	0.5516(5)	0.4795(3)	0.0159(10)
C15	0.2716(4)	0.5454(4)	0.5472(3)	0.0105(9)
C16	0.4250(4)	0.9027(5)	0.4517(3)	0.0170(10)
C17	0.5371(4)	0.8689(5)	0.5093(3)	0.0170(10)
C18	0.6126(4)	0.9660(5)	0.5582(3)	0.0187(11)

Table 5. Bond lengths (Å).

S1-C1	1.641(4)	N1-C1	1.359(5)
N1-N3	1.402(5)	N1-C2	1.411(6)
C1-C3	1.508(6)	S2-C2	1.649(4)
N2-C2	1.330(6)	N2-C3	1.468(5)
N2-H3	0.72(5)	C3-C15	1.524(6)
C3-C4	1.534(6)	N3-H2	0.82(5)
N3-H1	0.89(5)	C4-C5	1.381(6)
C4-C9	1.400(6)	C5-C6	1.392(6)
C5-H5	0.95	C6-C7	1.386(7)
C6-H6	0.95	C8-C9	1.382(6)
C8-C7	1.396(6)	C8-H8	0.95
C7-H7	0.95	C9-C10	1.475(6)
C10-C11	1.388(6)	C10-C15	1.400(6)
C11-C12	1.394(6)	C11-H11	0.95
C12-C13	1.391(6)	C12-H12	0.95
C13-C14	1.392(7)	C13-H13	0.95
C14-C15	1.382(6)	C14-H14	0.95
C16-C17	1.378(6)	C16-C18	1.394(7)
C16-H16	0.95	C17-C18	1.380(7)
C17-H17	0.95	C18-H18	0.95

Table 6. Bond angles (°).

C1-N1-N3	126.4(4)	C1-N1-C2	113.5(4)
N3-N1-C2	120.1(4)	N1-C1-C3	106.1(4)
N1-C1-S1	124.5(3)	C3-C1-S1	129.3(3)
C2-N2-C3	113.9(4)	C2-N2-H3	121.(4)
C3-N2-H3	125.(4)	N2-C2-N1	105.1(4)
N2-C2-S2	129.9(4)	N1-C2-S2	125.0(4)
N2-C3-C1	101.2(3)	N2-C3-C15	113.6(3)
C1-C3-C15	114.5(4)	N2-C3-C4	113.6(3)
C1-C3-C4	112.8(3)	C15-C3-C4	101.7(3)
N1-N3-H2	102.(3)	N1-N3-H1	107.(3)
H2-N3-H1	108.(5)	C5-C4-C9	121.6(4)
C5-C4-C3	127.9(4)	C9-C4-C3	110.5(4)
C4-C5-C6	118.3(4)	C4-C5-H5	120.8
C6-C5-H5	120.8	C7-C6-C5	120.5(4)
C7-C6-H6	119.8	C5-C6-H6	119.8
C9-C8-C7	118.8(4)	C9-C8-H8	120.6
C7-C8-H8	120.6	C6-C7-C8	121.0(4)
C6-C7-H7	119.5	C8-C7-H7	119.5
C8-C9-C4	119.8(4)	C8-C9-C10	131.8(4)
C4-C9-C10	108.4(4)	C11-C10-C15	120.8(4)
C11-C10-C9	130.1(4)	C15-C10-C9	109.0(4)
C10-C11-C12	118.7(4)	C10-C11-H11	120.7
C12-C11-H11	120.7	C13-C12-C11	120.2(4)
C13-C12-H12	119.9	C11-C12-H12	119.9
C12-C13-C14	121.0(4)	C12-C13-H13	119.5
C14-C13-H13	119.5	C15-C14-C13	118.9(4)
C15-C14-H14	120.6	C13-C14-H14	120.6
C14-C15-C10	120.3(4)	C14-C15-C3	129.2(4)
C10-C15-C3	110.4(4)	C17-C16-C18	120.6(4)
C17-C16-H16	119.7	C18-C16-H16	119.7

C16-C17-C18	119.8(5)	C16-C17-H17	120.1
C18-C17-H17	120.1	C17-C18-C16	119.6(4)
C17-C18-H18	120.2	C16-C18-H18	120.2

Table 7. Anisotropic atomic displacement parameters (Å²).

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	0.0115(5)	0.0120(6)	0.0149(6)	0.0021(5)	-0.0001(4)	0.0012(4)
N1	0.0134(18)	0.0051(19)	0.0128(19)	-0.0014(15)	0.0014(15)	-0.0013(14)
C1	0.0110(19)	0.012(2)	0.008(2)	-0.0009(17)	0.0033(16)	-0.0024(17)
S2	0.0124(5)	0.0116(6)	0.0157(6)	0.0008(5)	-0.0040(4)	-0.0024(4)
N2	0.0080(17)	0.011(2)	0.017(2)	0.0007(17)	0.0003(15)	-0.0001(16)
C2	0.012(2)	0.020(3)	0.006(2)	-0.0007(19)	0.0019(17)	0.0006(18)
C3	0.0098(16)	0.0040(17)	0.0138(18)	0.0022(15)	0.0005(14)	-0.0004(14)
N3	0.015(2)	0.013(2)	0.013(2)	0.0000(17)	0.0025(17)	-0.0018(17)
C4	0.0099(19)	0.007(2)	0.013(2)	0.0055(17)	0.0014(16)	0.0007(16)
C5	0.013(2)	0.010(2)	0.011(2)	-0.0016(19)	-0.0007(18)	0.0005(18)
C6	0.022(2)	0.009(2)	0.009(2)	-0.0005(18)	0.0040(19)	0.0004(18)
C8	0.016(2)	0.015(3)	0.020(3)	-0.002(2)	0.002(2)	-0.0075(19)
C7	0.014(2)	0.022(3)	0.023(3)	0.004(2)	0.011(2)	-0.002(2)
C9	0.010(2)	0.011(2)	0.014(2)	-0.0022(19)	-0.0006(17)	0.0029(17)
C10	0.012(2)	0.006(2)	0.013(2)	0.0041(18)	0.0005(17)	0.0031(17)
C11	0.013(2)	0.017(3)	0.018(3)	-0.006(2)	0.0018(19)	-0.0057(19)
C12	0.021(2)	0.012(3)	0.011(2)	-0.0003(19)	-0.0024(19)	0.0026(19)
C13	0.021(2)	0.012(3)	0.013(2)	0.003(2)	0.0075(19)	0.0056(19)
C14	0.010(2)	0.018(3)	0.020(3)	0.008(2)	0.0049(18)	0.0001(18)
C15	0.0109(19)	0.007(2)	0.012(2)	0.0008(17)	-0.0001(16)	0.0039(16)
C16	0.019(2)	0.017(3)	0.015(2)	0.002(2)	0.0049(19)	-0.008(2)
C17	0.021(2)	0.015(3)	0.016(2)	0.005(2)	0.007(2)	0.000(2)
C18	0.013(2)	0.024(3)	0.019(3)	0.006(2)	0.0032(19)	0.001(2)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$).

	x/a	y/b	z/c	U(eq)
H3	0.439(4)	0.569(5)	0.717(3)	0.002(13)
H2	0.398(4)	0.991(5)	0.630(4)	0.014(13)
H1	0.307(5)	1.009(5)	0.680(3)	0.016(13)
H5	0.1862	0.6726	0.8006	0.014
H6	0.0343	0.5473	0.8495	0.016
H8	-0.0036	0.3154	0.6153	0.021
H7	-0.0569	0.3691	0.7590	0.022
H11	0.0934	0.2956	0.4613	0.02
H12	0.2078	0.3106	0.3434	0.019
H13	0.3635	0.4676	0.3564	0.018
H14	0.4053	0.6150	0.4847	0.019
H16	0.3728	0.8358	0.4184	0.02
H17	0.5622	0.7793	0.5154	0.02
H18	0.6898	0.9434	0.5983	0.022