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Supporting Information

3,3'Azobis(6-amino-1,2,4,5-tetrazine): A Novel High-Nitrogen Energetic Material

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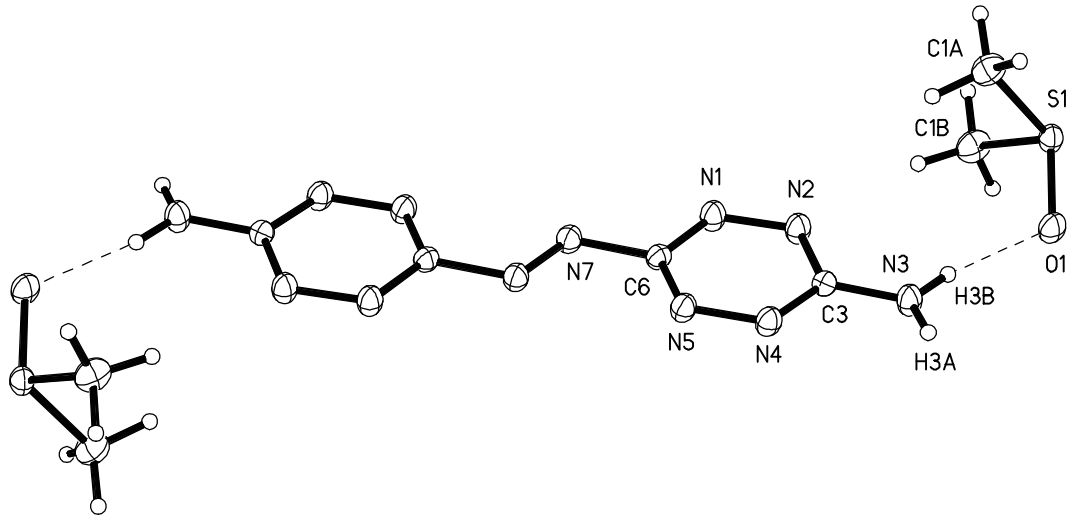
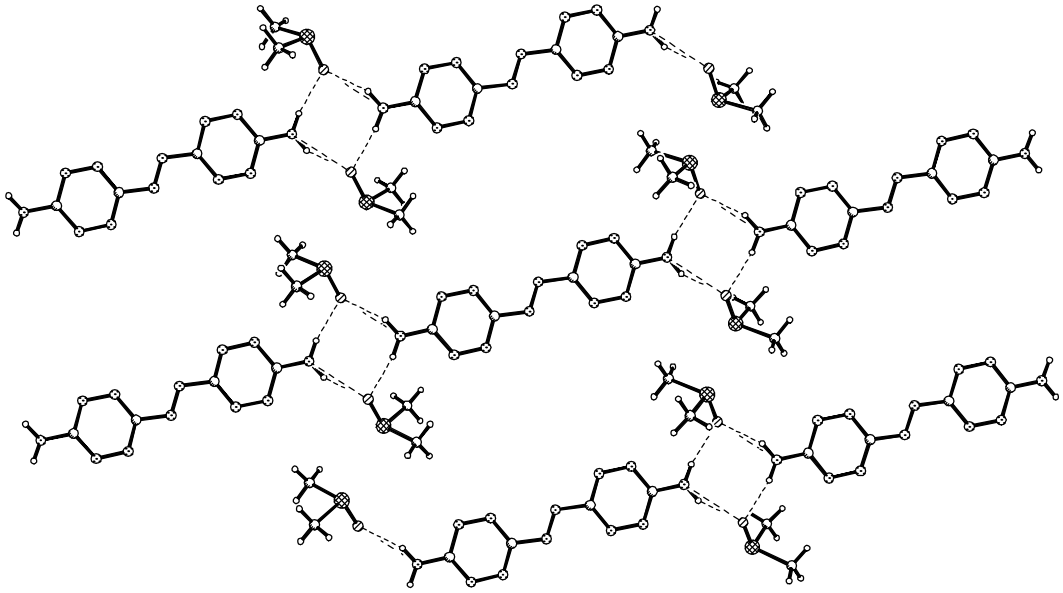
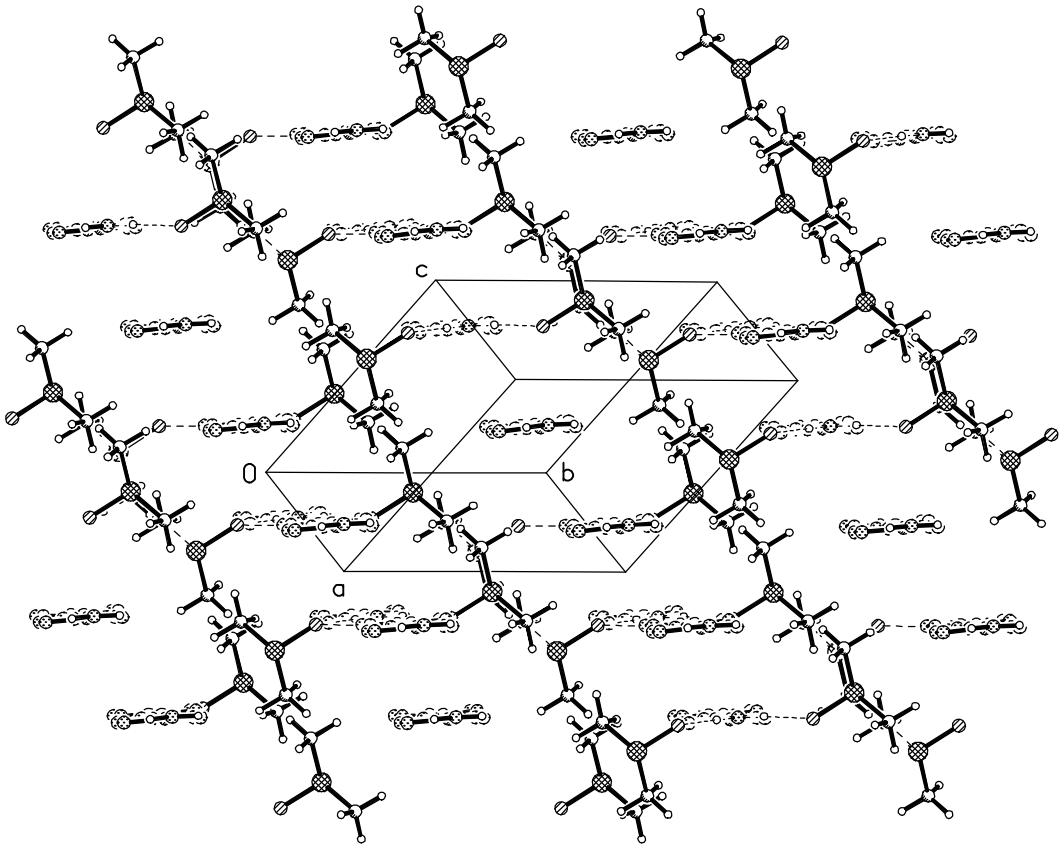


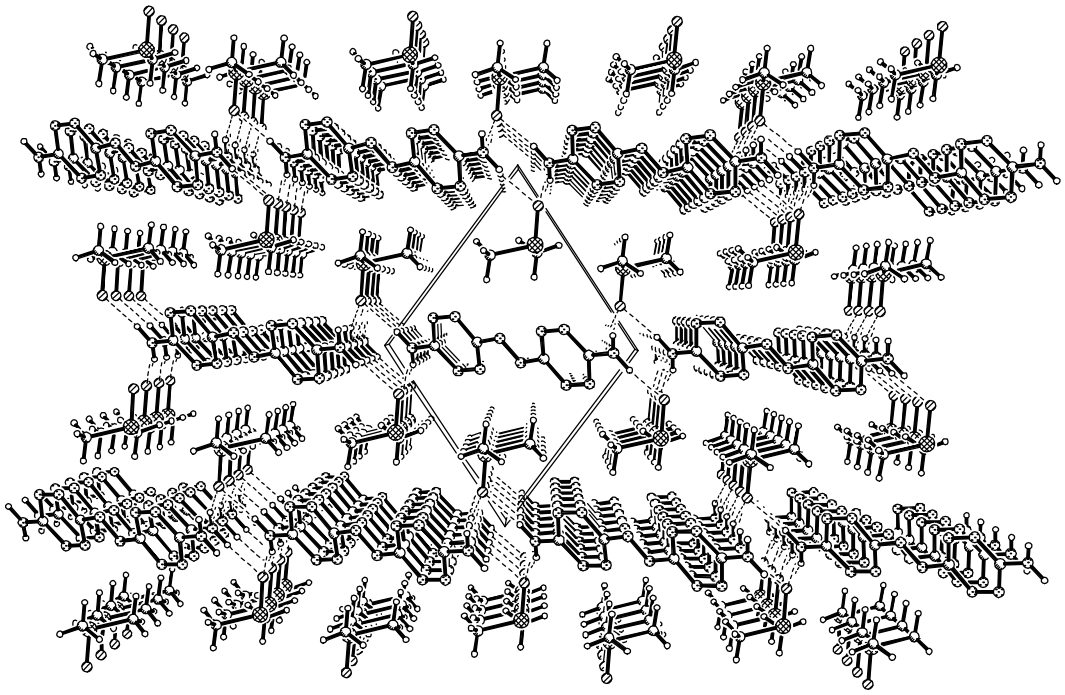
Supp. Fig. 1. An ORTEP drawing of the bis(DMSO)solvate of the diaminoazotetrazine, DAAT. The asymmetric unit in this crystal consists of the labelled atoms, namely one-half of the DAAT and one DMSO molecule.



Supp. Fig. 2. A segment of a sheet of essentially coplanar molecules of DAAT in the crystal assembly.



Supp. Fig. 3. A view of the full 3D assembly in the DAAT crystal. The planar sheets seen in Fig. 2 are now seen edge-on, and they are horizontal. The elongated azotetrazine molecules are seen end-on. They stack above one another, but with a shear offset, so they form an inclined stack of planar segments. In between these stacks lie wavy layers, also seen edge-on, comprised of the hydrocarbon portions of the DMSO molecules. The sulfoxide bonds project into the DAAT stacks, and link them together, by each accepting two hydrogen bonds from distinct DAAT molecules.



Supp. Fig. 4. A view of the full assembly down the **a** axis of the unit cell. The edge-on layers of DAAT and DMSO are horizontal, and alternate from top to bottom in this view.

Table 1. Crystal data and structure refinement for Diamino-azotetrazine/DMSO solvate.

Identification code	hisk24	
Empirical formula	C8 H16 N12 O2 S2	
Formula weight	376.45	
Temperature	294(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.3757(4) Å	α= 67.564(7)°
	b = 9.1971(10) Å	β= 75.634(7)°
	c = 9.3683(8) Å	γ = 76.442(7)°
Volume	409.65(6) $Å^3$	
Z	1	
Density (calculated)	1.526 Mg/m^3	
Absorption coefficient	3.260 mm^{-1}	
F(000)	196	
Crystal size	.40 x .22 x .14 mm^3	
Theta range for data collection	5.19 to 57.49°.	
Index ranges	-5<=h<=5, -9<=k<=9, -10<=l<=1	
Reflections collected	1392	
Reflections 'observed'	1082 [I>2sigma(I)]	
Independent reflections	1106 [R(int) = 0.0106]	
Completeness to theta = 57.49°	98.2 %	
Absorption correction	Integration	
Max. and min. transmission	0.6523 and 0.3176	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1106 / 0 / 118	
Goodness-of-fit on F^2	1.132	
Final R indices [I>2sigma(I)]	R1 = 0.0273, wR2 = 0.0736	
R indices (all data)	R1 = 0.0279, wR2 = 0.0745	
Extinction coefficient	0.048(3)	
Largest diff. peak and hole	0.145 and -0.245 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for hisk24. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	8036(3)	2013(2)	6276(2)	40(1)
N(2)	9769(3)	1209(2)	7185(2)	40(1)
C(3)	10642(4)	2027(2)	7853(2)	31(1)
N(3)	12294(4)	1231(3)	8819(2)	41(1)
N(4)	9963(3)	3627(2)	7565(2)	37(1)
N(5)	8218(3)	4389(2)	6662(2)	37(1)
C(6)	7274(4)	3552(2)	6079(2)	32(1)
N(7)	5377(3)	4279(2)	5101(2)	36(1)
S(1)	15188(1)	-3026(1)	8556(1)	35(1)
O(1)	14646(3)	-2073(2)	9632(2)	43(1)
C(1A)	15911(5)	-1670(3)	6614(3)	51(1)
C(1B)	12089(5)			

Hydrogen atoms	x	y	z	U(iso)
H(3A)	12930(50)	1740(30)	9210(30)	50
H(3B)	12870(50)	200(30)	9000(30)	50
H(1AA)	17517	-1308	6481	77
H(1AB)	14537	-776	6436	77
H(1AC)	16070	-2195	5878	77
H(1BA)	11259	-3892	9468	76
H(1BB)	12289	-3859	7739	76
H(1BC)	11040	-2272	8068	76

Table 3. Bond lengths [Å] and angles [°] for hisk24.

N(1)-N(2)	1.315(2)	N(5)-C(6)	1.338(3)
N(1)-C(6)	1.331(3)	C(6)-N(7)	1.415(3)
N(2)-C(3)	1.360(3)	N(7)-N(7)#1	1.246(3)
C(3)-N(3)	1.316(3)	S(1)-O(1)	1.5097(15)
C(3)-N(4)	1.365(3)	S(1)-C(1B)	1.773(2)
N(4)-N(5)	1.311(2)	S(1)-C(1A)	1.777(2)
N(2)-N(1)-C(6)	118.06(17)	N(1)-C(6)-N(5)	125.59(18)
N(1)-N(2)-C(3)	116.86(17)	N(1)-C(6)-N(7)	112.80(17)
N(3)-C(3)-N(2)	117.88(19)	N(5)-C(6)-N(7)	121.56(18)
N(3)-C(3)-N(4)	117.68(19)	N(7)#1-N(7)-C(6)	114.1(2)
N(2)-C(3)-N(4)	124.43(18)	O(1)-S(1)-C(1B)	105.12(10)
N(5)-N(4)-C(3)	116.95(16)	O(1)-S(1)-C(1A)	106.43(10)
N(4)-N(5)-C(6)	117.88(17)	C(1B)-S(1)-C(1A)	97.50(12)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for hisk24. The anisotropic 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}
N(1)	46(1)	35(1)	47(1)	-17(1)	-22(1)	0(1)
N(2)	46(1)	34(1)	48(1)	-18(1)	-22(1)	1(1)
C(3)	30(1)	33(1)	31(1)	-12(1)	-7(1)	-3(1)
N(3)	45(1)	36(1)	52(1)	-20(1)	-24(1)	1(1)
N(4)	44(1)	34(1)	39(1)	-13(1)	-16(1)	-4(1)
N(5)	45(1)	33(1)	38(1)	-12(1)	-17(1)	-2(1)
C(6)	35(1)	32(1)	30(1)	-12(1)	-9(1)	-4(1)
N(7)	40(1)	34(1)	38(1)	-13(1)	-14(1)	-2(1)
S(1)	39(1)	30(1)	38(1)	-11(1)	-15(1)	-1(1)
O(1)	51(1)	43(1)	46(1)	-20(1)	-23(1)	-3(1)
C(1A)	61(2)	49(1)	40(1)	-9(1)	-7(1)	-15(1)
C(1B)	53(2)	60(2)	52(1)	-24(1)	-13(1)	-21(1)