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1,3-Benzothiazol-2(3*H*)-one–1,3-benzothiazole-2(3*H*)-thione (1/1)

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Cocrystallization of 2-hydroxybenzothiazole and 2-mercaptobenzothiazole gives the title complex, $C_7H_5NS_2{\cdot}C_7H_5NOS$. The molecules are linked by N—H···S and N—H···O hydrogen bonds, forming discrete molecular pairs.

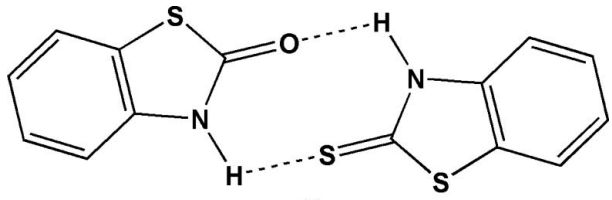
Key indicators

Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.134
Data-to-parameter ratio = 17.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In this paper, we describe the structure of (I), which formed by cocrystallization of 2-hydroxybenzothiazole (HBT) and 2-mercaptobenzothiazole (MBT).



(I)

The molecular structure of (I) is shown in Fig. 1. The values of the geometric parameters are comparable with the reported averages in the literature (Allen *et al.*, 1987). The HBT and MBT molecules are linked into discrete molecular pairs by N—H···O and N—H···S hydrogen bonds (Table 1). Weak π–π interactions between adjacent dimers are observed along the *b* axis (Fig. 2). The centroid-to-centroid distance between the benzene ring of MBT and the thialzole ring of an adjacent HBT molecules is 3.663 (1) Å.

Experimental

A mixture of 2-hydroxybenzothiazole (0.076 g, 0.5 mmol), 2-mercaptobenzothiazole (0.083 g, 0.5 mmol) and ethanol (10 ml) was stirred at 323 K for 1 h. The solution was then filtered and the filtrate was kept in a container. After 3 d, orange crystals of (I) suitable for X-ray analysis were obtained.

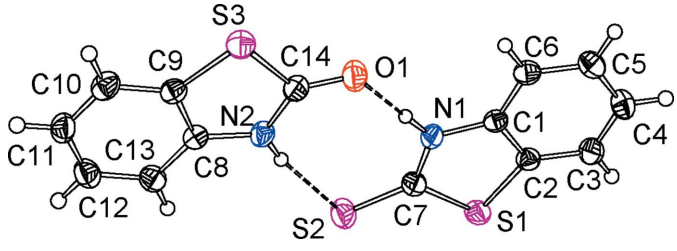


Figure 1
The asymmetric unit of (I), with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

Crystal data

$C_7H_5NS_2{\cdot}C_7H_5NOS$
M_r = 318.42
Monoclinic, $P2_1/c$
a = 12.078 (5) Å
b = 6.793 (3) Å
c = 17.271 (7) Å
β = 96.820 (6)°
V = 1407.1 (10) Å^3
Z = 4
D_x = 1.503 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 130 (2) K
Prism, orange
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.882, T_{max} = 0.925
10515 measured reflections
3206 independent reflections
2512 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.134
S = 1.07
3206 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 0.5291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	1.96	2.809 (3)	167
N2—H2A···S2	0.86	2.54	3.394 (2)	170

All H atoms were placed at calculated positions, and refined with isotropic displacement parameters using a riding model [C—H = 0.93 Å and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N)].

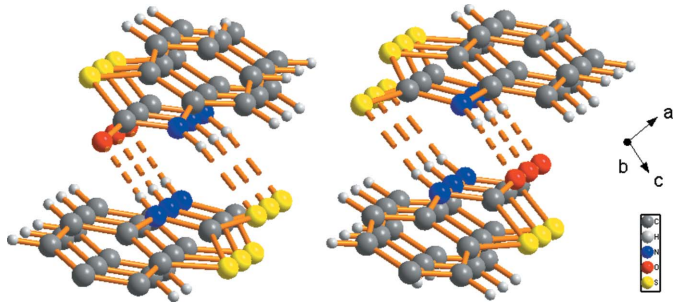


Figure 2
View of the three-dimensional packing. Hydrogen bonds are shown as dashed lines.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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