

ment parameters. Successful convergence of the full-matrix least-squares refinement on F^2 (SHELXL93; Sheldrick, 1993) was indicated by the maximum shift/error for the last cycle. The highest peaks in the final difference Fourier map were in the vicinity of the Ag atom; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

Data collection: CAD-4 Software (Enraf–Nonius, 1989). Cell refinement: CAD-4 Software. Molecular graphics: ORTEPII (Johnson, 1971). Software used to prepare material for publication: CIFTAB in SHELXL93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: BK1228). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,2'-Biphenylbis(η-cyclopentadienyl)-titanium

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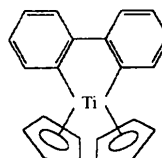
Abstract

The Ti atom in the title compound, [Ti(η-C₅H₅)₂-(C₁₂H₈)], has a distorted tetrahedral coordination and is attached to two cyclopentadienyl rings and to two C atoms in the 2 and 2' positions of the biphenyl ligand. The two eclipsed cyclopentadienyl (Cp) rings are bent back to make room for the σ-bonded biphenyl ligand. The Cp(centroid)—Ti—Cp(centroid) angles are in the range 135.7(2)–137.3(2)° for the three independent molecules in the asymmetric unit.

Comment

In recent years, the number of studies of cyclic organometallic compounds of transition metals has increased because of their special activation of C—H bonds and also because of their action in cycloaddition reactions and the disproportionation of alkenes. Compounds of type [Cp₂TiR₂] (where Cp is cyclopentadienyl and R is alkyl or aryl) have been studied extensively (Rausch & Klemann, 1971; Sonogashira & Hagihara, 1966; Atwood, Hunter, Alt & Rausch, 1976; Fachinetti, Floriani, Marchetti & Mellini, 1978; Bristow, Lappert, Martin, Atwood & Hunter, 1984; Engelhardt, Leung, Papisergino, Raston, Twiss & White, 1987).

The crystal structure of the title compound, (I), comprises three neutral molecules (A, B and C) per asymmetric unit. The molecular geometries of these three independent molecules are quite similar.



(I)

The coordination geometry of the Ti atom can be described as a distorted tetrahedron involving two C atoms of biphenyl and two Cp rings, if the centroid of each Cp ring is considered to occupy one coordination site (Fig. 1). The Ti atom forms an unstrained five-

membered ring with the biphenyl ligand. The ring plane defined by the atoms Ti, C(11), C(16), C(17) and C(22) bisects the $Cp(1)$ —Ti— $Cp(2)$ angles, where $Cp(1)$ and $Cp(2)$ are the centroids of the C(1)—C(5) and C(6)—C(10) rings, respectively, and is perpendicular to the plane formed by the Ti atom and the centroids of the two Cp rings; the dihedral angles between these planes are 90.7 (2), 88.9 (2) and 90.3 (2)° for molecules A, B and C, respectively.

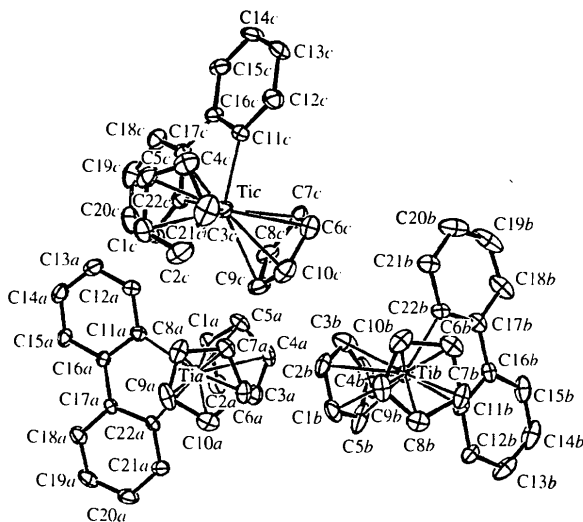


Fig. 1. ORTEP (Johnson, 1976) drawing of the three independent molecules (A, B and C) in the asymmetric unit, showing the atomic numbering and displacement ellipsoids at 20% probability, as viewed down the c axis.

The Ti atom is bonded to atoms C(11) and C(22) of the biphenyl ligand and the Ti— C_{σ} bond lengths are consistent with reported Ti— C_{sp^2} distances (Atwood, Hunter, Alt & Rausch, 1976; Fachinetti, Floriani, Marchetti & Mellini, 1978; Kocman, Rucklidge, O'Brien & Santo, 1971). The Ti— C_{Cp} bond lengths, which range from 2.325 (5) to 2.384 (5) Å, are similar to those found in the compounds reported above. The average distance of the Ti atom from the centroids of the Cp rings is 2.049 (3) Å.

The Cp rings of each molecule are nearly eclipsed, with staggered angles of 8.9 (9), 1.5 (13) and 0.6 (6)° for A, B and C, respectively.

Experimental

The title compound, (I), was prepared by Schleyer's method (Neugebauer, Kos & Schleyer, 1982).

Crystal data

[Ti(C₅H₅)₂(C₁₂H₈)]
 $M_r = 330.29$

Cu $K\alpha$ radiation
 $\lambda = 1.54184$ Å

Monoclinic
 $P2_1/c$
 $a = 16.531$ (4) Å
 $b = 13.224$ (2) Å
 $c = 22.633$ (2) Å
 $\beta = 87.85$ (2)°
 $V = 4944$ (1) Å³
 $Z = 12$
 $D_x = 1.331$ Mg m⁻³
 D_m not measured

Data collection

Enraf-Nonius CAD-4
diffractometer
 $\omega/2\theta$ scans
Absorption correction:
empirical via ψ scans
(North, Phillips &
Mathews, 1968)
 $T_{min} = 0.415$, $T_{max} =$
0.994
6801 measured reflections
5945 independent reflections

Refinement

Refinement on F
 $R = 0.071$
 $wR = 0.075$
 $S = 2.49$
4659 reflections
622 parameters
H atoms: see below
Unit weights applied

Cell parameters from 25
reflections
 $\theta = 18$ –36°
 $\mu = 4.36$ mm⁻¹
 $T = 293$ K
Block
0.26 × 0.14 × 0.10 mm
Orange

4464 observed reflections
[$I > 3\sigma(I)$]
 $R_{int} = 0.045$
 $\theta_{max} = 55$ °
 $h = 0 \rightarrow 17$
 $k = 0 \rightarrow 14$
 $l = -25 \rightarrow 25$
3 standard reflections
frequency: 60 min
intensity decay: 2.1%

(Δ/σ)_{max} = 0.76
 $\Delta\rho_{max} = 0.78$ e Å⁻³
 $\Delta\rho_{min} = -0.76$ e Å⁻³
Extinction correction: none
Atomic scattering factors
from *International Tables*
for *X-ray Crystallography*
(1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$B_{eq} = (4/3)\sum_i \sum_j \beta_{ij} a_i \cdot a_j$$

	x	y	z	B_{eq}
TiA	0.08941 (8)	0.0504 (1)	0.17801 (6)	3.21 (3)
C(1A)	0.0498 (5)	-0.1107 (6)	0.1451 (4)	4.7 (2)
C(2A)	-0.0181 (5)	-0.0674 (7)	0.1714 (4)	5.0 (2)
C(3A)	-0.0045 (6)	-0.0539 (7)	0.2324 (4)	5.4 (2)
C(4A)	0.0743 (7)	-0.0910 (7)	0.2425 (4)	5.8 (2)
C(5A)	0.1068 (6)	-0.1256 (6)	0.1891 (4)	5.4 (2)
C(6A)	0.1325 (6)	0.1193 (7)	0.2675 (3)	5.0 (2)
C(7A)	0.2019 (5)	0.0920 (7)	0.2339 (4)	5.2 (2)
C(8A)	0.2074 (6)	0.1516 (8)	0.1843 (4)	6.1 (2)
C(9A)	0.1422 (6)	0.2156 (7)	0.1860 (4)	6.5 (2)
C(10A)	0.0972 (6)	0.1965 (6)	0.2382 (4)	5.6 (2)
C(11A)	0.1369 (5)	0.0437 (6)	0.0876 (3)	3.7 (2)
C(12A)	0.2073 (5)	-0.0013 (7)	0.0651 (4)	4.6 (2)
C(13A)	0.2267 (6)	-0.0046 (7)	0.0048 (4)	5.7 (2)
C(14A)	0.1755 (6)	0.0413 (8)	-0.0338 (4)	5.9 (2)
C(15A)	0.1055 (5)	0.0877 (7)	-0.0134 (3)	4.7 (2)
C(16A)	0.0864 (5)	0.0933 (6)	0.0476 (3)	3.7 (2)
C(17A)	0.0123 (5)	0.1414 (6)	0.0724 (3)	3.5 (2)
C(18A)	-0.0412 (5)	0.1977 (7)	0.0382 (4)	5.2 (2)
C(19A)	-0.1090 (5)	0.2383 (7)	0.0639 (4)	5.8 (2)
C(20A)	-0.1261 (6)	0.2317 (8)	0.1239 (4)	6.4 (3)
C(21A)	-0.0726 (5)	0.1777 (7)	0.1583 (4)	5.2 (2)
C(22A)	-0.0036 (4)	0.1345 (6)	0.1342 (3)	3.6 (2)
TiB	0.26250 (8)	0.0862 (1)	0.48344 (6)	3.26 (3)
C(1B)	0.1958 (7)	0.1732 (8)	0.4094 (4)	6.9 (3)
C(2B)	0.2601 (6)	0.1309 (9)	0.3837 (3)	6.3 (3)
C(3B)	0.2512 (8)	0.0302 (9)	0.3859 (4)	10.8 (3)
C(4B)	0.1746 (8)	0.0161 (7)	0.4146 (4)	11.7 (3)
C(5B)	0.1445 (5)	0.105 (1)	0.4297 (4)	9.8 (4)

C(6B)	0.3721 (5)	0.1130 (7)	0.5477 (4)	5.1 (2)	C(17)—C(18)	1.409 (6)	1.415 (8)	1.411 (7)
C(7B)	0.3013 (5)	0.1555 (7)	0.5737 (3)	5.0 (2)	C(18)—C(19)	1.356 (7)	1.403 (8)	1.399 (7)
C(8B)	0.2800 (5)	0.2351 (6)	0.5378 (4)	5.0 (2)	C(19)—C(20)	1.379 (7)	1.332 (9)	1.356 (8)
C(9B)	0.3339 (6)	0.2411 (7)	0.4908 (4)	5.8 (2)	C(20)—C(21)	1.397 (7)	1.402 (10)	1.382 (8)
C(10B)	0.3890 (5)	0.1650 (8)	0.4946 (4)	5.9 (2)	C(21)—C(22)	1.371 (6)	1.375 (6)	1.403 (6)
C(11B)	0.1758 (4)	0.0204 (6)	0.5459 (3)	3.6 (2)	C(17)—C(22)	1.415 (5)	1.374 (6)	1.392 (6)
C(12B)	0.1076 (5)	0.0644 (7)	0.5716 (3)	4.7 (2)	C(11)—Ti—C(22)	80.8 (2)	79.6 (2)	79.2 (2)
C(13B)	0.0552 (5)	0.0095 (9)	0.6083 (4)	7.1 (3)	Cp(1)—Ti—Cp(2)	136.3 (2)	135.7 (2)	137.3 (2)
C(14B)	0.0714 (6)	-0.092 (1)	0.6197 (4)	7.8 (3)	C(11)—Ti—Cp(1)	106.0 (2)	105.4 (2)	106.1 (2)
C(15B)	0.1388 (6)	-0.1345 (7)	0.5944 (4)	6.1 (2)	C(22)—Ti—Cp(1)	106.3 (2)	107.1 (2)	105.5 (2)
C(16B)	0.1932 (5)	-0.0842 (6)	0.5578 (3)	3.9 (2)	C(11)—Ti—Cp(2)	107.7 (2)	107.9 (2)	106.4 (2)
C(17B)	0.2661 (5)	-0.1256 (6)	0.5286 (4)	4.3 (2)	C(22)—Ti—Cp(2)	106.3 (2)	107.0 (2)	107.3 (2)
C(18B)	0.2880 (6)	-0.2281 (7)	0.5363 (5)	6.7 (2)	C(11)—C(16)—C(17)	117.3 (4)	116.3 (4)	114.6 (4)
C(19B)	0.3585 (6)	-0.2619 (7)	0.5060 (5)	8.7 (3)	C(22)—C(17)—C(16)	118.0 (4)	119.1 (4)	118.3 (4)
C(20B)	0.4053 (6)	-0.2026 (8)	0.4716 (5)	7.9 (3)	C(2)—C(1)—C(5)	107.9 (4)	111.4 (5)	108.3 (6)
C(21B)	0.3816 (5)	-0.1019 (7)	0.4639 (4)	5.4 (2)	C(1)—C(2)—C(3)	108.5 (5)	108.6 (5)	106.8 (6)
C(22B)	0.3124 (4)	-0.0646 (6)	0.4917 (3)	3.8 (2)	C(2)—C(3)—C(4)	107.0 (5)	104.1 (5)	108.9 (6)
TiC	0.57694 (9)	0.1924 (1)	0.26542 (6)	3.93 (3)	C(3)—C(4)—C(5)	107.6 (5)	109.0 (5)	107.5 (6)
C(1C)	0.5896 (7)	0.3363 (8)	0.2038 (5)	7.0 (3)	C(1)—C(5)—C(4)	108.9 (5)	106.8 (5)	108.5 (5)
C(2C)	0.5897 (7)	0.3687 (7)	0.2624 (5)	8.1 (3)	C(7)—C(6)—C(10)	106.7 (4)	107.4 (7)	108.9 (5)
C(3C)	0.6605 (7)	0.3306 (8)	0.2864 (5)	8.1 (3)	C(6)—C(7)—C(8)	108.9 (5)	106.5 (6)	106.6 (5)
C(4C)	0.7021 (6)	0.2740 (8)	0.2436 (5)	6.3 (3)	C(7)—C(8)—C(9)	107.7 (5)	109.2 (6)	107.8 (5)
C(5C)	0.6590 (6)	0.2791 (7)	0.1924 (4)	5.9 (2)	C(8)—C(9)—C(10)	107.8 (4)	109.1 (6)	109.9 (5)
C(6C)	0.5545 (6)	0.1411 (7)	0.3655 (4)	5.6 (2)	C(6)—C(10)—C(9)	108.9 (4)	107.6 (7)	106.8 (5)
C(7C)	0.5191 (6)	0.0667 (7)	0.3299 (4)	5.2 (2)				
C(8C)	0.4568 (5)	0.1141 (8)	0.3009 (4)	5.6 (2)				
C(9C)	0.4548 (5)	0.2136 (7)	0.3184 (4)	5.8 (2)				
C(10C)	0.5148 (7)	0.2314 (7)	0.3580 (4)	6.6 (3)				
C(11C)	0.6568 (5)	0.0674 (6)	0.2515 (3)	3.9 (2)				
C(12C)	0.7211 (6)	0.0360 (8)	0.2861 (4)	5.8 (2)				
C(13C)	0.7690 (5)	-0.0461 (8)	0.2703 (4)	6.1 (2)				
C(14C)	0.7566 (5)	-0.0979 (7)	0.2190 (5)	6.3 (2)				
C(15C)	0.6936 (5)	-0.0703 (6)	0.1832 (4)	4.9 (2)				
C(16C)	0.6450 (5)	0.0118 (6)	0.1989 (3)	3.7 (2)				
C(17C)	0.5740 (5)	0.0449 (6)	0.1648 (3)	3.7 (2)				
C(18C)	0.5531 (6)	-0.0045 (7)	0.1123 (4)	5.4 (2)				
C(19C)	0.4834 (6)	0.0261 (9)	0.0840 (4)	6.9 (3)				
C(20C)	0.4383 (6)	0.1042 (9)	0.1057 (4)	7.1 (3)				
C(21C)	0.4592 (5)	0.1553 (8)	0.1562 (4)	5.9 (2)				
C(22C)	0.5288 (5)	0.1271 (6)	0.1858 (4)	4.1 (2)				

† Cp(1) and Cp(2) are the centroids of the C(1)—C(5) and C(6)—C(10) rings, respectively.

The structure was solved by direct and Fourier methods and refined by full-matrix least squares. Non-H atoms were allowed to refine with anisotropic displacement parameters. H atoms were located from the difference Fourier maps and included in the structure-factor calculations, but were not refined. All calculations were performed on a DEC PDP11/44 computer.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1985). Cell refinement: *CAD-4 Software*. Program(s) used to solve structure: *SDP-Plus* (B. A. Frenz & Associates Inc., 1985). Program(s) used to refine structure: *SDP-Plus*. Molecular graphics: *ORTEPII* (Johnson, 1976).

The authors thank Professor Rong-jun Yin for the samples and the National Laboratory of Applied Organic Chemistry for financial support.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1327). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 2. Selected geometric parameters (\AA , $^\circ$) for molecules A, B and C

	Molecule		
	A	B	C
Ti—C(11)	2.166 (4)	2.158 (5)	2.131 (5)
Ti—C(22)	2.168 (4)	2.168 (5)	2.175 (4)
Ti—C(1)	2.358 (5)	2.342 (5)	2.364 (5)
Ti—C(2)	2.373 (5)	2.336 (5)	2.342 (6)
Ti—C(3)	2.384 (5)	2.343 (5)	2.350 (6)
Ti—C(4)	2.380 (5)	2.358 (5)	2.370 (5)
Ti—C(5)	2.360 (5)	2.351 (6)	2.392 (5)
Ti—C(6)	2.354 (5)	2.392 (8)	2.381 (5)
Ti—C(7)	2.353 (6)	2.350 (8)	2.387 (6)
Ti—C(8)	2.374 (5)	2.347 (6)	2.355 (5)
Ti—C(9)	2.361 (5)	2.373 (8)	2.325 (5)
Ti—C(10)	2.370 (5)	2.359 (14)	2.357 (5)
Ti—Cp(1)†	2.049 (5)	2.051 (5)	2.046 (6)
Ti—Cp(2)†	2.051 (5)	2.050 (9)	2.045 (5)
C(1)—C(2)	1.376 (7)	1.318 (7)	1.394 (9)
C(1)—C(5)	1.410 (7)	1.308 (7)	1.392 (8)
C(2)—C(3)	1.419 (7)	1.341 (7)	1.402 (9)
C(3)—C(4)	1.418 (7)	1.413 (7)	1.386 (8)
C(4)—C(5)	1.384 (8)	1.318 (8)	1.385 (7)
C(6)—C(7)	1.399 (8)	1.408 (15)	1.414 (7)
C(6)—C(10)	1.360 (8)	1.403 (12)	1.377 (8)
C(7)—C(8)	1.374 (7)	1.383 (11)	1.390 (9)
C(8)—C(9)	1.369 (7)	1.364 (9)	1.374 (7)
C(9)—C(10)	1.395 (7)	1.363 (10)	1.383 (7)
C(11)—C(12)	1.387 (6)	1.379 (6)	1.408 (6)
C(11)—C(16)	1.416 (6)	1.440 (6)	1.417 (6)
C(12)—C(13)	1.389 (7)	1.381 (11)	1.383 (10)
C(13)—C(14)	1.381 (7)	1.400 (9)	1.371 (8)
C(14)—C(15)	1.373 (7)	1.353 (9)	1.391 (8)
C(15)—C(16)	1.407 (6)	1.371 (8)	1.389 (7)
C(16)—C(17)	1.473 (6)	1.461 (6)	1.496 (6)

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Bis(1,2-di-4-pyridylethane-*N:N'*)-cadmium(II) tetracyanonickelate(II) *m*-Xylene Solvate

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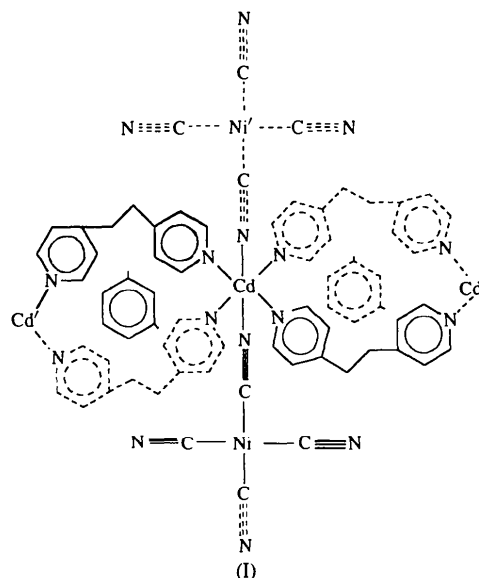
Abstract

The title compound, bis(1,2-di-4-pyridylethane-*N:N'*)-cadmium(II) tetracyanonickelate(II) di-*m*-xylene solvate, $[\text{Cd}(\text{C}_{12}\text{H}_{12}\text{N}_2)_2][\text{Ni}(\text{CN})_4] \cdot 2\text{C}_8\text{H}_{10}$, is represented by the general Hofmann-type clathrate formula $\text{Cd}(\text{Ligand})_2\text{Ni}(\text{CN})_4 \cdot 2\text{Guest}$, where *Ligand* is 1,2-di-4-pyridylethane ($\text{C}_{12}\text{H}_{12}\text{N}_2$) and *Guest* is *m*-xylene (C_8H_{10}). It was seen that the structure of the title compound is of a new type and quite different from that of the Hofmann-type clathrates.

Comment

The title structure, (I), differs from that of the Hofmann-type clathrate. In the well known Hofmann-type clathrate, *Ligand* is either bidentate (having two donor atoms) or a monodentate pair (having one donor atom each) and results in a three-dimensional metal complex host structure accommodating the aromatic *Guest* molecule. Cd atoms are in an octahedral environment formed by coordination to four N atoms of the cyanide groups and two N atoms of the ligand molecules. However, in the new type of host structure presented here, each Cd atom is coordinated octahedrally

by four N atoms of the ligand molecules and two N atoms of the cyanide groups. The other two cyanide groups of the $\text{Ni}(\text{CN})_4$ moiety have free nitrogen ends.



Of the six N atoms coordinating the Cd atom, two are from the cyanide groups, with a Cd—N3 distance of 2.320 (4) Å, and four are from pyridyl rings, with distances Cd—N2 2.422 (5) and Cd—N1 2.345 (5) Å (Fig. 1). The Ni atom is coordinated to the four C atoms of the cyanide groups in a square plane, with distances Ni—C13 1.852 (5) and Ni—C14 1.874 (7) Å. In the cyanide groups, the C—N distances are 1.139 (7) (C13—N3) and 1.150 (8) Å (C14—N4), with angles Cd—N3—C13 164.2 (5), Ni—C14—N4 179.1 (5) and Ni—C13—N3 178.2 (6)°. In the pyridyl rings, the distances N1—

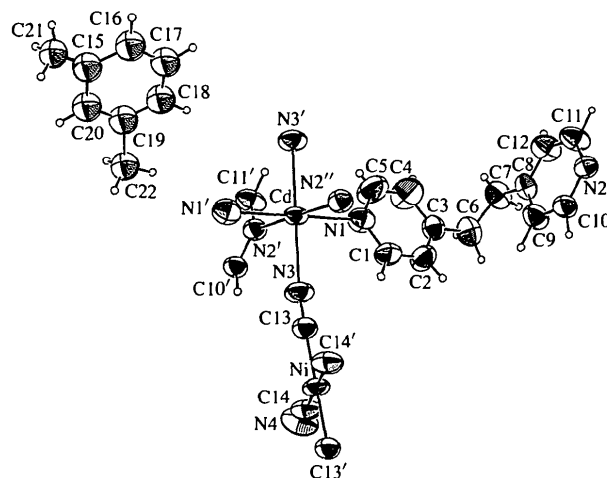


Fig. 1. A perspective view of the molecular structure of the title complex with the atom-numbering scheme. The displacement ellipsoids are plotted at the 50% probability level and the displacement parameters of the *Guest* atoms were fixed at 5 Å² for clarity.