in molecular properties. No experimental evidence for the energy barrier in $Ru(C_5H_5)_2$ seems to be available, but a theoretical study by Carter & Murrell (1980) indicates that the stabilization of the eclipsed orientation is about 2 kJ mol^{-1} greater than in $Fe(C_5H_5)_2$.

This kind of dependence of crystal structure on the preferred orientation and energy barrier of the free molecules is strongly supported by recent lattice-energy calculations by Brock (1981). For a crystal built from metallocene molecules with free rotation of the rings but with variable metal–C distances and atomic charges, the monoclinic structure with centrosymmetric molecules is more stable than the orthorhombic one with eclipsed molecules by several kJ mol^{-1} for all reasonable values of the parameters. Any observed energetic preference for the orthorhombic structure would then have to be attributed to an intrinsic preference of the free molecules for the eclipsed orientation.

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Clathrate Inclusion Compounds of Bis(isothiocyanato)-tetrakis(4-methylpyridine)nickel(II).

V.* Bis(isothiocyanato)tetrakis(4-methylpyridine)nickel(II)–Naphthalene (1:2)

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Abstract

The structure of $[Ni(C_6H_7N)_4(NCS)_2].2C_{10}H_8$ has been determined by X-ray diffraction and refined to $R = 0.065$ for 4402 observed reflections. A layer-type packing of host Ni(4-methylpyridine)$_4$(NCS)$_2$ molecules occurs. Three symmetrically independent guest naphthalene molecules occupy cavities between these layers. Crystal data: $C_{26}H_{28}N_6NiS_2.2C_{10}H_8$, $M_r = 803.7$, is monoclinic, space group $C2/c$, with $a = 16.266$ (14), $b = 16.456$ (15), $c = 31.929$ (11) Å, $\beta = 89.26$ (8)°, $U = 8545$ Å^3, $D_c = 1.249$ Mg m^{-3}, $Z = 8$, $F(000) = 3376$, μ(Cu $K\alpha$) = 1.74 mm^{-1}.

Introduction

Ni(4-MePy)$_4$(NCS)$_2$† clathrates with isomeric 2- or 1-methylnaphthalenes as guest components (Lipkowski, Sgarabotto & Andreetti, 1980, 1982) crystallize with layer-type molecular packing. Substitution of the guest with a smaller molecule, like

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* Part IV: Lipkowski & Andreetti (1982).

† 4-MePy = 4-methylpyridine (MeC$_5$H$_4$N).

o-xylene, leads to a disordered arrangement of the guest in the clathrate (Lipkowski & Andreetti, 1982). The naphthalene molecule is a little smaller than the methylnaphthalenes, and is symmetrical. Preliminary observations have suggested that the structure of Ni(4-MePy)$_4$(NCS)$_2$.2(naphthalene) is significantly different from those studied previously; even the visible spectrum of the crystalline phase is shifted significantly towards higher frequencies (Guarino, Occhiucci, Possagno & Bassanelli, 1977).

Experimental

Single crystals were synthesized by mixing equal amounts of methanolic solutions of Ni(4-MePy)$_4$(NCS)$_2$ saturated at 313K and naphthalene (2M) and cooling the mixture down to room temperature.

Preliminary cell parameters and space-group information were obtained from Weissenberg photographs. A crystal 0·3 × 0·3 × 0·15 mm was mounted along [110] inside a Lindemann-glass capillary tube together with a small amount of the mother liquor. The crystal seemed to be triclinic and 8243 independent reflections were measured ($\theta \leq 55°$) on a computer-controlled Siemens AED diffractometer (Cu $K\alpha$ radiation). The ω–2θ and five-points techniques (Hoppe, 1969) were used. 6563 unique reflections having $I \geq 2\sigma(I)$ were used in the structure determination. The structure was solved from three-dimensional Patterson and electron-density syntheses using SHELX (Sheldrick, 1975). Blocked full-matrix least-squares refinement of the non-H atoms with isotropic thermal parameters led to $R = 0·107$. At this stage the non-H atoms were assigned anisotropic thermal parameters and H atoms were included 'riding' on their C atoms in calculated positions (C–H = 1·08 Å). For the methyl groups regular tetrahedral geometry was assumed, the groups being refined as rigid moieties. At the end of the refinement, monoclinic symmetry, space group $C2/c$ was deduced. The final refinement was carried out in this space group (cell transformation matrix: 101/101/010), the number of unique observed reflections being 4402 and the consistency index* of the intensity data being 0·056. The final R was 0·065 ($R_w = 0·060$). The site occupation factors for the guest naphthalene molecules were 1·00 (1) (molecule A), 1·02 (1) (molecule B) and 1·02 (1) (molecule C). The weighting

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* The consistency index is defined as:

$$R = \sqrt{\frac{\sum N \sum (F_{mean} - F)^2}{\sum (N-1).\sum F^2}}$$

where the inner summations are over the N equivalent reflections averaged to give F_{mean} and the outer summations are over all unique reflections.

Table 1. *Final fractional atomic coordinates* ($\times 10^5$ *for* Ni *and* S; $\times 10^4$ *for* N *and* C) *and equivalent isotropic temperature factors* (*Hamilton*, 1959) *with e.s.d.'s in parentheses*

	x	y	z	B_{eq} (Å^2)
Ni	27706 (4)	10812 (4)	62572 (2)	4·67 (4)
N(1)	2847 (2)	1154 (2)	5612 (1)	5·4 (2)
N(2)	2683 (2)	1004 (2)	6908 (1)	4·5 (2)
N(3)	2300 (2)	−123 (2)	6201 (1)	4·7 (2)
N(4)	3988 (2)	627 (2)	6272 (1)	4·8 (2)
N(5)	3244 (2)	2282 (2)	6311 (1)	4·8 (2)
N(6)	1567 (2)	1567 (2)	6249 (1)	4·9 (2)
S(1)	26723 (12)	10302 (11)	47540 (4)	10·3 (1)
S(2)	25009 (8)	11103 (8)	77741 (3)	6·8 (1)
C(1)	2769 (2)	1105 (2)	5261 (1)	5·0 (2)
C(2)	2609 (2)	1046 (2)	7262 (1)	4·3 (2)
C(3)	1776 (3)	−339 (3)	5898 (1)	5·4 (2)
C(4)	1464 (3)	−1103 (3)	5852 (1)	6·1 (3)
C(5)	1681 (3)	−1710 (3)	6134 (2)	6·0 (3)
C(6)	2228 (3)	−1490 (3)	6448 (1)	5·8 (2)
C(7)	2512 (3)	−707 (3)	6471 (1)	4·9 (2)
C(8)	1365 (4)	−2579 (3)	6105 (2)	8·9 (3)
C(9)	4298 (3)	131 (3)	5974 (1)	5·3 (2)
C(10)	5097 (3)	−122 (3)	5957 (1)	5·5 (2)
C(11)	5637 (3)	128 (3)	6262 (1)	5·5 (2)
C(12)	5321 (3)	650 (3)	6567 (1)	5·5 (2)
C(13)	4521 (3)	880 (3)	6563 (1)	5·1 (2)
C(14)	6523 (3)	−142 (4)	6263 (2)	8·9 (4)
C(15)	3813 (3)	2562 (3)	6046 (1)	5·8 (2)
C(16)	4117 (3)	3337 (3)	6059 (1)	6·6 (3)
C(17)	3823 (3)	3882 (3)	6359 (1)	6·1 (2)
C(18)	3236 (3)	3583 (3)	6630 (1)	5·8 (2)
C(19)	2956 (3)	2803 (3)	6602 (1)	5·3 (2)
C(20)	4152 (4)	4739 (3)	6389 (2)	9·8 (4)
C(21)	1393 (3)	2225 (3)	6017 (1)	5·2 (2)
C(22)	649 (3)	2619 (3)	6043 (1)	5·9 (3)
C(23)	30 (3)	2328 (3)	6308 (1)	5·8 (2)
C(24)	216 (3)	1641 (3)	6539 (1)	5·7 (2)
C(25)	976 (3)	1279 (3)	6504 (1)	5·1 (2)
C(26)	−783 (3)	2756 (4)	6351 (2)	8·6 (3)

Guest naphthalene

Molecule A

	x	y	z	B_{eq} (Å^2)
C(27)	5760 (3)	−2255 (3)	7496 (1)	6·2 (3)
C(28)	6482 (3)	−1830 (4)	7496 (1)	7·0 (3)
C(29)	6479 (3)	−983 (4)	7493 (1)	6·9 (3)
C(30)	5770 (4)	−571 (3)	7496 (1)	6·6 (3)
C(31)	5000	−990 (4)	7500	5·2 (4)
C(32)	5000	−1838 (4)	7500	4·9 (4)

Molecule B

	x	y	z	B_{eq} (Å^2)
C(33)	5844 (3)	−2910 (4)	2397 (1)	7·4 (3)
C(34)	5420 (3)	−2211 (3)	2451 (1)	7·5 (3)
C(35)	4152 (3)	−4434 (4)	2602 (1)	7·2 (3)
C(36)	4584 (3)	−5129 (3)	2547 (1)	7·4 (3)
C(37)	5414 (2)	−3666 (3)	2450 (1)	5·2 (2)

Molecule C

	x	y	z	B_{eq} (Å^2)
C(38)	3753 (7)	3475 (7)	338 (2)	14·8 (8)
C(39)	4433 (13)	4136 (7)	318 (3)	20·1 (13)
C(40)	5112 (11)	3742 (7)	172 (3)	17·5 (12)
C(41)	5394 (7)	2945 (11)	27 (2)	17·8 (10)
C(42)	4965 (6)	1587 (8)	−69 (2)	11·3 (6)
C(43)	4304 (7)	1109 (6)	−27 (2)	11·2 (5)
C(44)	3560 (8)	1321 (7)	113 (3)	13·1 (7)
C(45)	3394 (5)	2053 (7)	229 (2)	11·0 (5)
C(46)	3993 (5)	2662 (5)	207 (2)	8·3 (4)
C(47)	4777 (6)	2490 (8)	66 (2)	10·6 (7)

scheme used was $w = 1/[\sigma^2(F) + 0.003\,F^2]$. Atomic parameters are listed in Table 1.*

Results and discussion

Molecular structure

The geometry of the host Ni(4-MePy)$_4$(NCS)$_2$ and guest naphthalene molecules is shown in Figs. 1 and 2. Structural parameters are listed in Tables 2 and 3.

The Ni(4-MePy)$_4$(NCS)$_2$ molecule is asymmetric and its conformation is similar to that found in the 1-methylnaphthalene (1-MeN) clathrate (Lipkowski, Sgarabotto & Andreetti, 1982). A significant conformational difference, however, occurs in the SCN–Ni–NCS subunit. In the present structure the two isothiocyanate groups are *trans*, whereas in the 1-MeN clathrate the S(1)–N(1)–N(2)–C(2) torsion angle is about 140°. The Ni has distorted octahedral coor-

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and temperature factors, details of rigid-body-motion analysis, and intermolecular contact distances have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36675 (36 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
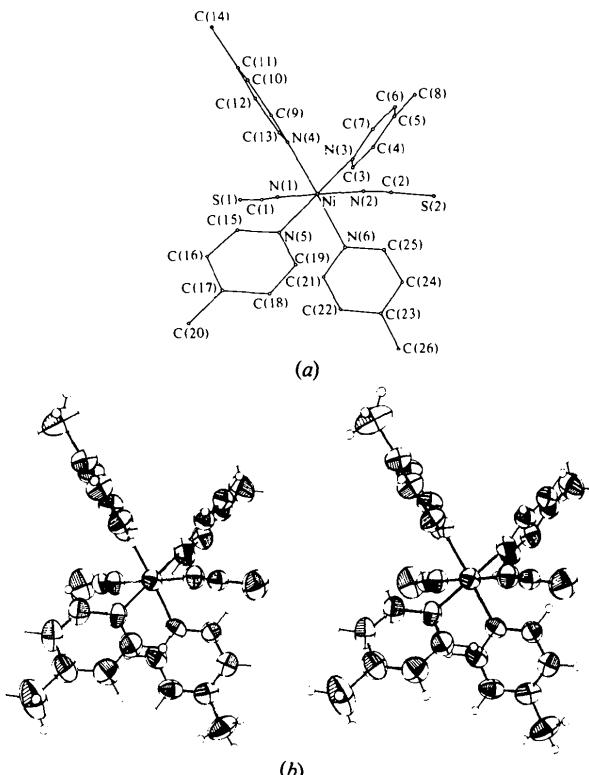
Fig. 1. The Ni(4-MePy)$_4$(NCS)$_2$ host molecule: (a) atom numbering, and (b) ORTEP (Johnson, 1965) stereoview. Ellipsoids of 50% probability are used for non-H atoms; the H atoms are indicated by spheres of 0.1 Å radius.
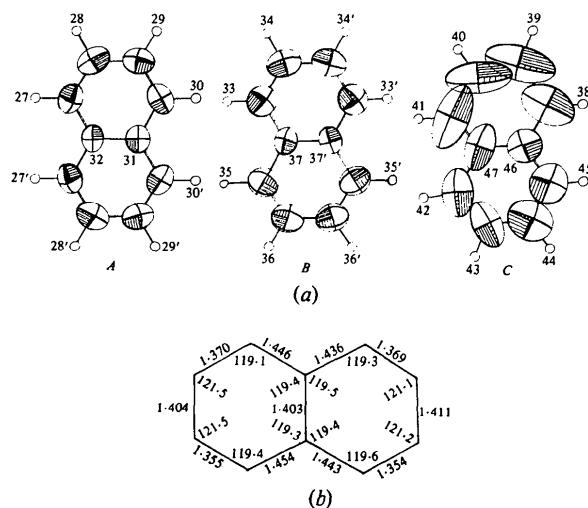
Fig. 2. (a) ORTEP plots of the three independent guest naphthalene molecules. Ellipsoids of 50% probability are used for C atoms. H atoms are represented by circles of 0.1 Å radius. Numbers shown denote the numbering of the C and H atoms. (b) Averaged geometry of molecules A and B (distances in Å, angles in °).

dination of the six N atoms. The mean Ni–N$_{4\text{-MePy}}$ distance is 2.124 (3) Å and is shorter than the corresponding value of 2.136 (4) Å in the 1-MeN clathrate. If this difference is significant it may be related to the spectral difference in the visible region between the two clathrate structures. The naphthalene clathrate has the $^3A_{2g} \rightarrow {}^3T_{1g}$ band shifted to higher frequencies (Guarino et al., 1977) which could be interpreted in terms of ligand–field influence over the central Ni atom.

The orientation of the 4-MePy ligands around the Ni–N bonds corresponds well with the minimum of the intramolecular van der Waals interaction energy (Lipkowski, 1981).

The guest naphthalene molecules are arranged in a very interesting way. Molecules A and B have twofold axial symmetry. The symmetry axis runs along the long axis of molecule B, but is perpendicular to that in molecule A. The averaged geometry of molecules A and B (Fig. 2b) does not differ significantly from that of perdeuteronaphthalene (Pawley & Yeats, 1969) or naphthalene itself [low-temperature study by Ponomarev, Filipenko & Atovmyan (1976)].

Packing

Discrete molecules of Ni(4-MePy)$_4$(NCS)$_2$ form layers perpendicular to c. Two different patterns formed by the guest molecules occur. At $z = \frac{1}{4}$ and $\frac{3}{4}$ symmetric and well ordered guest molecules A and B are arranged alternately parallel and perpendicular to the twofold axis. However, at $z = 0$ and $\frac{1}{2}$ guest molecules C are arranged in centrosymmetric pairs but, as seen in Fig. 3, show significant disordering.

Table 2. *Bond distances (Å), angles (°) and selected torsion angles (°) with e.s.d.'s in parentheses*

Values in square brackets are corrected for libration (Schomaker & Trueblood, 1968)

Host Ni(4-MePy)$_4$(NCS)$_2$

Ni—N(1)	2·065 (3)	Ni—N(2)	2·086 (4)
N(1)—C(1)	1·132 (6)	N(2)—C(2)	1·137 (6)
C(1)—S(1)	1·633 (5)	C(2)—S(2)	1·645 (4)

Ni—N(1)—C(1)	167·7 (3)	Ni—N(2)—C(2)	172·7 (3)

Ni—N(3)	2·133 (3)	Ni—N(4)	2·117 (3)
N(3)—C(3)	1·345 (5) [1·360]	N(4)—C(9)	1·347 (5) [1·362]
N(3)—C(7)	1·339 (5) [1·353]	N(4)—C(13)	1·345 (5) [1·360]
C(3)—C(4)	1·364 (7) [1·375]	C(9)—C(10)	1·365 (6) [1·377]
C(4)—C(5)	1·393 (7) [1·408]	C(10)—C(11)	1·382 (6) [1·398]
C(5)—C(6)	1·397 (7) [1·412]	C(11)—C(12)	1·392 (6) [1·408]
C(5)—C(8)	1·523 (7) [1·534]	C(11)—C(14)	1·508 (7) [1·521]
C(6)—C(7)	1·371 (7) [1·381]	C(12)—C(13)	1·355 (6) [1·367]

Ni—N(5)	2·129 (3)	Ni—N(6)	2·116 (3)
N(5)—C(15)	1·328 (5) [1·348]	N(6)—C(21)	1·344 (5) [1·358]
N(5)—C(19)	1·344 (5) [1·364]	N(6)—C(25)	1·338 (5) [1·350]
C(15)—C(16)	1·369 (5) [1·381]	C(21)—C(22)	1·374 (7) [1·385]
C(16)—C(17)	1·392 (7) [1·413]	C(22)—C(23)	1·392 (7) [1·404]
C(17)—C(18)	1·372 (7) [1·392]	C(23)—C(24)	1·385 (7) [1·400]
C(17)—C(20)	1·512 (7) [1·526]	C(23)—C(26)	1·503 (7) [1·514]
C(18)—C(19)	1·365 (6) [1·378]	C(24)—C(25)	1·376 (6) [1·386]

N(1)—Ni—N(3)	89·3 (1)	N(1)—Ni—N(4)	90·0 (1)
N(1)—Ni—N(5)	90·6 (1)	N(1)—Ni—N(6)	90·5 (1)

N(3)—C(3)—C(4)	124·1 (4)	N(4)—C(9)—C(10)	124·1 (4)
C(3)—C(4)—C(5)	120·0 (4)	C(9)—C(10)—C(11)	119·6 (4)
C(4)—C(5)—C(6)	116·6 (4)	C(10)—C(11)—C(12)	116·4 (4)
C(5)—C(6)—C(7)	120·0 (4)	C(11)—C(12)—C(13)	120·8 (4)
C(6)—C(7)—N(3)	123·4 (4)	C(12)—C(13)—N(4)	123·2 (4)
C(7)—N(3)—C(3)	116·4 (4)	C(13)—N(4)—C(9)	115·9 (3)
C(4)—C(5)—C(8)	123·1 (5)	C(10)—C(11)—C(14)	122·0 (4)

N(5)—C(15)—C(16)	123·6 (4)	N(6)—C(21)—C(22)	122·6 (4)
C(15)—C(16)—C(17)	120·0 (4)	C(21)—C(22)—C(23)	120·3 (4)
C(16)—C(17)—C(18)	115·7 (4)	C(22)—C(23)—C(24)	116·3 (4)
C(17)—C(18)—C(19)	121·7 (4)	C(23)—C(24)—C(25)	120·8 (4)
C(18)—C(19)—N(5)	122·1 (4)	C(24)—C(25)—N(6)	122·3 (4)
C(19)—N(5)—C(15)	116·9 (4)	C(25)—N(6)—C(21)	117·8 (4)
C(16)—C(17)—C(20)	121·7 (4)	C(22)—C(23)—C(26)	121·5 (4)

N(1)—Ni—N(3)—C(3)	−38 (1)	N(1)—Ni—N(4)—C(9)	−35 (1)
N(1)—Ni—N(5)—C(15)	−36 (1)	N(1)—Ni—N(6)—C(21)	−47 (1)
C(1)—N(1)—Ni—N(3)	32 (1)	C(2)—N(2)—Ni—N(3)	−142 (1)

Guest naphthalene

Molecule *A*

C(27)—C(28)	1·367 (8) [1·377]	C(30)—C(31)	1·430 (6) [1·440]
C(28)—C(29)	1·394 (10) [1·410]	C(31)—C(32)	1·395 (9) [1·411]
C(29)—C(30)	1·338 (8) [1·348]	C(32)—C(27)	1·414 (6) [1·425]

C(27)—C(28)—C(29)	120·6 (5)	C(30)—C(31)—C(32)	118·8 (3)
C(28)—C(29)—C(30)	120·7 (5)	C(31)—C(32)—C(27)	119·0 (3)
C(29)—C(30)—C(31)	120·7 (5)	C(32)—C(27)—C(28)	120·2 (5)

Molecule *B*

C(33)—C(34)	1·351 (8) [1·360]	C(35)—C(37)	1·456 (8) [1·467]
C(34)—C(34)	1·398 (9) [1·412]	C(35)—C(36)	1·353 (8) [1·362]
C(33)—C(37)	1·436 (7) [1·446]	C(36)—C(36)	1·382 (10) [1·397]
C(37)—C(37)	1·380 (8) [1·395]		

C(33)—C(34)—C(34)	121·6 (4)	C(33)—C(37)—C(35)	120·3 (4)
C(34)—C(33)—C(37)	118·4 (5)	C(37)—C(35)—C(36)	118·0 (6)
C(33)—C(37)—C(37)	120·0 (5)	C(35)—C(36)—C(36)	122·3 (6)

Molecule *C*

C(38)—C(39)	1·552 (21) [1·586]	C(42)—C(43)	1·338 (15) [1·367]
C(38)—C(46)	1·454 (20) [1·480]	C(43)—C(44)	1·331 (17) [1·361]
C(39)—C(40)	1·358 (24) [1·388]	C(44)—C(45)	1·288 (16) [1·315]
C(40)—C(41)	1·463 (21) [1·493]	C(45)—C(46)	1·399 (14) [1·429]
C(41)—C(47)	1·257 (17) [1·285]	C(46)—C(47)	1·376 (12) [1·407]
C(47)—C(42)	1·576 (17) [1·609]		

C(38)—C(39)—C(40)	104·8 (1·0)	C(42)—C(43)—C(44)	127·3 (1·0)
C(39)—C(40)—C(41)	141·9 (1·4)	C(43)—C(44)—C(45)	121·9 (1·1)
C(40)—C(41)—C(47)	104·8 (1·1)	C(44)—C(45)—C(46)	120·8 (0·9)
C(41)—C(47)—C(46)	130·2 (1·2)	C(45)—C(46)—C(47)	120·7 (0·9)
C(47)—C(46)—C(38)	121·9 (0·9)	C(46)—C(47)—C(42)	117·3 (0·9)
C(46)—C(38)—C(39)	116·4 (1·0)	C(47)—C(42)—C(43)	112·0 (0·8)

Table 3. *Selected least-squares planes and atomic deviations (Å)*

(I) $-0·7523X - 1·1596Y + 31·7936Z = 19·5623$

N(3)	−0·006 (3)	N(5)	−0·006 (3)
N(4)	0·006 (3)	N(6)	0·006 (3)
Ni*	−0·003 (1)		

(II) $15·1407X - 5·9989Y + 1·2221Z = 4·3091$

N(1)	−0·005 (3)	N(3)	0·005 (3)
N(2)	−0·005 (3)	N(5)	0·005 (3)
Ni*	0·003 (1)		

(III) $5·9094X + 15·2830Y + 2·5168Z = 4·8760$

N(1)	−0·018 (3)	N(4)	0·018 (3)
N(2)	−0·018 (3)	N(6)	0·018 (3)
Ni*	−0·012 (1)		

(IV) $-12·4720X + 4·0456Y + 18·6162Z = 8·6260$

N(3)	0·000 (3)	C(6)	−0·004 (3)
C(3)	0·002 (3)	C(7)	0·002 (3)
C(4)	−0·004 (3)	C(8)*	−0·007 (5)
C(5)	0·005 (4)	Ni*	0·004 (1)

(V) $3·8133X + 13·0198Y - 17·9370Z = -8·9071$

N(4)	−0·006 (3)	C(12)	0·003 (3)
C(9)	0·001 (3)	C(13)	0·005 (3)
C(10)	0·007 (3)	C(14)*	−0·024 (5)
C(11)	−0·009 (3)	Ni*	0·148 (1)

(VI) $11·7511X - 4·8862Y + 20·2340Z = 15·4648$

N(5)	−0·002 (3)	C(18)	0·002 (3)
C(15)	−0·002 (3)	C(19)	−0·002 (3)
C(16)	0·002 (3)	C(20)*	0·026 (5)
C(17)	−0·002 (3)	Ni*	−0·076 (1)

(VII) $5·6755X + 9·5600Y + 23·6215Z = 17·1412$

N(6)	0·007 (3)	C(24)	−0·004 (3)
C(21)	−0·011 (4)	C(25)	−0·001 (3)
C(22)	0·005 (3)	C(26)*	0·051 (5)
C(23)	0·002 (3)	Ni*	0·245 (1)

(VIII) $0·1189X + 0·0185Y + 31·9285Z = 24·0020$

C(27)	−0·004 (3)	C(32)	0·000 (2)
C(28)	0·005 (4)	C(27)*	0·003 (3)
C(29)	0·003 (4)	C(28)*	−0·004 (4)
C(30)	−0·001 (4)	C(29)*	0·007 (4)
C(31)	0·002 (2)	C(30)*	0·006 (4)

(IX) $3·8982X + 0·0192Y + 31·0948Z = 9·7268$

C(33)	−0·001 (5)	C(33)*	−0·018 (5)
C(34)	0·003 (3)	C(34)*	−0·020 (3)
C(35)	0·001 (4)	C(35)*	−0·026 (4)
C(36)	0·002 (3)	C(36)*	−0·030 (3)
C(37)	−0·005 (3)	C(37)*	−0·017 (3)

(X) $4·5548X - 3·5997Y + 29·9583Z = 1·4828$

C(38)	−0·012 (6)	C(43)	−0·003 (6)
C(39)	0·002 (10)	C(44)	0·002 (8)
C(40)	0·014 (9)	C(45)	0·010 (6)
C(41)	−0·005 (8)	C(46)	−0·002 (5)
C(42)	0·001 (7)	C(47)	−0·006 (7)

Selected dihedral angles (°)

|			
(I)–(IV)	52·5 (8)	(VIII)–(IX)	14 (2)
(I)–(V)	51·0 (7)	(VIII)–(X)	21 (3)
(I)–(VI)	52·4 (8)	(IX)–(X)	13 (2)
(I)–(VII)	47·5 (9)		

* Atoms not included in the least-squares calculation.

Fig. 3. The molecular packing viewed along [110]. The shortest intermolecular distances between non-H atoms are: host–host, $C(6)\cdots C(26) = 3.49$ (1) Å; host–guest molecule C, $C(22)\cdots C(41) = 3.40$ (2) and $C(22)\cdots C(47) = 3.43$ (2) Å. A list of intermolecular contacts including also those involving H atoms in geometrically calculated positions has been deposited. There are no significant differences between these distances and the corresponding sums of van der Waals radii.

The structure thus contains three different types of cavities; two of them have twofold axial symmetry (occupied by naphthalene molecules A and B); the third is centrosymmetric and is occupied by two naphthalene molecules (C). There is certainly an analogy with the previously studied layer-type structures of the $Ni(4-MePy)_4(NCS)_2$ clathrates (Lipkowski, Sgarabotto & Andreetti, 1982), especially when the naphthalene clathrate structure is viewed along [110] (Fig. 3), but one important point should be stressed: Namely, clathration of different guest molecules involves, in each case, adaptation of the host structure, which is thus extremely versatile, in order to absorb very different guests. The conformation of the pyridine rings and of the isothiocyanate groups may be significantly changed in order to shape the cavities appropriately. The same type of molecular packing of the host may thus produce different sets of cavities available for guest molecules. In the 2-MeN clathrate (space group $P\bar{1}$) one type of cavity has been found (Lipkowski et al., 1980), in the 1-MeN and o-xylene clathrate ($P2_1/c$) there are two (Lipkowski, Sgarabotto & Andreetti, 1982; Lipkowski & Andreetti, 1982), and in the present structure three different cavities can be distinguished. The geometry of these 'sorption centers' for guest molecules is of great importance especially when considering clathration of mixtures of different guests. Then each type of cavity can show its own selectivity with respect to a given mixture of possible guests.

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