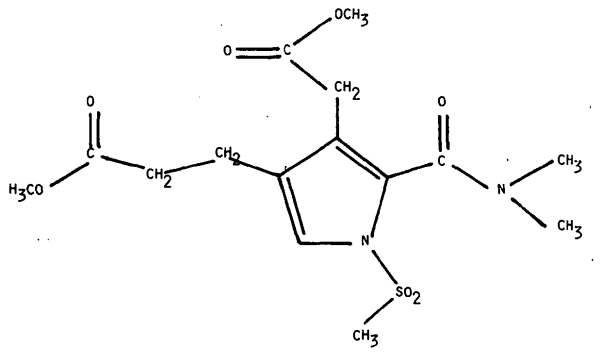
with scattering factors taken from *International Tables for X-ray Crystallography* (1974).



(I)

Final atomic parameters are listed in Table 1* and molecular geometry is in Table 2. The molecular structure and atomic numbering are illustrated in Fig. 1.

* Lists of structure factors, H-atom coordinates and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51523 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. The geometry and conformation of the *N*-methylsulfonyl (*N*-mesyl) group are in good agreement with other examples reviewed by Kálmán, Párkányi & Schawartz (1977). Structural characteristics of the carboxylic amide group are reviewed by Chakrabarti & Dunitz (1982); the sterically-induced out-of-plane twist observed here is common in tertiary aryl carboxamides.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1989). C**45**, 694–695

The structure of $[CdNi(CN)_4(C_6H_8N_2)(NH_3)]$: Corrigendum.

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Abstract

The crystal structure of this compound, recently described in space group $Pna2_1$, has been more satisfactorily refined in *Pnma*. The final R is 0·019 for 104 parameters, compared to an R of 0·033 for 171 parameters in $Pna2_1$. The revised structure shows more reasonable interatomic distances involving the bridging C—N groups and a planar rather than a non-planar pyridine ring.

The structure of this polymeric compound, *catena*-poly-[tri-μ-cyano-(ammine)(2-amino-3-methylpyridine)cadmium-μ-cyano-nickel], has recently been described (Hökelek & Ülkü, 1988; hereinafter, HU) in the non-centrosymmetric space group $Pna2_1$ [orthorhombic; $a = 13{\cdot}535$ (1), $b = 13{\cdot}607$ (1), $c = 7{\cdot}645$ (1) Å, $Z = 4$] and refined to an R of 0·033 for 1632 'observed' reflections. It is properly described in the centrosymmetric space group *Pnam* (transformed here to the conventional *Pnma*, No. 62).

Initial coordinates in *Pnma* were obtained from the values in Table 2 of HU by decrementing the z's by about 0·64 (so that most of the atoms lie at $z = 0{\cdot}25$ or $z = 0{\cdot}75$), interchanging y and z, and averaging N(1) with N(3), N(2) with N(4), C(1) with C(3), and C(2) with C(4). Least-squares refinement with anisotropic U_{ij}'s, including an extinction

* Contribution No. 7852.

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parameter, quickly led to an R of 0·023 for 1624 reflections recovered from SUP 44753. (Eight entries in SUP 44753 were illegible.) Difference maps then clearly indicated the positions of all the H atoms except those on the NH_3 group N(5), which were represented by a ring of essentially uniform electron density (0·3 e Å^{-3}). This group was modeled by six half-weight H atoms; the remaining H atoms were placed in idealized positions (C—H, 0·96; N—H, 0·90 Å) and not further adjusted. The total number of parameters was 104 (compared with 171 for the earlier, $Pna2_1$, model). Final full-matrix refinement led to an R of 0·019 with a maximum shift/σ value of 0·03. The *Pnma* coordinates are given in Table 1.*

There are small but highly significant (in terms of the e.s.d.'s) changes in a number of the bond lengths (see Table 2). The largest changes involve the bridging C—N groups, which appeared to show wide ranges of Ni—C, Cd—N and C—N distances in the $Pna2_1$ description but are entirely regular now. The atoms of these C—N groups were the only ones that needed to be modeled as structurally distinct pairs in the $Pna2_1$ description; because of the very large correlations within each pair [the two atoms of a pair, such as N(1) and N(3), are in fact indistinguishable, as shown by the *Pnma* refinement], these atoms showed large e.s.d.'s in all coordinates (HU, Table 2) and even larger displacements from their true positions. For the remaining atoms, which lie on mirror planes in the *Pnma* description and hence were modeled as single atoms in $Pna2_1$, the near-singularities involved the out-of-plane coordinates z; accordingly, the e.s.d.'s of their z coordinates, but not of x and y, are large (see HU, Table 2) and the reported values of z are perturbed. These out-of-plane perturbations do not have large effects on the bond lengths; however, other details of the structure are affected. For example, in the $Pna2_1$ description, atom C(8) of the pyridine ring appears to be highly pyramidal, lying 0·23 Å from the plane of its three neighbors; in the revised *Pnma* description the pyridine ring is, as expected, planar (by symmetry).

The earlier authors do not indicate why they selected space group $Pna2_1$ rather than *Pnma*; both carry the same systematic absences. The irregular distances involving the C—N groups, the non-planarity of the pyridine ring, and the peculiar e.s.d.'s resulting from the $Pna2_1$ refinement might well have suggested that the space group was incorrect. In any event, workers should be continually alert to the problem of assigning the correct space group, and to the dangers of an incorrect assignment.

Table 1. *Coordinates* (× 10^5) *and* U_{eq} *values* (Å^2 × 10^4), *space group Pnma*

	x	y	z	U_{eq}*
Ni	26345 (3)	−25000	23981 (3)	197 (1)
Cd	1365 (2)	25000	16036 (2)	181 (1)
N(1,3)	13578 (16)	2942 (31)	14903 (17)	323 (5)
N(2,4)	−10826 (16)	3023 (30)	17126 (18)	333 (5)
N(5)	−62 (27)	25000	−880 (24)	319 (7)
N(6)	3847 (23)	25000	33238 (22)	282 (6)
N(7)	−12589 (28)	25000	37677 (28)	510 (11)
C(1,3)	18532 (17)	−7782 (33)	18187 (18)	245 (5)
C(2,4)	34209 (18)	−7707 (33)	29673 (18)	252 (5)
C(5)	13549 (31)	25000	35840 (30)	375 (9)
C(6)	16645 (38)	25000	45376 (37)	604 (14)
C(7)	9448 (46)	25000	52695 (34)	675 (18)
C(8)	−260 (42)	25000	50507 (33)	484 (12)
C(9)	−2963 (31)	25000	40421 (28)	332 (8)
C(10)	−8200 (52)	25000	58303 (40)	788 (19)

* $U_{eq} = \frac{1}{3}\sum_i\sum_j[U_{ij}(a_i^*a_j^*)(\mathbf{a}_i.\mathbf{a}_j)]$.

Table 2. *Bond lengths* (Å) *from the Pnma (this investigation) and the* $Pna2_1$ *(Hökelek & Ülkü, 1988) refinements*

Bond	*Pnma*	$Pna2_1$
Ni—C(1,3)	1·863 (2)	1·877 (16), 1·860 (14)
—C(2,4)	1·866 (2)	1·835 (15), 1·903 (16)
Cd—N(1,3)	2·366 (2)	2·392 (16), 2·351 (14)
—N(2,4)	2·360 (2)	2·308 (13), 2·417 (17)
—N(5)	2·310 (3)	2·317 (6)
—N(6)	2·365 (3)	2·365 (4)
N(1,3)—C(1,3)	1·150 (3)	1·125 (20), 1·162 (18)
N(2,4)—C(2,4)	1·146 (3)	1·205 (25), 1·077 (25)
N(6)—C(5)	1·360 (5)	1·350 (9)
—C(9)	1·344 (5)	1·362 (7)
C(5)—C(6)	1·364 (7)	1·383 (9)
C(6)—C(7)	1·393 (7)	1·363 (12)
C(7)—C(8)	1·347 (7)	1·427 (15)
C(8)—C(9)	1·420 (6)	1·407 (10)
—C(10)	1·510 (8)	1·527 (14)
C(9)—N(7)	1·355 (6)	1·343 (8)

I thank W. P. Schaefer for helpful comments.

Reference

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* Lists of anisotropic U_{ij} values and coordinates for the H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51446 (2 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1989). C**45**, 695

Cubic structure of sodium calcium germanate $Na_{3.70}Ca_{1.15}Ge_3O_9$. Erratum.

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(*Received* 24 *January* 1989)

Abstract

A printer's error is corrected. In Table 1 of the paper by Nishi & Takéuchi [*Acta Cryst.* (1988), C**44**, 1867–1869] the y coordinate of O(4) is illegible. It should read 2196 (6).

All relevant information is contained in the *Abstract*.

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