

The N–Ni–N bond angles are in the range 86.11 (6)–93.89 (6)°, close to 90°. The Ni–N(azide) bond lengths are 2.1112 (17) Å, similar to the Ni–N(triazole) bond lengths, compared with the Ni–N(azide) bond lengths of 2.100 (3) and 2.108 (3) Å in the monodentate coordination azide complex $[\text{Ni}(\text{N}_3)_2(\text{bte})_2]_n$ (Zhu *et al.*, 2006). The azide ligand is almost linear [bond angle N7–N8–N9 = 177.2 (3)°], in good agreement with the results usually obtained for monodentate azide complexes. The Ni1–N7–N8 bond angle is 129.58 (14)°.

Because the methyl C atom of bbtz can rotate freely to adjust itself to the coordination environment, bbtz can exhibit *trans-gauche* and *gauche-gauche* conformations (Li *et al.*, 2005). The bbtz ligands of (I) exhibit the *trans-gauche* conformation, similar to the free bbtz molecule (Peng *et al.*, 2004). The three rings (two triazole rings and one benzene ring) of one bbtz ligand are not coplanar. The dihedral angle between the two triazole planes is 63.70 (9)° in (I), but 0° in free bbtz due to symmetry. The dihedral angles between the benzene ring plane and the N1–N3/C9/C10 and N4–N6/C11/C12 triazole planes in (I) are 66.46 (9) and 66.10 (7)°, respectively, compared with 77.81 (9)° in free bbtz (Peng *et al.*, 2004).

As illustrated in Fig. 2, each bbtz ligand in (I) coordinates to Ni^{II} atoms through its two 4-position triazole N atoms, thus acting as a bridging bidentate ligand to form a two-dimensional neutral (4,4)-network. The networks contain nearly square grids (52-membered rings), with an Ni^{II} atom at each corner and a bbtz ligand at each edge connecting two Ni^{II} atoms. As a consequence of the crystal structure symmetry, the edge lengths are equal, with a value of 14.3646 (15) Å. The diagonal lengths of the nearly square grid are 20.542 (2) and 20.084 (2) Å, and the angles of the square are 88.7 (1) and 91.3 (1)°.

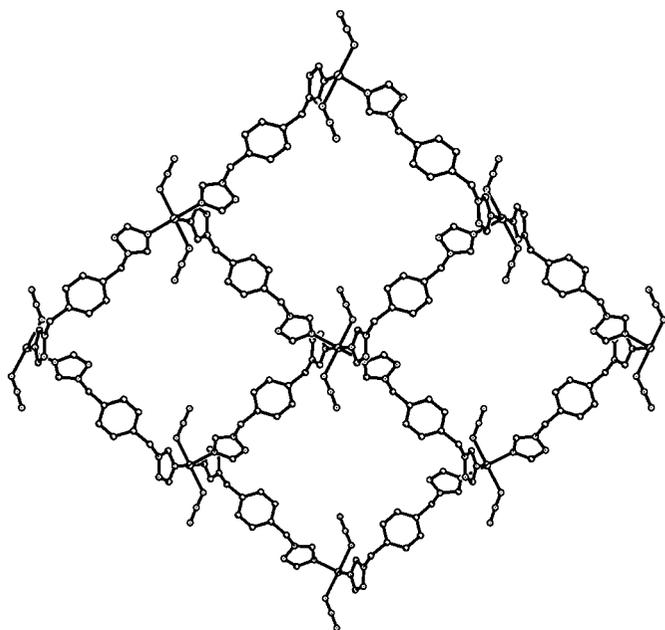


Figure 2
A view of the two-dimensional (4,4)-network of (I) along the *c* direction.

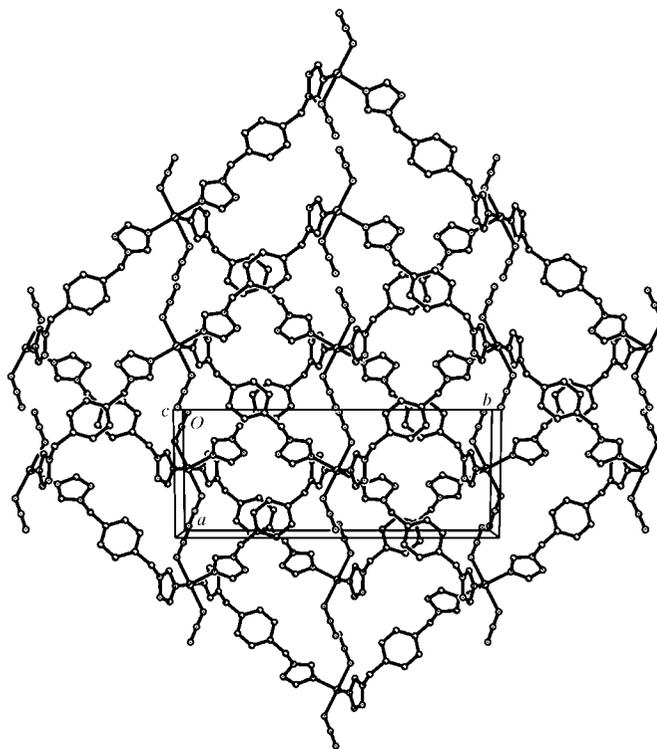


Figure 3
The cell packing of (I).

The nearly square grid sheets are stacked in an offset fashion parallel to the *c* direction. The offset half-cell superpositions of each pair of adjacent networks divide the voids into smaller rectangles whereby the azide anions of one sheet project into the holes of the next sheet. In the superposition structure, the sheets are arranged in an ...*A–B–A–B*... sequence (Fig. 3).

Complex (I) has a two-dimensional (4,4)-network, while $[\text{Ni}(\text{NCO})_2(\text{bte})_2]_n$ and $[\text{Ni}(\text{N}_3)_2(\text{bte})_2]_n$ (Zhu *et al.*, 2006) form one-dimensional double chains. The reason may be that bte is more flexible than bbtz.

Experimental

A H₂O–MeOH solution (20 ml, 1:1 *v/v*) of Ni(NO₃)₂·6H₂O (0.145 g, 0.50 mmol) was added to one leg of a H-shaped tube, and a H₂O–MeOH solution (20 ml, 1:1 *v/v*) of bbtz (0.240 g, 1.00 mmol) and NaN₃ (0.065 g, 1.00 mmol) was added to the other leg of the tube. After several weeks, well shaped blue single crystals of (I) were obtained. Analysis found: C 46.21, H 3.83, N 40.38%; calculated for C₂₄H₂₄N₁₈Ni: C 46.25, H 3.88, N 40.46%.

Crystal data

$[\text{Ni}(\text{N}_3)_2(\text{C}_{12}\text{H}_{12}\text{N}_6)_2]$	$V = 1378.3 (4) \text{ \AA}^3$
$M_r = 623.32$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.2566 (14) \text{ \AA}$	$\mu = 0.76 \text{ mm}^{-1}$
$b = 20.542 (3) \text{ \AA}$	$T = 193 (2) \text{ K}$
$c = 8.3351 (14) \text{ \AA}$	$0.40 \times 0.30 \times 0.18 \text{ mm}$
$\beta = 102.850 (4)^\circ$	

Data collection

Rigaku Mercury CCD area-detector diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\min} = 0.752$, $T_{\max} = 0.876$

15202 measured reflections
3157 independent reflections
2850 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.102$
 $S = 1.08$
3157 reflections

196 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.44 \text{ e } \text{\AA}^{-3}$

Table 1

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

Ni1—N6 ⁱ	2.1012 (16)	Ni1—N3	2.1162 (16)
Ni1—N7	2.1112 (17)		
N6 ⁱ —Ni1—N7	88.23 (6)	N8—N7—Ni1	129.58 (14)
N6 ⁱ —Ni1—N3	88.09 (6)	N9—N8—N7	177.2 (3)
N7—Ni1—N3	86.11 (6)		

Symmetry code: (i) $x + 1, -y + \frac{3}{2}, z - \frac{1}{2}$.

H atoms were placed in idealized positions and refined as riding, with C—H distances of 0.95 (triazole and benzene) and 0.99 \AA (methyl), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV3092). Services for accessing these data are described at the back of the journal.

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