Supporting Information

The N-H…S hydrogen bonding pattern in trithiocyanuric acid in crystalline state: geometric, topological, and energetic analysis of trithiocyanuric acid cocrystals

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Table S1. Geometric parameters for the structure (**I**).

Bond Lengths			
Atoms	*Length [Å]*	*Atoms*	*Length [Å]*
S(2) - C(2)	1.702(11)	N(5) - C(4)	1.3672(17)
S(6) - C(6)	1.644(6)	N(11) - C(12)	1.3309(17)
S(4) - C(4)	1.628(8)	N(11) - C(16)	1.3229(18)
S(13) - S(13)^{i}	2.0400(9)	C(2) - S(3)	1.614(11)
S(13) - C(13)	1.7807(14)	N(14) - C(13)	1.3278(19)
N(3) - C(2)	1.3551(16)	N(14) - C(15)	1.327(2)
N(3) - C(4)	1.3704(16)	C(13) - C(12)	1.3836(18)
N(1) - C(2)	1.3633(15)	C(6) - S(5)	1.665(6)
N(1) - C(6)	1.3690(15)	C(4) - S(1)	1.648(8)
N(5) - C(6)	1.3580(16)	C(16) - C(15)	1.379(2)
Bond Angles			
Atoms	*Angle [˚]*	*Atoms*	*Angle [˚]*
C(13) - S(13) - S(13)^{i}	103.92(5)	S(6) - C(6) - S(5)	3.4(6)
C(2) - N(3) - C(4)	125.70(11)	N(1) - C(6) - S(6)	123.1(2)
C(2) - N(1) - C(6)	124.24(11)	N(1) - C(6) - S(5)	121.6(2)
C(6) - N(5) - C(4)	125.90(11)	N(5) - C(6) - S(6)	121.8(2)
C(16) - N(11) - C(12)	117.25(12)	N(5) - C(6) - N(1)	115.03(11)
N(3) - C(2) - S(2)	123.7(4)	N(5) - C(6) - S(5)	123.4(2)
N(3) - C(2) - N(1)	115.38(10)	N(11) - C(12) - C(13)	121.16(12)
N(3) - C(2) - S(3)	122.1(4)	S(4) - C(4) - S(1)	7.7(7)
N(1) - C(2) - S(2)	120.8(4)	N(3) - C(4) - S(4)	123.7(3)
N(1) - C(2) - S(3)	122.5(4)	N(3) - C(4) - S(1)	123.0(3)
S(3) - C(2) - S(2)	4.1(8)	N(5) - C(4) - S(4)	122.6(3)
C(15) - N(14) - C(13)	115.85(13)	N(5) - C(4) - N(3)	113.60(11)
N(14) - C(13) - S(13)	113.80(10)	N(5) - C(4) - S(1)	123.3(3)
N(14) - C(13) - C(12)	122.06(13)	N(11) - C(16) - C(15)	120.91(14)
C(12)- C(13) - S(13)	124.13(11)	N(14) - C(15) - C(16)	122.76(14)
Torsion Angles			
Atoms	*Angle [˚]*	*Atoms*	*Angle [˚]*
S(13)^{i} - S(13) - C(13) - N(14)	-167.09(10)	C(6) - N(1) - C(2) - S(3)	-178.6(4)
S(13)^{i} - S(13) - C(13) - C(12)	13.67(12)	C(6) - N(5) - C(4) - S(4)	-172.4(4)
S(13) - C(13) - C(12) - N(11)	178.55(10)	C(6) - N(5) - C(4) - N(3)	2.66(19)
N(11) - C(16) - C(15) - N(14)	-1.3(3)	C(6) - N(5) - C(4) - S(1)	178.4(4)
C(2) - N(3) - C(4) - S(4)	174.9(4)	C(12) - N(11) - C(16) - C(15)	1.3(2)
C(2) - N(3) - C(4) - N(5)	-0.15(19)	C(4) - N(3) - C(2) - S(2)	175.1(4)
C(2) - N(3) - C(4) - S(1)	-176.0(4)	C(4) - N(3) - C(2) - N(1)	-2.87(18)

C(2) - N(1) - C(6) - S(6)	176.5(3)	C(4) - N(3) - C(2) - S(3)	179.5(4)
C(2) - N(1) - C(6) - N(5)	-1.72(18)	C(4) - N(5) - C(6) - S(6)	179.9(3)
C(2) - N(1) - C(6) - S(5)	-179.9(3)	C(4) - N(5) - C(6) - N(1)	-1.80(19)
N(14) - C(13) - C(12) - N(11)	-0.6(2)	C(4) - N(5) - C(6) - S(5)	176.3(4)
C(13) - N(14) - C(15) - C(16)	0.3(3)	C(16) - N(11) - C(12) - C(13)	-0.42(19)
C(6) - N(1) - C(2) - S(2)	-174.2(4)	C(15) - N(14) - C(13) - S(13)	-178.57(12)
C(6) - N(1) - C(2) - N(3)	3.85(17)	C(15) - N(14) - C(13) - C(12)	0.7(2)

symmetry: [i] 1-x,+y,3/2-z

Table S2. Geometric parameters for the structure (**II**).

Bond Lengths			
Atoms	*Length [Å]*	*Atoms*	*Length [Å]*
S(4) - C(4)	1.6649(14)	N(3) - C(2)	1.3716(18)
S(6) - C(6)	1.6382(14)	N(3) - C(4)	1.3639(18)
S(2) - C(2)	1.6558(14)	C(17) - C(12)^{i}	1.437(2)
N(1) - C(2)	1.3640(19)	C(17) - C(16)^{i}	1.4249(19)
N(1) - C(6)	1.3752(18)	C(12) - C(13)	1.423(2)
N(5) - C(4)	1.3542(19)	C(13) - C(14)	1.361(2)
N(5) - C(6)	1.3804(18)	C(16) - C(15)	1.359(2)
N(11) - C(17)	1.3463(19)	C(14) - C(15)	1.425(2)
N(11) - C(12)	1.3488(18)		
Bond Angles			
Atoms	*Angle [˚]*	*Atoms*	*Angle [˚]*
C(2) - N(1) - C(6)	124.72(12)	C(13) - C(12) - C(17)^{i}	119.58(13)
C(4) - N(5) - C(6)	125.63(12)	C(14) - C(13) - C(12)	119.65(13)
C(17) - N(11) - C(12)	117.46(12)	C(15) - C(16) - C(17)^{i}	119.93(13)
C(4) - N(3) - C(2)	124.87(13)	N(5) - C(4) - S(4)	123.04(11)
N(1) - C(2) - S(2)	122.66(11)	N(5) - C(4) - N(3)	115.02(12)
N(1) - C(2) - N(3)	115.42(12)	N(3) - C(4) - S(4)	121.94(11)
N(3) - C(2) - S(2)	121.91(11)	C(13) - C(14) - C(15)	120.90(14)
N(11) - C(17) - C(12)^{i}	121.49(13)	C(16) - C(15) - C(14)	121.13(13)
N(11) - C(17) - C(16)^{i}	119.70(13)	N(1) - C(6) - S(6)	124.26(11)
C(16)1 - C(17) - C(12)^{i}	118.81(13)	N(1) - C(6) - N(5)	114.27(12)
N(11) - C(12) - C(17)^{i}	121.04(13)	N(5) - C(6) - S(6)	121.46(11)
N(11) - C(12) - C(13)	119.38(13)		
Torsion Angles			
Atoms	*Angle [˚]*	*Atoms*	*Angle [˚]*
N(11) - C(12) - C(13) - C(14)	-179.97(12)	C(12) - C(13) - C(14) - C(15)	-0.3(2)
C(2) - N(1) - C(6) - S(6)	-177.46(10)	C(13) - C(14) - C(15) - C(16)	0.7(2)

C(2) - N(1) - C(6) - N(5)	1.55(19)	C(4) - N(5) - C(6) - S(6)	176.69(11)
C(2) - N(3) - C(4) - S(4)	177.80(10)	C(4) - N(5) - C(6) - N(1)	-2.4(2)
C(2) - N(3) - C(4) - N(5)	-2.1(2)	C(4) - N(3) - C(2) - S(2)	-177.85(10)
C(17) - N(11) - C(12) - C(17)^{i}	-1.1(2)	C(4) - N(3) - C(2) - N(1)	1.5(2)
C(17) - N(11) - C(12) - C(13)	178.30(12)	C(6) - N(1) - C(2) - S(2)	178.15(10)
C(17)1 - C(12) - C(13) - C(14)	-0.6(2)	C(6) - N(1) - C(2) - N(3)	-1.2(2)
C(17)1 - C(16) - C(15) - C(14)	-0.1(2)	C(6) - N(5) - C(4) - S(4)	-177.31(11)
C(12) - N(11) - C(17) - C(12)^{i}	1.1(2)	C(6) - N(5) - C(4) - N(3)	2.6(2)
C(12) - N(11) - C(17) - C(16)^{i}	-179.51(12)		

symmetry: ^{i}1-x,1-y,1-z

Table S3. Geometric parameters for the structure (**III**).

Bond Lengths			
Atoms	*Lengths [Å]*	*Atoms*	*Lengths [Å]*
S(6) - C(6)	1.6577(17)	N(5) - C(4)	1.369(2)
S(17) - C(17)	1.6624(18)	N(14) - C(13)	1.333(2)
S(2) - C(2)	1.6529(17)	N(14) - C(15)	1.323(3)
S(4) - C(4)	1.6372(18)	N(17) - C(17)	1.305(2)
N(3) - C(4)	1.373(2)	N(11) - C(12)	1.333(2)
N(3) - C(2)	1.352(2)	N(11) - C(16)	1.332(2)
N(1) - C(6)	1.359(2)	C(12) - C(17)	1.497(2)
N(1) - C(2)	1.366(2)	C(12) - C(13)	1.386(2)
N(5) - C(6)	1.360(2)	C(15) - C(16)	1.382(3)
Bond Angles			
Atoms	*Angle [˚]*	*Atoms*	*Angle [˚]*
C(2) - N(3) - C(4)	125.33(14)	N(17) - C(17) - C(12)	114.98(16)
C(6) - N(1) - C(2)	124.26(15)	C(12) - C(17) - S(17)	121.08(13)
C(6) - N(5) - C(4)	125.87(16)	N(14) - C(13) - C(12)	122.01(16)
C(15) - N(14) - C(13)	116.40(16)	N(3) - C(4) - S(4)	123.75(13)
C(16) - N(11) - C(12)	115.94(16)	N(5) - C(4) - S(4)	122.64(14)
N(11) - C(12) - C(17)	117.36(15)	N(5) - C(4) - N(3)	113.61(15)
N(11) - C(12) - C(13)	121.53(15)	N(3) - C(2) - S(2)	123.44(12)
C(13) - C(12) - C(17)	121.11(15)	N(3) - C(2) - N(1)	115.72(15)
N(1) - C(6) - S(6)	122.15(13)	N(1) - C(2) - S(2)	120.84(13)
N(1) - C(6) - N(5)	115.09(15)	N(14) - C(15) - C(16)	121.65(17)
N(5) - C(6) - S(6)	122.76(13)	N(11) - C(16) - C(15)	122.39(19)
N(17) - C(17) - S(17)	123.94(14)		
Torsion Angles			
Atoms	*Angle [˚]*	*Atoms*	*Angle [˚]*
N(14) - C(15) - C(16) - N(11)	-2.6(4)	C(13) - C(12) - C(17) - N(17)	-172.75(18)

N(11) - C(12) - C(17) - S(17)	-172.70(14)	C(4) - N(3) - C(2) - S(2)	-178.20(15)
N(11) - C(12) - C(17) - N(17)	7.6(3)	C(4) - N(3) - C(2) - N(1)	1.2(3)
N(11) - C(12) - C(13) - N(14)	-1.2(3)	C(4) - N(5) - C(6) - S(6)	179.94(15)
C(12) - N(11) - C(16) - C(15)	2.8(4)	C(4) - N(5) - C(6) - N(1)	-0.5(3)
C(6) - N(1) - C(2) - S(2)	175.81(14)	C(2) - N(3) - C(4) - S(4)	-178.78(15)
C(6) - N(1) - C(2) - N(3)	-3.6(3)	C(2) - N(3) - C(4) - N(5)	1.2(3)
C(6) - N(5) - C(4) - S(4)	178.38(15)	C(2) - N(1) - C(6) - S(6)	-177.16(14)
C(6) - N(5) - C(4) - N(3)	-1.6(3)	C(2) - N(1) - C(6) - N(5)	3.3(3)
C(17) - C(12) - C(13) - N(14)	179.19(16)	C(15) - N(14) - C(13) - C(12)	1.4(3)
C(13) - N(14) - C(15) - C(16)	0.4(3)	C(16) - N(11) - C(12) - C(17)	178.7(2)
C(13) - C(12) - C(17) - S(17)	7.0(2)	C(16)- N(11) - C(12) - C(13)	-1.0(3)

Table S4. Geometric parameters for the structure (**IV**).

Bond Lengths			
Atoms	*Length [Å]*	*Atoms*	*Length [Å]*
S(6) - C(6)	1.6614(12)	N(11) - C(12)	1.3554(16)
S(2) - C(2)	1.6458(12)	N(3) - C(4)	1.3685(15)
S(4) - C(4)	1.652(8)	N(3) - C(2)	1.3688(14)
O(11) - N(11)	1.3013(13)	N(14) - C(15)	1.3397(16)
N(5) - C(4)	1.3693(15)	N(14) - C(13)	1.3413(16)
N(5) - C(6)	1.3580(14)	C(4) - S(1)	1.641(9)
N(1) - C(2)	1.3735(15)	C(16) - C(15)	1.3727(17)
N(1) - C(6)	1.3618(15)	C(12) - C(13)	1.3758(18)
N(11) - C(16)	1.3587(15)		
Bond Angles			
Atom	*Angle [˚]*	*Atom*	*Angle [˚]*
C(6) - N(5) - C(4)	125.34(10)	S(1) - C(4) - S(4)	4.4(10)
C(6)- N(1) - C(2)	124.25(10)	N(1) - C(2) - S(2)	122.56(9)
O(11) - N(11) - C(16)	120.56(10)	N(3)- C(2) - S(2)	122.20(9)
O(11) - N(11) - C(12)	120.60(10)	N(3) - C(2) - N(1)	115.25(10)
C(12) - N(11) - C(16)	118.84(10)	N(11) - C(16) - C(15)	119.44(11)
C(4) - N(3) - C(2)	124.94(10)	N(5) - C(6) - S(6)	122.03(9)
C(15) - N(14) - C(13)	115.81(11)	N(5) - C(6) - N(1)	115.63(10)
N(5) - C(4) - S(4)	121.6(4)	N(1) - C(6) - S(6)	122.34(9)
N(5) - C(4) - S(1)	123.5(4)	N(14) - C(15) - C(16)	123.26(11)
N(3) - C(4) - S(4)	123.9(4)	N(11) - C(12) - C(13)	118.98(11)
N(3) - C(4) - N(5)	114.49(10)	N(14) - C(13) - C(12)	123.64(12)
N(3) - C(4) - S(1)	121.9(4)		
Torsion Angles			

Atoms	*Angle [˚]*	*Atoms*	*Angle [˚]*
O(11) - N(11) - C(16) - C(15)	-179.12(11)	C(2) - N(3) - C(4) - N(5)	-3.26(17)
O(11) - N(11) - C(12) - C(13)	-179.80(11)	C(2) - N(3) - C(4) - S(1)	174.5(6)
N(11) - C(16) - C(15) - N(14)	-1.71(19)	C(16) - N(11) - C(12) - C(13)	-0.51(18)
N(11) - C(12) - C(13) - N(14)	-0.6(2)	C(6) - N(5) - C(4) - S(4)	-179.4(6)
C(4) - N(5) - C(6) - S(6)	177.28(9)	C(6) - N(5) - C(4) - N(3)	3.09(17)
C(4) - N(5) - C(6) - N(1)	-2.40(17)	C(6) - N(5) - C(4) - S(1)	-174.7(6)
C(4) - N(3) - C(2) - S(2)	-177.71(9)	C(6) - N(1) - C(2) - S(2)	178.56(9)
C(4) - N(3) - C(2) - N(1)	2.72(17)	C(6) - N(1) - C(2) - N(3)	-1.88(16)
C(2) - N(1) - C(6) - S(6)	-177.95(9)	C(15) - N(14) - C(13) - C(12)	0.5(2)
C(2) - N(1) - C(6) - N(5)	1.72(16)	C(12) - N(11) - C(16) - C(15)	1.60(17)
C(2) - N(3) - C(4) - S(4)	179.2(6)	C(13) - N(14) - C(15) - C(16)	0.62(18)

Table S5. Selected intermolecular interaction with sulfur atom for structures (I) – (IV) [Å, °].

SULFUR – SULFUR INTERACTIONS						
		d(C-S)	**d(S…S)**	**<(C-S…S)**	***symmetry***	
I	C4-S4…S6	1.637(1)	3.724(1)	126(1)	*1-x,2-y,-z*	
II	C4-S4…S6	1.665(1)	3.799(1)	155(1)	*-x,1-y,-z*	
	C2-S2…S4	1.656(1)	3.748(1)	156(1)	*1-x,2-y,-z*	
IV	C2-S2…S4	1.646(1)	3.464(5)	125(1)	*x,1/2-y,-1/2+z*	
	C6-S6…S4	1.661(1)	3.798(1)	157(1)	*2-x,1-y,1-z*	
SULFUR…π STACKING INTERACTIONS						
		d(Y-X)	**d(X…Cg)**	**d(Y…Cg)**	**<(Y-X…Cg)**	**symmetry**
I	C6-S6…Cg2	1.654(1)	3.717(1)	4.486(1)	106(1)	*x,-1+y,z*
	C2-S2…Cg1	1.659(1)	3.451(1)	4.253(1)	107(1)	*x,1+y,z*
	C2-S2…Cg2	1.659(1)	3.427(1)	4.021(1)	98(1)	*1/2-x,3/2-y,-z*
II	C4-S4…Cg7	1.664(1)	3.753(1)	4.383(2)	101(1)	*-x,2-y,-z*
	C4-S4…Cg7	1.664(1)	3.608(1)	3.723(2)	81(1)	*1-x,1-y,-z*
III	C2-S2…Cg1	1.653(1)	3.646(1)	4.397(1)	106(1)	*1-x,1-y,-z*
	C6-S6…Cg1	1.658(1)	3.882(1)	4.336(1)	94(1)	*x,y,z*
IV	C6-S6…Cg1	1.661(1)	3.320(1)	3.690(1)	89(1)	*1+x,y,z*