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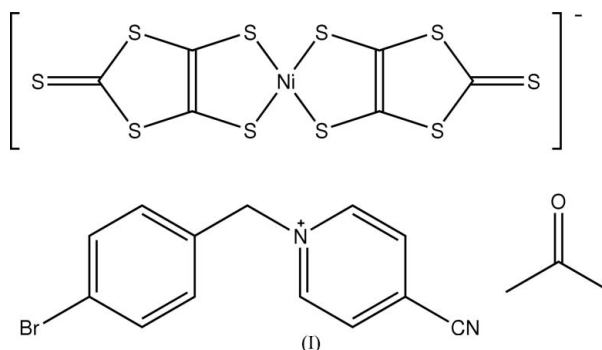
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å  
 $R$  factor = 0.055  
 $wR$  factor = 0.105  
Data-to-parameter ratio = 15.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.***N*-(4-Bromobenzyl)-4-cyanopyridinium bis(2-thioxo-1,3-dithiole-4,5-dithiolato)-nickelate(III) acetone solvate**

The title compound,  $(\text{C}_{13}\text{H}_{10}\text{BrN}_2)[\text{Ni}(\text{C}_3\text{S}_5)_2]\cdot\text{C}_3\text{H}_6\text{O}$ , is a new ionic complex in which the  $\text{Ni}^{\text{III}}$  atom exhibits a square-planar coordination involving four S atoms from two 2-thioxo-1,3-dithiole-4,5-dithiolate (dmit) ligands. In the crystal structure, weak  $\text{S}\cdots\text{S}$  and hydrogen-bonding interactions form a three-dimensional supramolecular network.

## Comment

The syntheses and characterization of bis-dithiolate metal complexes and their analogs have been actively studied for a long time because of their properties and potential applications such as in conducting or magnetic materials and non-linear optics (NLO) (Cassoux, 1999). 2-Thioxo-1,3-dithiole-4,5-dithiolate (dmit) metal complexes are well known as molecular conductors (Akutagawa & Nakamura, 2000).



In order to study the interplay of magnetic properties, the title compound, (I), was synthesized. Its structure is found to comprise three separate components (Fig. 1), namely the  $[\text{Ni}^{\text{III}}(\text{dmit})_2]^-$  anion, the *N*-(4-bromobenzyl)-4-cyanopyridinium cation and an acetone solvent molecule. The  $\text{Ni}^{\text{III}}$  ion adopts square-planar coordination involving four S atoms of two dmit ligands. All three components of the structure stack in columns down the *a* axis (Fig. 2). The columns are stabilized by hydrogen bonding (Table 2) and weak  $\text{S}\cdots\text{N}$  and  $\text{S}\cdots\text{S}$  interactions [ $\text{S}8\cdots\text{N}2 = 3.192(5)$  Å and  $\text{S}7\cdots\text{S}7^i = 3.582(3)$  Å; symmetry code: (i)  $-x + 2, -y + 2, -z + 1$ ], resulting in a three-dimensional supramolecular network structure.

## Experimental

4,5-Bis(thiobenzoyl)-1,3-dithiole-2-thione (812 mg, 2.0 mmol; Wang *et al.*, 1998) was suspended in dry methanol (20 ml) and sodium (92 mg, 4.0 mmol) was added under a nitrogen atmosphere at room temperature to give a bright-red solution.  $\text{NiCl}_2\cdot 6\text{H}_2\text{O}$  (238 mg, 1 mmol) was then added, followed successively by  $\text{I}_2$  (127 mg, 0.5 mmol) and a solution of *N*-(4-bromobenzyl)-4-cyanopyridinium

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bromide (2 mmol, 0.380 g) in methanol at an interval of approximately 20 min. The solution was stirred for a further 30 min and the resulting solid collected by filtration. Single crystals of (I) were obtained by evaporation of a dilute acetone solution over 1–2 weeks at room temperature.

#### Crystal data

$(C_{13}H_{10}BrN_2)[Ni(C_3S_5)_2] \cdot C_3H_6O$	$V = 1505.3 (7) \text{ \AA}^3$
$M_r = 783.66$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.729 \text{ Mg m}^{-3}$
$a = 9.197 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.601 (3) \text{ \AA}$	$\mu = 2.69 \text{ mm}^{-1}$
$c = 15.714 (4) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 98.265 (5)^\circ$	Needle, black
$\beta = 92.767 (4)^\circ$	$0.3 \times 0.1 \times 0.1 \text{ mm}$
$\gamma = 95.821 (5)^\circ$	

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer	7546 measured reflections
$\varphi$ and $\omega$ scans	5213 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	2680 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.739$ , $T_{\max} = 0.760$	$R_{\text{int}} = 0.063$
	$\theta_{\max} = 25.0^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 0.04P]$
$R[F^2 > 2\sigma(F^2)] = 0.055$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 0.99$	$\Delta\rho_{\max} = 0.55 \text{ e \AA}^{-3}$
5213 reflections	$\Delta\rho_{\min} = -0.49 \text{ e \AA}^{-3}$
330 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ni1—S7	2.1545 (16)	Ni1—S4	2.1605 (16)
Ni1—S5	2.1547 (16)	Ni1—S6	2.1649 (16)
S7—Ni1—S5	86.20 (6)	S7—Ni1—S6	92.71 (6)
S7—Ni1—S4	178.59 (6)	S5—Ni1—S6	177.58 (7)
S5—Ni1—S4	93.18 (6)	S4—Ni1—S6	87.96 (6)

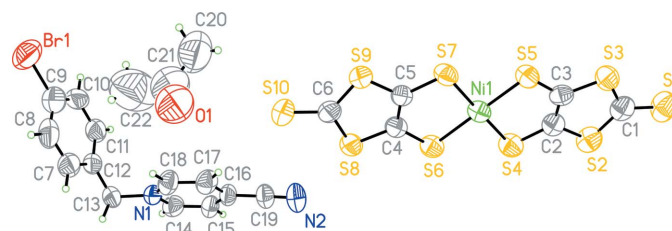
**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C15—H15 $\cdots$ N2 <sup>i</sup>	0.93	2.50	3.290 (8)	143
C14—H14 $\cdots$ O1 <sup>ii</sup>	0.93	2.55	3.135 (8)	121
C13—H13B $\cdots$ O1 <sup>ii</sup>	0.97	2.46	3.230 (9)	136

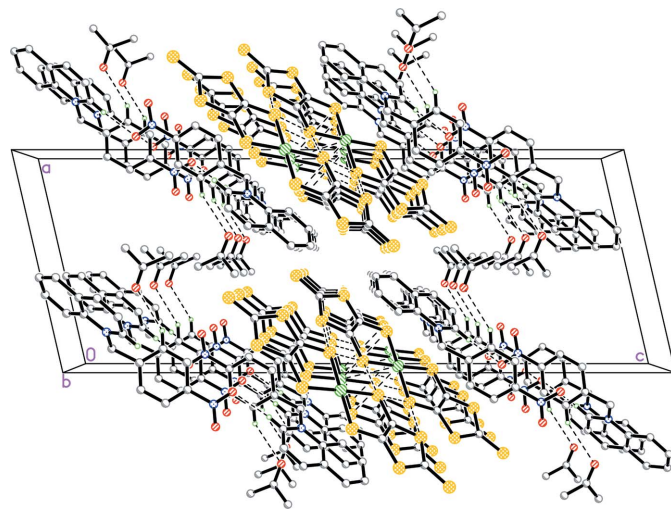
Symmetry codes: (i)  $-x, -y + 1, -z + 1$ ; (ii)  $x - 1, y, z$ .

All H atoms were refined using a riding model, with  $C-H = 0.93 \text{ \AA}$  and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$  for aromatic H atoms,  $C-H = 0.97 \text{ \AA}$  and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$  for  $\text{CH}_2$  H atoms, and  $C-H = 0.96 \text{ \AA}$  and  $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$  for methyl H atoms.



**Figure 1**

The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.



**Figure 2**

The packing of (I), viewed along the  $b$  axis. Hydrogen atoms not involved in hydrogen bonds have been omitted for clarity. Dashed lines indicate hydrogen-bonding and weak  $S \cdots S$  and  $S \cdots N$  interactions.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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