N11	-- H112 .. S5	1.000(4)	2.471(4)	3.373(4)	149.8(4)	3_756
N12	-- H121 .. S1	0.999(4)	2.471(4)	3.377(4)	150.6(4)	3_756
N12	-- H122 .. S1	1.001(5)	2.425(4)	3.412(4)	169.0(4)	1_455

Translation of Symmetry Code to Equiv.Pos for TC7_150K

a =[3_555.00]	= -x,-y,-z	m =[4_545.00]	= x,-1/2-y,1/2+z
b =[2_655.00]	= 1-x,1/2+y,1/2-z	n =[4_645.00]	= 1+x,-1/2-y,1/2+z
c =[1_455.00]	= -1+x,y,z	o =[1_656.00]	= 1+x,y,1+z
d =[1_454.00]	= -1+x,y,-1+z	p =[1_656.00]	= 1+x,y,1+z
e =[3_655.00]	= 1-x,-y,-z	r =[4_544.00]	= x,-1/2-y,-1/2+z
f =[3_655.00]	= 1-x,-y,-z	u =[3_655.00]	= 1-x,-y,-z
g =[4_444.00]	= -1+x,-1/2-y,-1/2+z	v =[2_645.00]	= 1-x,-1/2+y,1/2-z
h =[1_655.00]	= 1+x,y,z	w =[2_645.00]	= 1-x,-1/2+y,1/2-z
k =[3_756.00]	= 2-x,-y,1-z	x =[4_444.00]	= -1+x,-1/2-y,-1/2+z
l =[4_544.00]	= x,-1/2-y,-1/2+z	y =[3-756.00]	= 2-x,-y,1-z

Table **S6** - Thiourea cyclooctanone at 293 K

Figure **S6** - Thiourea cyclooctanone at 293 K. Atom numbering and anisotropic displacement parameter.

Table **S6a** - Crystal Data and Details of the Structure Determination for TCO8_293K

Table **S6b** - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for TCO8_293K

Table **S6c** - Hydrogen Atom Positions and Isotropic Displacement Parameters for TCO8_293K

Table **S6d** - (An)isotropic Displacement Parameters for TCO8_293K

Table **S6e** - Bond Distances (Angstrom) for TCO8_293K

Table **S6f** - Bond Angles (Degrees) for TCO8_293K

Table **S6g** - Torsion Angles (Degrees) for TCO8_293K

Table **S6h** - Contact Distances(Angstrom) for TCO8_293K

Table **S6i** - Hydrogen Bonds (Angstrom, Deg) for TCO8_293K

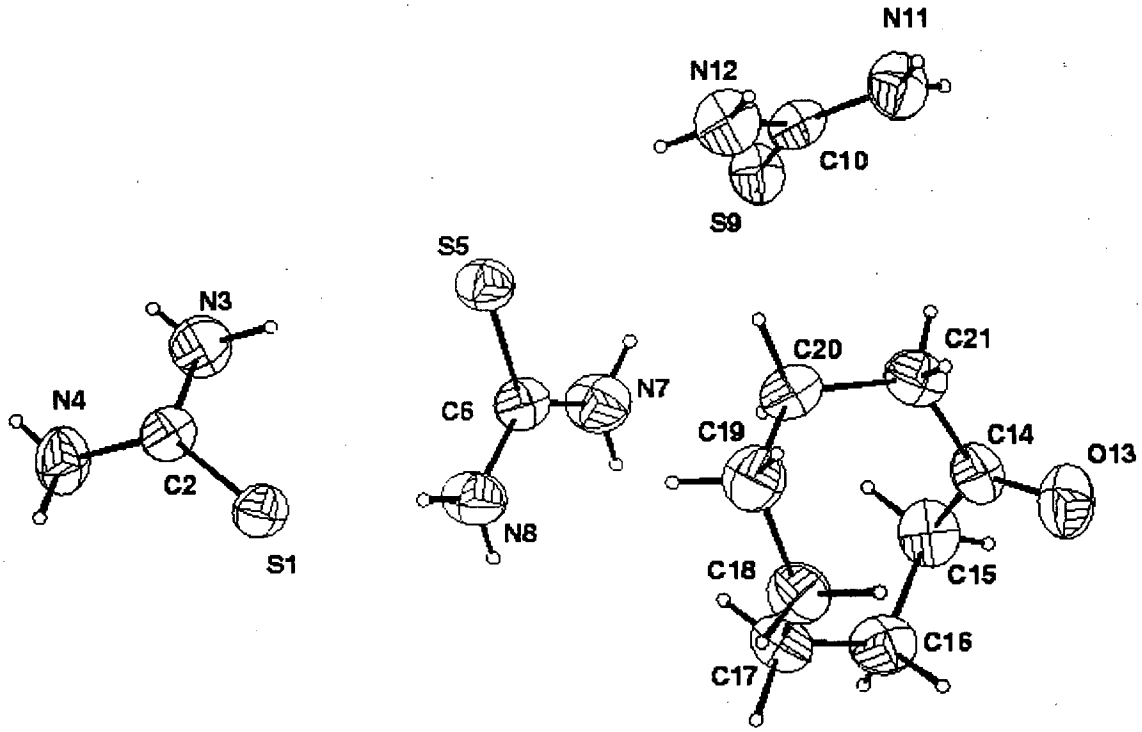

Figure S6 - Thiourea cyclooctanone at 293 K. Atom numbering and anisotropic displacement parameter.

Table **S6a** - Crystal Data and Details of the Structure Determination for TCO8_293K

Crystal Data			
Empirical Formula		C8 H14 O, 3(C H4 N2 S)	
Formula Weight			354.59
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	12.2365(15)	15.631(2)	10.3603(13)
alpha, beta, gamma [deg]	90	111.816(11)	90
V [Ang**3]			1839.7(4)
Z			4
D(obs), D(calc) [g/cm**3]			0.000, 1.280
F(000)			760
Mu(CuKa) [/mm]			3.8
Crystal Size [mm]		0.20 x 0.30 x 0.60	
Data Collection			
Temperature (K)			293
Radiation [Angstrom]		CuKa	1.54180
Theta Min-Max [Deg]			2.2, 74.3
Scan,(Type & Range) [Deg]		0.55 + 0.20 Tan(Theta)	
Dataset		-15: 0 ; -19: 0 ; -11: 12	
Tot., Uniq. Data, R(int)		4068, 3741, 0.040	
Observed data [F > 3.0 sigma(I)]			3428
Refinement			
Nref, Npar			3428, 191
R, wR, S		0.0680, 0.0750, 1.07	
w = Chebychev polynomial with 3 parameters Carruthers & Watkin , 1979		6.83 4.70 4.98	
Max. and Av. Shift/Error			0.01, 0.00
Min. and Max. resd. dens. [e/Ang^3]			-0.65, 0.67

Table **S6b** - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for TC08_293K

Atom	x	y	z	U(eq) [Ang^2]
O13	0.04555(15)	-0.06710(11)	0.1602(2)	0.0691(6)
C14	0.11660(17)	-0.01754(13)	0.1464(2)	0.0511(6)
C15	0.12311(19)	0.07209(13)	0.2013(2)	0.0572(7)
C16	0.1837(2)	0.07602(14)	0.3590(2)	0.0595(7)
C17	0.3148(2)	0.05585(16)	0.4165(2)	0.0625(7)
C18	0.3469(2)	-0.03584(15)	0.3903(2)	0.0593(7)
C19	0.3952(2)	-0.04574(18)	0.2756(3)	0.0659(8)
C20	0.3220(2)	-0.00949(18)	0.1350(2)	0.0633(8)
C21	0.1965(2)	-0.04350(17)	0.0732(2)	0.0627(7)
S1	0.85876(4)	0.14292(3)	0.46915(5)	0.0461(2)
N3	0.85670(18)	0.23495(13)	0.2542(2)	0.0615(6)
N4	1.01658(16)	0.25245(12)	0.4531(2)	0.0581(6)
C2	0.91423(17)	0.21545(11)	0.3861(2)	0.0430(5)
S5	0.57078(4)	0.15348(3)	0.07841(5)	0.0482(2)
N7	0.40026(17)	0.23201(13)	0.1303(2)	0.0602(6)
N8	0.56825(17)	0.20804(12)	0.31832(18)	0.0582(6)
C6	0.50838(17)	0.20124(11)	0.1830(2)	0.0442(5)
S9	0.21498(4)	0.19731(3)	-0.21114(5)	0.0476(2)
N11	0.13645(17)	0.04564(12)	-0.3148(2)	0.0610(6)
N12	0.33347(17)	0.05357(11)	-0.1915(2)	0.0582(6)
C10	0.22893(16)	0.09108(11)	-0.24091(18)	0.0430(5)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table **S6c** - Hydrogen Atom Positions and Isotropic Displacement Parameters for TCO8_293K

Atom	x	y	z	U(iso) [Ang^2]
H151	0.16812(19)	0.10837(13)	0.1588(2)	0.0660
H152	0.04132(19)	0.09497(13)	0.1745(2)	0.0660
H161	0.1732(2)	0.13510(14)	0.3896(2)	0.0721
H162	0.1440(2)	0.03395(14)	0.3998(2)	0.0721
H171	0.3456(2)	0.06558(16)	0.5193(2)	0.0730
H172	0.3543(2)	0.09617(16)	0.3727(2)	0.0730
H181	0.4077(2)	-0.05759(15)	0.4786(2)	0.0681
H182	0.2743(2)	-0.07169(15)	0.3654(2)	0.0681
H191	0.4738(2)	-0.01692(18)	0.3074(3)	0.0781
H192	0.4054(2)	-0.10831(18)	0.2632(3)	0.0781
H201	0.3621(2)	-0.02332(18)	0.0692(2)	0.0789
H202	0.3182(2)	0.05400(18)	0.1444(2)	0.0789
H211	0.2005(2)	-0.10740(17)	0.0741(2)	0.0741
H212	0.1607(2)	-0.02282(17)	-0.0250(2)	0.0741
H31	0.88580	0.27200	0.21300	0.0723
H32	0.78920	0.21080	0.20780	0.0723
H41	1.04480	0.28940	0.41070	0.0679
H42	1.05630	0.24010	0.54010	0.0679
H71	0.36920	0.25620	0.18440	0.0735
H72	0.35960	0.22820	0.04140	0.0735
H81	0.63980	0.18810	0.35480	0.0701
H82	0.53640	0.23230	0.37140	0.0701
H111	0.14400	-0.00850	-0.32960	0.0723
H112	0.06720	0.06950	-0.34890	0.0723
H121	0.39590	0.08310	-0.14350	0.0692
H122	0.34030	-0.00050	-0.20690	0.0692

The temperature factor has the form of EXP(-T) where $T = 8\pi^2 U \sin^2(\theta/\lambda)$ for isotropic Atoms

Table **S6d** - (An)isotropic Displacement Parameters for TCO8_293K

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)

O13	0.0595(9)	0.0570(9)	0.0912(12)	-0.0082(8)	0.0284(8)	-0.0116(7)
C14	0.0459(9)	0.0480(10)	0.0520(10)	0.0006(8)	0.0097(8)	-0.0008(8)
C15	0.0557(11)	0.0420(10)	0.0701(13)	0.0055(9)	0.0190(10)	0.0074(8)
C16	0.0734(14)	0.0452(11)	0.0654(12)	-0.0067(9)	0.0323(11)	0.0054(9)
C17	0.0649(13)	0.0678(13)	0.0508(11)	-0.0113(9)	0.0170(10)	-0.0073(11)
C18	0.0540(11)	0.0656(13)	0.0515(11)	0.0115(9)	0.0117(9)	0.0097(9)
C19	0.0498(11)	0.0769(15)	0.0707(14)	-0.0037(11)	0.0220(10)	0.0110(10)
C20	0.0632(12)	0.0762(15)	0.0593(12)	-0.0032(11)	0.0330(10)	-0.0020(11)
C21	0.0629(12)	0.0711(14)	0.0527(11)	-0.0120(10)	0.0200(10)	-0.0040(11)
S1	0.0563(3)	0.0390(3)	0.0457(3)	0.0024(2)	0.0221(2)	-0.0068(2)
N3	0.0689(11)	0.0621(11)	0.0511(9)	0.0138(8)	0.0194(8)	-0.0111(8)
N4	0.0550(10)	0.0501(9)	0.0654(11)	0.0116(8)	0.0179(8)	-0.0107(7)
C2	0.0515(9)	0.0311(8)	0.0500(9)	0.0006(6)	0.0231(8)	0.0011(7)
S5	0.0514(3)	0.0497(3)	0.0450(3)	-0.0027(2)	0.0197(2)	0.0061(2)
N7	0.0600(10)	0.0622(11)	0.0610(10)	-0.0054(8)	0.0255(8)	0.0122(8)
N8	0.0640(10)	0.0637(11)	0.0482(9)	-0.0066(8)	0.0223(8)	0.0055(8)
C6	0.0550(10)	0.0327(8)	0.0490(10)	0.0002(7)	0.0241(8)	-0.0017(7)
S9	0.0474(3)	0.0353(3)	0.0589(3)	-0.0035(2)	0.0182(2)	0.0025(2)
N11	0.0630(10)	0.0424(9)	0.0804(13)	-0.0166(8)	0.0299(9)	-0.0049(7)
N12	0.0610(10)	0.0443(9)	0.0687(11)	0.0031(7)	0.0235(8)	0.0133(7)
C10	0.0540(10)	0.0378(9)	0.0460(9)	0.0025(7)	0.0289(8)	0.0028(7)

The temperature factor has the form of EXP(-*T*) where

$T = 8\pi^2 U \sin^2(\theta/\lambda)$ for isotropic atoms

$T = \sum_{ij} h_i\, h_j\, U_{ij}\, a_i^*\, a_j^*$ for anisotropic atoms.

a_i^* are reciprocal axial lengths and h_i are the reflection indices.

Table **S6e** - Bond Distances (Angstrom) for TCO8_293K

S1	-C2	1.709(2)	S5	-C6	1.712(2)
S9	-C10	1.7090(18)	N3	-C2	1.319(3)
N4	-C2	1.319(3)	N7	-C6	1.320(3)
N8	-C6	1.323(3)	N11	-C10	1.314(3)
N12	-C10	1.325(3)	O13	-C14	1.212(3)

C19	-C20	1.508(4)	C14	-C15	1.503(3)
C14	-C21	1.499(3)	C15	-C16	1.524(3)
C16	-C17	1.522(4)	C17	-C18	1.537(3)
C18	-C19	1.519(4)	C20	-C21	1.523(4)

Table **S6f** - Bond Angles (Degrees) for TCO8_293K

S1	-C2	-N3	121.05(17)	S1	-C2	-N4	120.21(15)
S5	-C6	-N8	120.29(17)	N7	-C6	-N8	119.0(2)
S5	-C6	-N7	120.75(16)	N11	-C10	-N12	118.99(17)
S9	-C10	-N11	120.54(16)	N3	-C2	-N4	118.73(19)
S9	-C10	-N12	120.47(15)	C15	-C14	-C21	119.4(2)
O13	-C14	-C21	121.2(2)	O13	-C14	-C15	119.4(2)
C14	-C15	-C16	112.30(17)	C15	-C16	-C17	115.67(19)
C16	-C17	-C18	115.18(19)	C17	-C18	-C19	115.6(2)
C18	-C19	-C20	116.9(2)	C19	-C20	-C21	114.8(2)
C14	-C21	-C20	115.99(18)				

Table **S6g** - Torsion Angles (Degrees) for TCO8_293K

O13	-C14	-C21	-C20	-141.5(2)	O13	-C14	-C15	-C16	75.5(3)
C21	-C14	-C15	-C16	-105.7(2)	C15	-C14	-C21	-C20	39.7(3)
C14	-C15	-C16	-C17	68.2(3)	C15	-C16	-C17	-C18	-64.1(2)
C16	-C17	-C18	-C19	103.5(2)	C17	-C18	-C19	-C20	-53.8(3)
C18	-C19	-C20	-C21	-56.2(3)	C19	-C20	-C21	-C14	68.0(3)

Table **S6h** - Contact Distances (Angstrom) for TCO8_293K

S1	.N3_k	3.524(2)	O13	.N11_b	3.208(3)
S1	.N8	3.462(2)	O13	.N4_a	3.041(3)
S1	.N11_j	3.364(2)	S5	.N3	3.528(2)
S5	.N12_j	3.4928(19)	S5	.N8_q	3.4475(19)
S9	.N7	3.462(2)	S9	.N7_q	3.439(2)
S9	.C16_u	3.665(2)	N3	.S5	3.528(2)
S9	.N4_s	3.530(2)	N3	.S1_l	3.524(2)
S9	.N4_t	3.532(2)	N4	.S9_o	3.532(2)
N4	.O13_n	3.041(3)	N4	.S9_i	3.530(2)

N7	.S9	3.462(2)	N7	.S9_d	3.439(2)
N8	.S5_r	3.4475(19)	N8	.S1	3.462(2)
N11	.O13_c	3.208(3)	N11	.S1_v	3.364(2)
N12	.S5_h	3.4928(19)	C14	.C18	3.019(3)
C14	.O13_c	3.331(3)	C14	.C14_c	3.348(3)
C16	.S9_d	3.665(2)	C16	.C20	3.599(3)
O13	.C14_c	3.331(3)	C18	.C14	3.019(3)
C20	.C16	3.599(3)			

Table **S6i** - Hydrogen Bonds (Angstrom, Deg) for TCO8_293K

D	H	A	D - H	H -- A	D --- A	D H A	Symm(A)
N3	-- H31 ..	S1	0.8703	2.7639	3.524(2)	146.79	4_554
N3	-- H32 ..	S5	0.8722	2.6609	3.528(2)	172.57	.
N4	-- H41 ..	O13	0.8709	2.4879	3.041(3)	122.06	2_655
N4	-- H41 ..	S9	0.8709	2.8154	3.532(2)	140.63	4_655
N4	-- H42 ..	S9	0.8720	2.6721	3.530(2)	168.10	1_656
N7	-- H71 ..	S9	0.8717	2.6035	3.439(2)	160.89	4_555
N7	-- H72 ..	S9	0.8711	2.6017	3.462(2)	169.66	.
N8	-- H81 ..	S1	0.8721	2.5926	3.462(2)	174.83	.
N8	-- H82 ..	S5	0.8703	2.7007	3.4475(19)	144.65	4_555
N11	-- H111 ..	S1	0.8711	2.5436	3.364(2)	157.33	3_655
N11	-- H112 ..	S1	0.8715	2.7933	3.635(2)	162.91	1_454
N12	-- H121 ..	S5	0.8727	2.7237	3.557(2)	160.29	.
N12	-- H122 ..	S5	0.8699	2.7563	3.4928(19)	143.31	3_655

Translation of Symmetry Code to Equiv.Pos for TCO8_293K

```
a =[  2_645.00 ]  = 1-x,-1/2+y,1/2-z
b =[  3_555.00 ]  = -x,-y,-z
c =[  3_555.00 ]  = -x,-y,-z
d =[  4_555.00 ]  = x,1/2-y,1/2+z
e =[  1_455.00 ]  = -1+x,y,z
f =[  3_656.00 ]  = 1-x,-y,1-z
g =[  3_656.00 ]  = 1-x,-y,1-z
h =[  3_655.00 ]  = 1-x,-y,-z
i =[  1_656.00 ]  = 1+x,y,1+z
l =[  4_554.00 ]  = x,1/2-y,-1/2+z
m =[  1_655.00 ]  = 1+x,y,z
n =[  2_655.00 ]  = 1-x,1/2+y,1/2-z
o =[  4_655.00 ]  = 1+x,1/2-y,1/2+z
s =[  1_454.00 ]  = -1+x,y,-1+z
t =[  4_454.00 ]  = -1+x,1/2-y,-1/2+z
```

Table **S7** - Thiourea cyclooctanone at 280 K

Figure **S7** - Thiourea cyclooctanone at 280 K. Atom numbering and anisotropic displacement parameter.

Table **S7a** - Crystal Data and Details of the Structure Determination for TCO8_280K

Table **S7b** - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for TCO8_280K

Table **S7c** - Hydrogen Atom Positions and Isotropic Displacement Parameters for TCO8_280K

Table **S7d** - (An)isotropic Displacement Parameters for TCO8_280K

Table **S7e** - Bond Distances (Angstrom) for TCO8_280K

Table **S7f** - Bond Angles (Degrees) for TCO8_280K

Table **S7g** - Torsion Angles (Degrees) for TCO8_280K

Table **S7h** - Contact Distances(Angstrom) for TCO8_280K

Table **S7i** - Hydrogen Bonds (Angstrom, Deg) for TCO8_280K

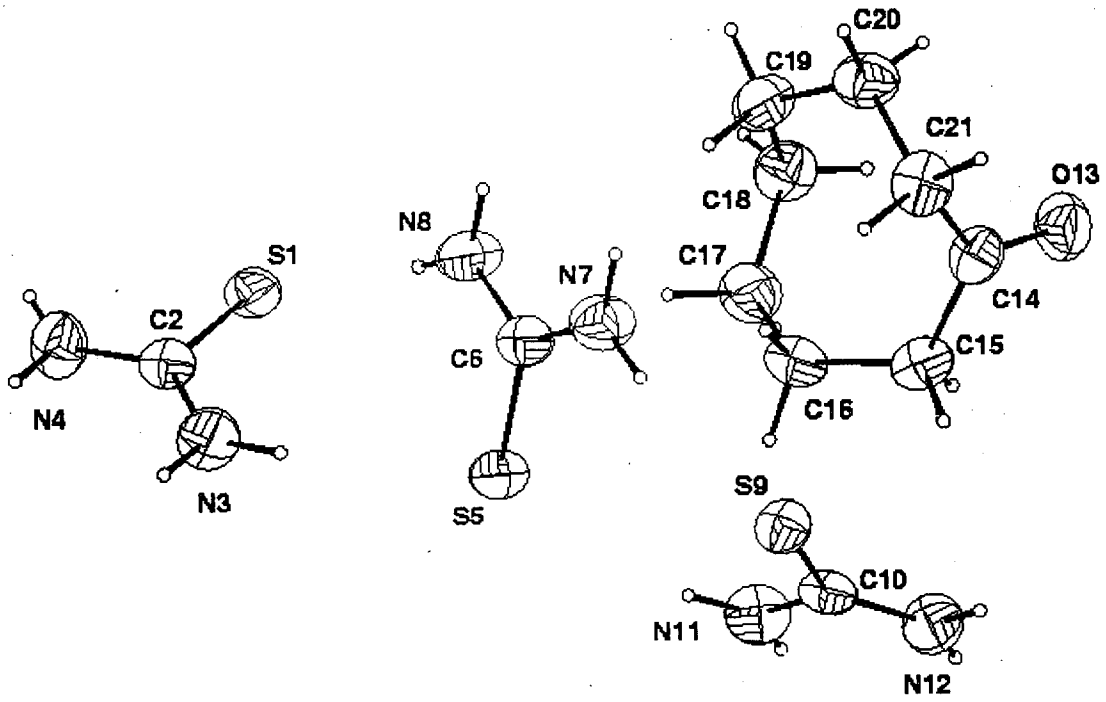

Figure S7 - Thiourea cyclooctanone at 280 K. Atom numbering and anisotropic displacement parameter.

Table S7a Crystal Data and Details of the Structure Determination for TCO8_280K

Crystal Data			
Empirical Formula		C8 H14 O, 3(C H4 N2 S)	
Formula Weight			354.59
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	12.219(7)	15.6205(17)	10.3555(14)
alpha, beta, gamma [deg]	90	111.823(8)	90
V [Ang**3]			1834.9(11)
Z			4
D(obs), D(calc) [g/cm**3]			0.000, 1.284
F(000)			760
Mu(CuKa) [/mm]			3.8
Crystal Size [mm]		0.16 x 0.19 x 0.80	
Data Collection			
Temperature (K)			280
Radiation [Angstrom]		CuKa	1.54180
Theta Min-Max [Deg]			2.2, 74.3
Scan,(Type & Range) [Deg]		0.53 + 0.17 Tan(Theta)	
Dataset		-15: 14 ; -19: 1 ; -1: 12	
Tot., Uniq. Data, R(int)		4835, 4005, 0.040	
Observed data [F > 3.0 sigma(I)]			3636
Refinement			
Nref, Npar			3636, 191
R, wR, S		0.0354, 0.0436, 0.90	
w = Chebychev polynomial with 3 parameters Carruthers & Watkin , 1979		5.31 3.86 3.96	
Max. and Av. Shift/Error			0.09, 0.00
Min. and Max. resd. dens. [e/Ang^3]			-0.80, 0.38

Table **S7a** - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for TCO8_280K

Atom	x	y	z	U(eq) [Ang^2]
O13	0.04549(9)	-0.06715(7)	0.15947(13)	0.0648(3)
C14	0.11643(11)	-0.01743(9)	0.14609(13)	0.0485(4)
C15	0.19716(13)	-0.04339(11)	0.07307(14)	0.0595(5)
C16	0.32241(13)	-0.00917(12)	0.13470(15)	0.0595(5)
C17	0.39595(13)	-0.04578(12)	0.27521(17)	0.0628(5)
C18	0.34690(13)	-0.03570(10)	0.38992(14)	0.0561(4)
C19	0.31448(13)	0.05620(10)	0.41640(15)	0.0589(4)
C20	0.18333(13)	0.07618(9)	0.35853(15)	0.0560(4)
C21	0.12292(12)	0.07256(9)	0.20055(15)	0.0542(4)
S1	0.85818(3)	0.14261(2)	0.46981(3)	0.0448(1)
N3	0.85589(12)	0.23519(9)	0.25474(13)	0.0596(4)
N4	1.01610(10)	0.25272(8)	0.45437(13)	0.0565(4)
C2	0.91380(11)	0.21547(7)	0.38705(13)	0.0420(3)
S5	0.57056(3)	0.15341(2)	0.07867(3)	0.0468(1)
N7	0.39979(11)	0.23230(8)	0.13048(13)	0.0578(4)
N8	0.56773(11)	0.20788(8)	0.31895(12)	0.0570(4)
C6	0.50833(11)	0.20127(7)	0.18343(13)	0.0433(4)
S9	0.21441(3)	0.19740(2)	-0.21056(3)	0.0465(1)
N11	0.33338(11)	0.05356(8)	-0.19165(13)	0.0563(4)
N12	0.13578(11)	0.04566(8)	-0.31523(14)	0.0588(4)
C10	0.22845(11)	0.09111(8)	-0.24108(12)	0.0420(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table **S7b** - Hydrogen Atom Positions and Isotropic Displacement Parameters for TCO8_280K

Atom	x	y	z	U(iso) [Ang^2]
H151	0.20162(13)	-0.10733(11)	0.07444(14)	0.0695
H152	0.16135(13)	-0.02301(11)	-0.02535(14)	0.0695
H161	0.36249(13)	-0.02255(12)	0.06867(15)	0.0736
H162	0.31835(13)	0.05430(12)	0.14466(15)	0.0736
H171	0.47477(13)	-0.01716(12)	0.30728(17)	0.0748
H172	0.40577(13)	-0.10841(12)	0.26261(17)	0.0748
H181	0.40753(13)	-0.05760(10)	0.47839(14)	0.0645
H182	0.27407(13)	-0.07150(10)	0.36461(14)	0.0645
H191	0.34508(13)	0.06590(10)	0.51920(15)	0.0682
H192	0.35407(13)	0.09670(10)	0.37278(15)	0.0682
H201	0.17240(13)	0.13515(9)	0.38936(15)	0.0682
H202	0.14351(13)	0.03380(9)	0.39881(15)	0.0682
H211	0.16840(12)	0.10871(9)	0.15830(15)	0.0626
H212	0.04106(12)	0.09562(9)	0.17330(15)	0.0626
H31	0.88500	0.27250	0.21360	0.0689
H32	0.78830	0.21100	0.20800	0.0689
H41	1.04440	0.28980	0.41200	0.0657
H42	1.05610	0.24030	0.54130	0.0657
H71	0.36880	0.25660	0.18460	0.0701
H72	0.35910	0.22860	0.04160	0.0701
H81	0.63920	0.18770	0.35580	0.0672
H82	0.53560	0.23230	0.37170	0.0672
H111	0.39600	0.08310	-0.14330	0.0671
H112	0.34040	-0.00050	-0.20740	0.0671
H121	0.14340	-0.00850	-0.33040	0.0708
H122	0.06640	0.06950	-0.34910	0.0708

The temperature factor has the form of EXP(-T) where $T = 8\pi^2 U \sin^2(\theta/\lambda)$ for isotropic Atoms

Table **S7c** - (An)isotropic Displacement Parameters for TCO8_280K

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O13	0.0582(5)	0.0567(6)	0.0798(7)	-0.0089(5)	0.0261(5)	-0.0113(5)

C14	0.0469(6)	0.0481(7)	0.0446(6)	0.0005(5)	0.0101(5)	-0.0007(5)
C15	0.0632(8)	0.0691(9)	0.0449(7)	-0.0104(6)	0.0186(6)	-0.0030(7)
C16	0.0614(8)	0.0750(10)	0.0513(7)	-0.0032(7)	0.0316(6)	-0.0023(7)
C17	0.0519(7)	0.0760(10)	0.0613(8)	-0.0041(7)	0.0219(6)	0.0080(7)
C18	0.0554(7)	0.0627(8)	0.0448(7)	0.0091(6)	0.0124(6)	0.0080(6)
C19	0.0659(8)	0.0632(8)	0.0448(7)	-0.0099(6)	0.0175(6)	-0.0057(7)
C20	0.0700(8)	0.0458(7)	0.0578(8)	-0.0064(6)	0.0302(7)	0.0030(6)
C21	0.0558(7)	0.0426(7)	0.0608(8)	0.0039(6)	0.0178(6)	0.0062(5)
S1	0.0566(2)	0.0409(2)	0.0393(2)	0.0022(1)	0.0205(1)	-0.0062(1)
N3	0.0696(7)	0.0617(7)	0.0449(6)	0.0124(5)	0.0182(5)	-0.0114(6)
N4	0.0582(6)	0.0504(6)	0.0571(7)	0.0105(5)	0.0169(5)	-0.0107(5)
C2	0.0515(6)	0.0337(5)	0.0438(6)	0.0013(4)	0.0211(5)	0.0019(5)
S5	0.0520(2)	0.0506(2)	0.0391(2)	-0.0024(1)	0.0186(1)	0.0055(1)
N7	0.0600(7)	0.0606(7)	0.0554(6)	-0.0050(5)	0.0246(5)	0.0107(5)
N8	0.0652(7)	0.0652(7)	0.0419(6)	-0.0058(5)	0.0214(5)	0.0065(6)
C6	0.0550(7)	0.0348(6)	0.0436(6)	-0.0004(5)	0.0223(5)	-0.0016(5)
S9	0.0489(2)	0.0377(2)	0.0514(2)	-0.0033(1)	0.0169(2)	0.0026(1)
N11	0.0618(7)	0.0456(6)	0.0613(7)	0.0031(5)	0.0228(5)	0.0118(5)
N12	0.0629(7)	0.0455(6)	0.0713(8)	-0.0157(5)	0.0288(6)	-0.0044(5)
C10	0.0548(6)	0.0400(6)	0.0394(6)	0.0019(4)	0.0269(5)	0.0027(5)

==========

The temperature factor has the form of EXP(-T) where

$T = 8\pi^2 U \sin^2(\theta/\lambda)$ for isotropic atoms

$T = \sum_{ij} h_i\, h_j\, U_{ij}\, a_i^*\, a_j^*$ for anisotropic atoms.

a_i^* are reciprocal axial lengths and h_i are the reflection indices.

Table **S7d** - Bond Distances (Angstrom) for TCO8_280K

S1	-C2	1.7102(16)	S5	-C6	1.7109(17)
S9	-C10	1.7106(16)	N3	-C2	1.3236(19)
N4	-C2	1.319(2)	C19	-C20	1.520(2)
N7	-C6	1.324(2)	N8	-C6	1.3227(19)
N11	-C10	1.327(2)	N12	-C10	1.315(2)
O13	-C14	1.210(2)	C14	-C15	1.505(2)
C14	-C21	1.506(2)	C15	-C16	1.520(3)
C16	-C17	1.510(2)	C17	-C18	1.525(2)
C18	-C19	1.541(2)	C20	-C21	1.525(2)

Table **S7e** - Bond Angles (Degrees) for TCO8_280K

S1	-C2	-N3	120.96(11)	S1	-C2	-N4	120.26(10)
S5	-C6	-N8	120.59(11)	N7	-C6	-N8	118.74(13)
S5	-C6	-N7	120.67(10)	N11	-C10	-N12	119.03(12)
S9	-C10	-N11	120.43(10)	N3	-C2	-N4	118.78(13)
S9	-C10	-N12	120.54(11)	O13	-C14	-C21	119.79(13)
C15	-C14	-C21	119.13(13)	O13	-C14	-C15	121.07(13)
C14	-C15	-C16	116.12(12)	C15	-C16	-C17	114.66(14)
C16	-C17	-C18	116.50(14)	C17	-C18	-C19	115.88(13)
C18	-C19	-C20	115.11(13)	C19	-C20	-C21	115.73(13)
C14	-C21	-C20	111.93(11)				

Table **S7f** - Torsion Angles (Degrees) for TCO8_280K

O13	-C14	-C21	-C20	75.40(18)	O13	-C14	-C15	-C16	-141.67(15)
C21	-C14	-C15	-C16	39.57(19)	C15	-C14	-C21	-C20	-105.82(15)
C14	-C15	-C16	-C17	68.47(19)	C15	-C16	-C17	-C18	-56.5(2)
C16	-C17	-C18	-C19	-53.7(2)	C17	-C18	-C19	-C20	103.56(16)
C18	-C19	-C20	-C21	-64.15(17)	C19	-C20	-C21	-C14	68.58(17)

Table **S7g** - Contact Distances (Angstrom) for TCO8_280K

S1	.N8	3.457(2)	O13	.C14_c	3.319(3)
S1	.N3_k	3.523(2)	O13	.N4_a	3.035(2)
S1	.N12_j	3.362(2)	S5	.N11_j	3.490(2)

S5	.N3	3.519(3)	S5	.N8_q	3.444(2)
S9	.N7	3.457(2)	S9	.N7_q	3.438(2)
S9	.N4_s	3.522(2)	N3	.S5	3.519(3)
S9	.N4_t	3.532(2)	N3	.S1_l	3.523(2)
S9	.C20_u	3.656(3)	N4	.O13_n	3.035(2)
N4	.S9_i	3.522(2)	N4	.S9_o	3.532(2)
N7	.S9	3.457(2)	N7	.S9_d	3.438(2)
N8	.S1	3.457(2)	N8	.S5_r	3.444(2)
N11	.S5_e	3.490(2)	N12	.S1_v	3.362(2)
N12	.O13_c	3.206(3)	C14	.O13_c	3.319(3)
C14	.C14_c	3.339(3)	C14	.C18	3.017(3)
C18	.C14	3.017(3)	C20	.S9_d	3.656(3)
O13	.N12_b	3.206(3)			

Table **S7h** - Hydrogen Bonds (Angstrom, Deg) for TCO8_280K

N3	-- H31	.. S1	0.8720	2.7612	3.523(2)	146.76	4_554
N3	-- H32	.. S5	0.8729	2.6519	3.519(3)	172.62	.
N4	-- H41	.. O13	0.8720	2.4785	3.035(2)	122.31	2_655
N4	-- H41	.. S9	0.8720	2.8154	3.532(2)	140.45	4_655
N4	-- H42	.. S9	0.8716	2.6643	3.522(2)	168.35	1_656
N7	-- H71	.. S9	0.8714	2.6032	3.438(2)	160.74	4_555
N7	-- H72	.. S9	0.8703	2.5980	3.457(2)	169.48	.
N8	-- H81	.. S1	0.8717	2.5886	3.457(2)	174.58	.
N8	-- H82	.. S5	0.8703	2.6986	3.444(2)	144.42	4_555
N11	-- H111	.. S5	0.8742	2.7192	3.555(2)	160.36	.
N11	-- H112	.. S5	0.8703	2.7545	3.490(2)	143.07	3_655
N12	-- H121	.. S1	0.8718	2.5401	3.362(2)	157.52	3_655
N12	-- H122	.. S1	0.8714	2.7833	3.625(3)	162.83	1_454
C16	-- H161	.. S5	1.000(2)	2.847(2)	3.717(3)	145.89(17)	3_655

Translation of Symmetry Code to Equiv.Pos

a =[2_645.00] = 1-x,-1/2+y,1/2-z
b =[3_555.00] = -x,-y,-z
c =[3_555.00] = -x,-y,-z
d =[4_555.00] = x,1/2-y,1/2+z
e =[3_655.00] = 1-x,-y,-z

```
f =[  3_656.00 ]   = 1-x,-y,1-z
g =[  3_656.00 ]   = 1-x,-y,1-z
h =[  1_455.00 ]   = -1+x,y,z
i =[  1_656.00 ]   = 1+x,y,1+z
l =[  4_554.00 ]   = x,1/2-y,-1/2+z
m =[  1_655.00 ]   = 1+x,y,z
n =[  2_655.00 ]   = 1-x,1/2+y,1/2-z
o =[  4_655.00 ]   = 1+x,1/2-y,1/2+z
s =[  1_454.00 ]   = -1+x,y,-1+z
t =[  4_454.00 ]   = -1+x,1/2-y,-1/2+z
```

Table **S8** - Thiourea cyclooctanone at 120 K

Figure **S8** - Thiourea cyclooctanone at 120 K. Atom numbering and anisotropic displacement parameter.

Table **S8a** - Crystal Data and Details of the Structure Determination for TCO8_120K

Table **S8b** - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for TCO8_120K

Table **S8c** - Hydrogen Atom Positions and Isotropic Displacement Parameters for TCO8_120K

Table **S8d** - (An)isotropic Displacement Parameters for TCO8_120K

Table **S8e** - Bond Distances (Angstrom) for TCO8_120K

Table **S8f** - Bond Angles (Degrees) for TCO8_120K

Table **S8g** - Torsion Angles (Degrees) for TCO8_120K

Table **S8h** - Contact Distances(Angstrom) for TCO8_120K

Table **S8i** - Hydrogen Bonds (Angstrom, Deg) for TCO8_120K

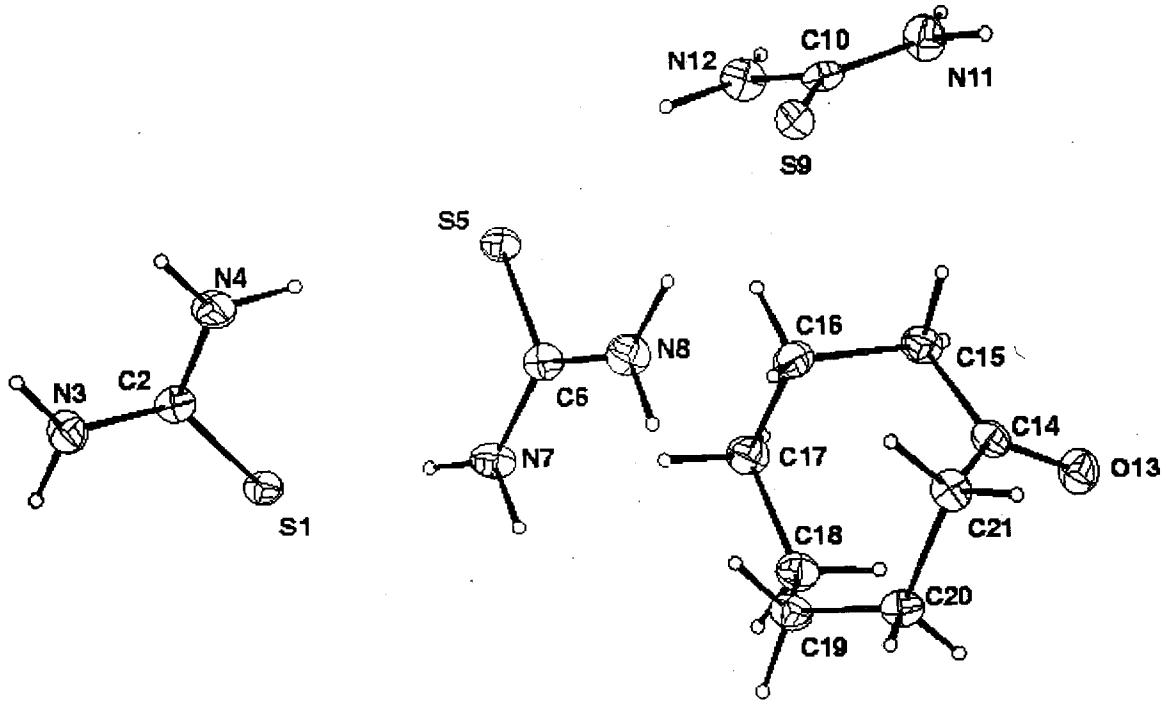

Figure S8 - Thiourea cyclooctanone at 120 K. Atom numbering and anisotropic displacement parameter.

Table **S8a** - Crystal Data and Details of the Structure Determination for TCO8_120K

Crystal Data			
Empirical Formula		C8 H14 O, 3(C H4 N2 S)	
Formula Weight			354.59
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	12.0830(14)	15.518(2)	10.2930(14)
alpha, beta, gamma [deg]	90	111.770(10)	90
V [Ang**3]			1792.3(4)
Z			4
D(obs), D(calc) [g/cm**3]			0.000, 1.314
F(000)			760
Mu(CuKa) [/mm]			3.9
Crystal Size [mm]		0.16 x 0.19 x 0.80	
Data Collection			
Temperature (K)			120
Radiation [Angstrom]		CuKa	1.54180
Theta Min-Max [Deg]			2.2, 74.3
Scan,(Type & Range) [Deg]		0.43 + 0.15 Tan(Theta)	
Dataset		-15: 14 ; -19: 1 ; -1: 12	
Tot., Uniq. Data, R(int)		4718, 3901, 0.050	
Observed data [F > 3.0 sigma(I)]			3798
Refinement			
Nref, Npar			3798, 191
R, wR, S		0.0380, 0.0434, 1.07	
w = Chebychev polynomial with 3 parameters Carruthers & Watkin , 1979		4.11 1.56 2.72	
Max. and Av. Shift/Error			0.67, 0.00
Min. and Max. resd. dens. [e/Ang^3]			-0.42, 0.42

Table **S8b** - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for TCO8_120K

Atom	x	y	z	U(eq) [Ang^2]
O13	0.45573(8)	0.06828(6)	0.34330(10)	0.0276(3)
C14	0.38383(11)	0.01783(8)	0.35763(12)	0.0211(3)
C15	0.30124(12)	0.04371(9)	0.43103(13)	0.0246(3)
C16	0.17468(11)	0.00746(9)	0.36781(13)	0.0241(4)
C17	0.09947(12)	0.04435(9)	0.22495(14)	0.0264(4)
C18	0.15152(11)	0.03486(9)	0.11061(13)	0.0239(3)
C19	0.18500(12)	-0.05782(9)	0.08465(14)	0.0248(3)
C20	0.31832(11)	-0.07715(8)	0.14309(13)	0.0234(3)
C21	0.37877(11)	-0.07365(8)	0.30357(13)	0.0223(3)
S1	-0.35535(3)	-0.14084(2)	0.02520(3)	0.0195(1)
N3	-0.51510(10)	-0.25351(7)	0.03903(12)	0.0254(3)
N4	-0.35286(11)	-0.23630(8)	0.24143(12)	0.0273(3)
C2	-0.41165(11)	-0.21543(8)	0.10765(13)	0.0195(3)
S5	-0.06964(3)	-0.15255(2)	0.41925(3)	0.0204(1)
N7	-0.06670(10)	-0.20747(8)	0.17626(11)	0.0262(3)
N8	0.10320(10)	-0.23339(7)	0.36718(12)	0.0257(3)
C6	-0.00664(12)	-0.20127(8)	0.31330(13)	0.0203(3)
S9	0.28889(3)	-0.19831(2)	0.70665(3)	0.0203(1)
N11	0.36710(10)	-0.04555(7)	0.81761(12)	0.0264(3)
N12	0.16630(10)	-0.05393(7)	0.69218(12)	0.0250(3)
C10	0.27341(11)	-0.09163(8)	0.74089(12)	0.0193(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table **S8c** - Hydrogen Atom Positions and Isotropic Displacement Parameters for TCO8_120K

Atom	x	y	z	U(iso) [Ang^2]
H151	0.33730(12)	0.02460(9)	0.53023(13)	0.0600
H152	0.29475(12)	0.10830(9)	0.42747(13)	0.0600
H161	0.13292(11)	0.01914(9)	0.43401(13)	0.0600
H162	0.18065(11)	-0.05627(9)	0.35715(13)	0.0600
H171	0.08791(12)	0.10742(9)	0.23740(14)	0.0600
H172	0.02027(12)	0.01492(9)	0.19117(14)	0.0600
H181	0.22613(11)	0.07072(9)	0.13868(13)	0.0600
H182	0.09241(11)	0.05792(9)	0.02094(13)	0.0600
H191	0.14536(12)	-0.09844(9)	0.12959(14)	0.0600
H192	0.15284(12)	-0.06839(9)	-0.01897(14)	0.0600
H201	0.33060(11)	-0.13632(8)	0.11078(13)	0.0600
H202	0.35819(11)	-0.03386(8)	0.10276(13)	0.0600
H211	0.46223(11)	-0.09663(8)	0.33330(13)	0.0600
H212	0.33274(11)	-0.11044(8)	0.34626(13)	0.0600
H31	-0.54780	-0.29730	0.08710	0.0600
H32	-0.56210	-0.23820	-0.06100	0.0600
H41	-0.38700	-0.28020	0.28740	0.0600
H42	-0.27540	-0.20780	0.29630	0.0600
H71	-0.02940	-0.23630	0.11530	0.0600
H72	-0.14910	-0.18350	0.13360	0.0600
H81	0.15030	-0.22880	0.46990	0.0600
H82	0.13940	-0.26180	0.30480	0.0600
H111	0.44780	-0.07310	0.85690	0.0600
H112	0.35770	0.01660	0.83770	0.0600
H121	0.15810	0.00840	0.71280	0.0600
H122	0.09420	-0.08780	0.63550	0.0600

The temperature factor has the form of EXP(-*T*) where $T = 8\pi^2 U \sin^2(\theta/\lambda)$ for isotropic Atoms

Table **S8d** - (An)isotropic Displacement Parameters for TCO8_120K

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O13	0.0285(5)	0.0219(5)	0.0329(5)	-0.0031(4)	0.0118(4)	-0.0055(4)

C14	0.0226(6)	0.0193(6)	0.0186(6)	0.0008(5)	0.0044(5)	0.0008(5)
C15	0.0279(6)	0.0255(6)	0.0203(6)	-0.0041(5)	0.0088(5)	-0.0019(5)
C16	0.0263(6)	0.0262(7)	0.0227(6)	-0.0005(5)	0.0126(5)	-0.0011(5)
C17	0.0248(6)	0.0295(7)	0.0247(6)	-0.0010(5)	0.0089(5)	0.0039(5)
C18	0.0262(6)	0.0239(6)	0.0202(6)	0.0032(5)	0.0070(5)	0.0033(5)
C19	0.0290(6)	0.0229(6)	0.0215(6)	-0.0026(5)	0.0082(5)	-0.0019(5)
C20	0.0296(6)	0.0181(6)	0.0239(6)	-0.0013(5)	0.0116(5)	0.0010(5)
C21	0.0246(6)	0.0158(6)	0.0248(6)	0.0015(5)	0.0073(5)	0.0016(5)
S1	0.0256(2)	0.0154(2)	0.0183(2)	0.0010(1)	0.0090(1)	-0.0026(1)
N3	0.0271(5)	0.0212(5)	0.0256(5)	0.0033(4)	0.0071(4)	-0.0047(4)
N4	0.0331(6)	0.0263(6)	0.0212(5)	0.0053(4)	0.0086(4)	-0.0055(5)
C2	0.0255(6)	0.0133(5)	0.0214(6)	-0.0003(4)	0.0105(5)	0.0011(5)
S5	0.0240(2)	0.0192(2)	0.0183(2)	-0.0010(1)	0.0082(1)	0.0020(1)
N7	0.0312(6)	0.0269(6)	0.0208(5)	-0.0023(4)	0.0101(4)	0.0028(5)
N8	0.0275(5)	0.0236(6)	0.0266(5)	-0.0023(4)	0.0109(4)	0.0048(4)
C6	0.0272(6)	0.0129(5)	0.0222(6)	-0.0001(4)	0.0108(5)	-0.0019(4)
S9	0.0230(2)	0.0144(2)	0.0226(2)	-0.0014(1)	0.0075(1)	0.0011(1)
N11	0.0283(6)	0.0194(5)	0.0318(6)	-0.0059(5)	0.0115(5)	-0.0018(4)
N12	0.0279(5)	0.0195(5)	0.0269(6)	0.0014(4)	0.0093(4)	0.0056(4)
C10	0.0268(6)	0.0169(6)	0.0182(5)	0.0014(4)	0.0130(5)	0.0014(5)

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The temperature factor has the form of EXP(-*T*) where

$T = 8\pi^2 U \sin^2(\theta/\lambda)$ for isotropic atoms

$T = \sum_{ij} h_i\, h_j\, U_{ij}\, a_i^*\, a_j^*$ for anisotropic atoms.

a_i^* are reciprocal axial lengths and h_i are the reflection indices.

Table **S8e** - Bond Distances (Angstrom) for TCO8_120K

S1	-C2	1.7178(14)	S5	-C6	1.7193(14)
S9	-C10	1.7171(13)	N3	-C2	1.3250(18)
N4	-C2	1.3342(17)	N7	-C6	1.3290(16)
N8	-C6	1.3310(19)	N11	-C10	1.3241(18)
N12	-C10	1.3369(18)	O13	-C14	1.2184(17)
C14	-C15	1.512(2)	C15	-C16	1.530(2)
C16	-C17	1.5247(19)	C17	-C18	1.533(2)
C18	-C19	1.544(2)	C19	-C20	1.526(2)
C20	-C21	1.5395(18)	C14	-C21	1.5177(18)

Table **S8f** - Bond Angles (Degrees) for TCO8_120K

S1	-C2	-N3	120.35(10)	S1	-C2	-N4	121.11(11)
S5	-C6	-N8	120.53(10)	N7	-C6	-N8	118.86(13)
S5	-C6	-N7	120.60(11)	N11	-C10	-N12	118.81(12)
S9	-C10	-N11	120.59(10)	N3	-C2	-N4	118.54(12)
S9	-C10	-N12	120.59(10)	C15	-C14	-C21	119.16(12)
O13	-C14	-C21	119.35(12)	O13	-C14	-C15	121.47(12)
C14	-C15	-C16	115.50(11)	C15	-C16	-C17	114.61(11)
C16	-C17	-C18	115.90(12)	C17	-C18	-C19	115.51(11)
C18	-C19	-C20	114.90(11)	C19	-C20	-C21	115.31(11)
C14	-C21	-C20	111.40(10)				

Table **S8g** - Torsion Angles (Degrees) for TCO8_120K

O13	-C14	-C21	-C20	-74.98(15)	O13	-C14	-C15	-C16	141.83(13)
C21	-C14	-C15	-C16	-39.56(16)	C15	-C14	-C21	-C20	106.37(13)
C14	-C15	-C16	-C17	-69.03(15)	C15	-C16	-C17	-C18	56.63(16)
C16	-C17	-C18	-C19	54.48(16)	C17	-C18	-C19	-C20	-104.76(14)
C18	-C19	-C20	-C21	64.89(15)	C19	-C20	-C21	-C14	-68.95(15)

Table **S8h** - Contact Distances (Angstrom) for TCO8_120K

S1	.N7	3.4101(14)	S1	.N4_k	3.4974(13)
S1	.N11_j	3.3428(12)	O13	.N3_a	2.9975(15)
S1	.C18_e	3.6440(15)	O13	.C14_c	3.2547(16)

S5	.C16_p	3.6807(15)	O13	.N11_b	3.1750(17)
S5	.N4	3.4791(15)	S5	.N7_q	3.4129(13)
S5	.N12_j	3.4572(12)	S5	.N12	3.5243(13)
S9	.N8_q	3.4114(14)	S9	.N8	3.4241(13)
S9	.C20_u	3.5872(14)	N3	.S9_i	3.4695(13)
S9	.N3_t	3.4894(14)	N3	.S9_n	3.4894(14)
S9	.N3_s	3.4695(13)	N3	.O13_m	2.9975(15)
N4	.S1_o	3.4975(13)	N4	.S5	3.4791(15)
N7	.S1	3.4101(14)	N7	.S5_r	3.4129(13)
N8	.S9	3.4241(13)	N8	.S9_g	3.4114(14)
N11	.S1_v	3.3428(12)	N11	.O13_c	3.1750(17)
N12	.S5	3.5243(13)	N12	.S5_d	3.4572(12)
C14	.O13_c	3.2547(16)	C14	.C18	3.0199(19)
C14	.C14_c	3.2671(18)	C16	.S5_d	3.6807(15)
C18	.S1_f	3.6439(15)	C18	.C14	3.0199(19)
C20	.S9_g	3.5872(14)			

Table **S8i** - Hydrogen Bonds (Angstrom, Deg) for TCO8_120K

D		H		A	D - H	H -- A	D --- A	D H A	Symm(A)
N3	--	H31	..	O13	1.0038	2.3475	2.9975(15)	121.55	2_545
N3	--	H31	..	S9	1.0038	2.6858	3.4894(14)	137.17	4_444
N3	--	H32	..	S9	1.0027	2.4800	3.4695(13)	168.97	1_454
N4	--	H41	..	S1	1.0015	2.6352	3.4975(13)	144.28	4_545
N4	--	H42	..	S5	0.9992	2.4868	3.4791(15)	172.02	.
N7	--	H71	..	S5	1.0034	2.5604	3.4129(13)	142.67	4_544
N7	--	H72	..	S1	0.9991	2.4148	3.4101(14)	174.04	.
N8	--	H81	..	S9	1.0003	2.4371	3.4241(13)	168.91	.
N8	--	H82	..	S9	1.0031	2.4536	3.4114(14)	159.52	4_544
N11	--	H111	..	S1	1.0023	2.5898	3.5614(14)	163.28	1_656
N11	--	H112	..	S1	1.0016	2.3956	3.3428(12)	157.45	3_556
N12	--	H121	..	S5	1.0030	2.6298	3.4572(12)	139.82	3_556
N12	--	H122	..	S5	0.9993	2.5719	3.5243(13)	159.28	.
C16	--	H161	..	S5	1.0034(19)	2.8299(15)	3.6807(15)	142.95(13)	3_556
C20	--	H201	..	S9	1.0061(18)	2.8604(14)	3.5872(14)	129.66(12)	4_544

Translation of Symmetry Code to Equiv.Pos for TCO8_120K

a =[2_555.00]	= -x,1/2+y,1/2-z	i =[1_454.00]	= -1+x,y,-1+z
b =[3_656.00]	= 1-x,-y,1-z	l =[1_455.00]	= -1+x,y,z
c =[3_656.00]	= 1-x,-y,1-z	m =[2_545.00]	= -x,-1/2+y,1/2-z
d =[3_556.00]	= -x,-y,1-z	n =[4_444.00]	= -1+x,-1/2-y,-1/2+z
e =[3_555.00]	= -x,-y,-z	o =[4_545.00]	= x,-1/2-y,1/2+z
f =[3_555.00]	= -x,-y,-z	s =[1_656.00]	= 1+x,y,1+z
g =[4_544.00]	= x,-1/2-y,-1/2+z	t =[4_645.00]	= 1+x,-1/2-y,1/2+z
h =[1_655.00]	= 1+x,y,z		

Powder pattern refinement for the high temperature phase of TCO8

Number of reflections: 22

Final values: (Standard errors on 2nd line)

Zero	Lambda	a	b	c	alpha	beta	gamma
.00716	1.54188	16.4182	16.4182	12.5472	90.00	90.00	120.00
.00372	.00000	.0048	.0048	.0039	.00	.00	.00

Volume: 2929.08 Å^3

H	K	L	2Th(obs)	2Th-Zero	2Th(Calc)	diff.
1	1	0	10.818	10.811	10.777	.033
0	1	2	15.424	15.417	15.438	-.021
2	1	1	18.043	18.036	17.956	.080
2	0	2	18.833	18.826	18.866	-.040
1	2	2	21.789	21.782	21.776	.005
1	1	3	23.877	23.869	23.878	-.009
3	1	2	26.796	26.789	26.701	.087
3	2	1	28.189	28.182	28.269	-.087
1	4	0	28.771	28.763	28.774	-.010
2	2	3	30.613	30.605	30.516	.090
0	2	4	31.140	31.133	31.166	-.033
1	4	3	36.140	36.133	36.043	.090
4	3	1	39.192	39.185	39.204	-.019
3	1	5	42.622	42.615	42.710	-.095
4	4	0	44.193	44.186	44.129	.057
4	3	4	48.571	48.563	48.575	-.011
4	4	3	49.602	49.595	49.472	.123
5	4	1	50.797	50.790	50.670	.120
1	6	4	51.244	51.237	51.218	.019
8	1	1	55.682	55.675	55.721	-.045
1	3	7	56.470	56.462	56.386	.076
5	4	4	58.700	58.693	58.632	.061