

S = 0.885

11 499 reflections

920 parameters

H atoms not refined

$$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 33.5904P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

Extinction correction:

SHELXL93

Extinction coefficient:

0.00109 (8)

Scattering factors from

International Tables for  
Crystallography (Vol. C)

Table 1. Selected bond lengths (Å)

Sr1—O17	2.456 (7)	Sr5—O16	2.588 (7)
Sr1—O12	2.488 (7)	Sr5—O22	2.615 (6)
Sr1—O112	2.510 (6)	Sr5—O32	2.737 (7)
Sr1—O13	2.551 (6)	Sr5—O36	2.751 (7)
Sr1—O24	2.564 (6)	Sr6—O28 <sup>v</sup>	2.412 (8)
Sr1—O211	2.642 (6)	Sr6—O19	2.469 (8)
Sr1—O33	2.919 (7)	Sr6—O111 <sup>ii</sup>	2.534 (6)
Sr1—O311	2.939 (7)	Sr6—O212 <sup>vi</sup>	2.548 (6)
Sr1—O34	2.948 (6)	Sr6—O18	2.550 (7)
Sr2—O27	2.543 (6)	Sr6—O210	2.629 (6)
Sr2—O16 <sup>i</sup>	2.567 (7)	Sr6—O38	2.802 (7)
Sr2—O22	2.584 (7)	Sr6—O310	2.812 (7)
Sr2—O21	2.586 (7)	Sr6—O312 <sup>vi</sup>	2.888 (8)
Sr2—O15	2.602 (7)	O11—C11	1.300 (12)
Sr2—O23	2.640 (7)	O21—C11	1.230 (11)
Sr2—O13	2.678 (6)	O12—C12	1.185 (12)
Sr2—O25	2.906 (8)	O22—C12	1.246 (12)
Sr3—O212 <sup>ii</sup>	2.530 (6)	O13—C13	1.326 (11)
Sr3—O29	2.554 (7)	O23—C13	1.210 (11)
Sr3—O210 <sup>iii</sup>	2.555 (7)	O14—C14	1.231 (11)
Sr3—O14 <sup>ii</sup>	2.607 (6)	O24—C14	1.250 (11)
Sr3—O18	2.610 (7)	O15—C15	1.239 (12)
Sr3—O111 <sup>ii</sup>	2.716 (6)	O25—C15	1.258 (12)
Sr3—O211 <sup>ii</sup>	2.718 (6)	O16—C16	1.246 (11)
Sr3—O24 <sup>ii</sup>	2.801 (6)	O26—C16	1.217 (11)
Sr4—O26 <sup>i</sup>	2.434 (7)	O17—C17	1.230 (11)
Sr4—O110 <sup>iii</sup>	2.476 (7)	O27—C17	1.291 (11)
Sr4—O27	2.519 (7)	O18—C18	1.260 (12)
Sr4—O14 <sup>ii</sup>	2.525 (6)	O28—C18	1.266 (12)
Sr4—O29	2.573 (7)	O19—C19	1.227 (12)
Sr4—O21	2.613 (7)	O29—C19	1.298 (12)
Sr4—O31	2.810 (7)	O110—C110	1.199 (12)
Sr4—O39	2.827 (7)	O210—C110	1.283 (12)
Sr4—O37	2.988 (9)	O111—C111	1.235 (12)
Sr5—O11	2.406 (7)	O211—C111	1.190 (11)
Sr5—O23 <sup>v</sup>	2.455 (7)	O112—C112	1.258 (11)
Sr5—O15	2.459 (7)	O212—C112	1.239 (12)
Sr5—O25 <sup>v</sup>	2.526 (8)		

Symmetry codes: (i)  $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ ; (ii)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ ; (iii)  $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$ ; (iv)  $\frac{3}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ ; (v)  $\frac{3}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$ ; (vi)  $1 - x, -y, 1 - z$ .

A preliminary reduction of the unit cell indicated the possibility of higher metric symmetry (orthorhombic C), but the  $R_{\text{int}}$  value was 0.223, cf.  $R_{\text{int}}$  was 0.038 for the chosen monoclinic cell. The intensity statistics indicated centrosymmetry. All non-H atoms were located from  $E$  maps and the subsequent  $\Delta\rho$  syntheses. Since the number of collected reflections satisfying the criterion  $I > 2\sigma(I)$  was not large enough, all furan rings were treated as residues of common geometry in the final steps of refinement [using the SADI command in SHELXL93 (Sheldrick, 1993)], and DELU was used to stabilize the anisotropic displacement parameters by restraining common components of neighbouring atoms to be approximately equal. The H atoms bonded to the furan rings were placed geometrically with a C—H distance of 0.93 Å. Their isotropic displacement parameters were taken to be 1.2 times those of their attached C atoms.

Data collection: *KM-4 Users Guide* (Kuma Diffraction, 1989). Cell refinement: *KM-4 Users Guide*. Data reduction: *KM-4 Users Guide*. Program(s) used to solve structure: SHELXS86 (Sheldrick, 1990).

Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: JZ1136). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1997). **C53**, 289–292

### [Bis(thiodiphenylphosphino-S)amido]-chlorobis(dimethylphenylphosphine-P)-nitridorhenium(V)

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## Abstract

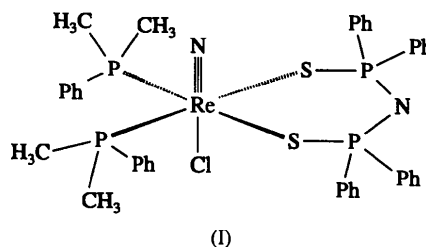
The title complex,  $[\text{ReNCl}(\text{C}_{24}\text{H}_{20}\text{NP}_2\text{S}_2)(\text{C}_8\text{H}_{11}\text{P})_2]$ , is formed during the reaction of  $[\text{ReNCl}_2(\text{Me}_2\text{PhP})_3]$  with a stoichiometric amount of  $\text{Na}(\text{SPh}_2\text{PNPPH}_2\text{S})$  in dichloromethane/methanol. The equatorial sphere of the six-coordinate complex is occupied by two  $\text{Me}_2\text{PhP}$  ligands and the tetraphenyldithioimidodiphosphinate anion, which binds in a bidentate manner via the sulfur donors. The chloro ligand is arranged in a position *trans* with respect to the terminal nitrido N atom, with exceptionally long Re—Cl bond lengths [2.598(4) and 2.632(5) Å for the two crystallographically independent molecules] due to the structural *trans* influence of 'N<sup>3-</sup>'.

### Comment

Recently, we have shown that [ReNCl<sub>2</sub>(Me<sub>2</sub>PhP)<sub>3</sub>] is a suitable starting material for obtaining rhenium mixed-ligand complexes which contain phosphines and chelating co-ligands (Abram & Ritter, 1993; Ritter & Abram, 1994). In contrast to similar reactions with [ReNCl<sub>2</sub>(Ph<sub>3</sub>P)<sub>2</sub>], where the equatorial coordination sphere is completely replaced by chelating ligands, the more basic Me<sub>2</sub>PhP ligand remains and mixed-ligand complexes are formed.

The reaction of [ReNCl<sub>2</sub>(Me<sub>2</sub>PhP)<sub>3</sub>] with one equivalent of sodium tetraphenyldithioimidodiphosphinate yields the yellow air-stable title compound, [ReNCl(SPh<sub>2</sub>PNPPh<sub>2</sub>S)(Me<sub>2</sub>PhP)<sub>2</sub>], (I). The formation of significant amounts of the bis-chelate [ReN(SPh<sub>2</sub>PNPPh<sub>2</sub>S)<sub>2</sub>] can only be observed when a large excess of the ligand, *i.e.* when the ratio of [ReNCl<sub>2</sub>(Me<sub>2</sub>PhP)<sub>3</sub>] to ligand is ten or higher, and long refluxing times are applied. The title compound is readily soluble in organic solvents such as CH<sub>2</sub>Cl<sub>2</sub> or CHCl<sub>3</sub> and only sparingly soluble in alcohols. The IR spectrum of the compound shows a narrow band for the ReN vibration at 1055 cm<sup>-1</sup>, which is the same value as observed for [ReNCl<sub>2</sub>(Me<sub>2</sub>PhP)<sub>3</sub>]. In the FAB<sup>+</sup> mass spectrum of the complex, rhenium-containing fragments can be observed at *m/z* = 924, 822 and 787, which can be assigned to [ReN(Me<sub>2</sub>PhP)<sub>2</sub>-(SPh<sub>2</sub>PNPPh<sub>2</sub>S)]<sup>+</sup>, [ReNCl(Me<sub>2</sub>PhP)(SPh<sub>2</sub>PNPPh<sub>2</sub>S)]<sup>+</sup> and [ReN(Me<sub>2</sub>PhP)(SPh<sub>2</sub>PNPPh<sub>2</sub>S)]<sup>+</sup>, respectively. No evidence could be found for the molecular ion peak. This agrees well with the results of mass spectrometry

studies on other six-coordinate rhenium-nitrido complexes where, in general, cleavage of the bond *trans* to the nitrido ligand is preferred (Abram & Ritter, 1993; Ritter & Abram, 1994; Hübener, Abram & Strähle, 1994).



Crystals of the title compound were obtained from a CH<sub>2</sub>Cl<sub>2</sub>/methanol solution. The triclinic unit cell contains two crystallographically independent [ReNCl(Me<sub>2</sub>PhP)<sub>2</sub>(SPh<sub>2</sub>PNPPh<sub>2</sub>S)] molecules (Fig. 1). The molecular geometry of the second molecule does not differ significantly and therefore will not be discussed in detail. Selected bond distances and angles are given in Table 1.

The Re atom is octahedrally coordinated, with the Me<sub>2</sub>PhP and chelating ligands in equatorial positions. Distortions from idealized octahedral geometry are evident. The N(11)—Re(1)—P(13) angle of 86.5(2)° is much smaller than those to the other equatorially coordinated donor atoms, which range between 95.3(2) and 106.4(2)°. The geometry of [ReNCl(Me<sub>2</sub>PhP)<sub>2</sub>-(SPh<sub>2</sub>PNPPh<sub>2</sub>S)] is thus similar to that of [ReNCl-

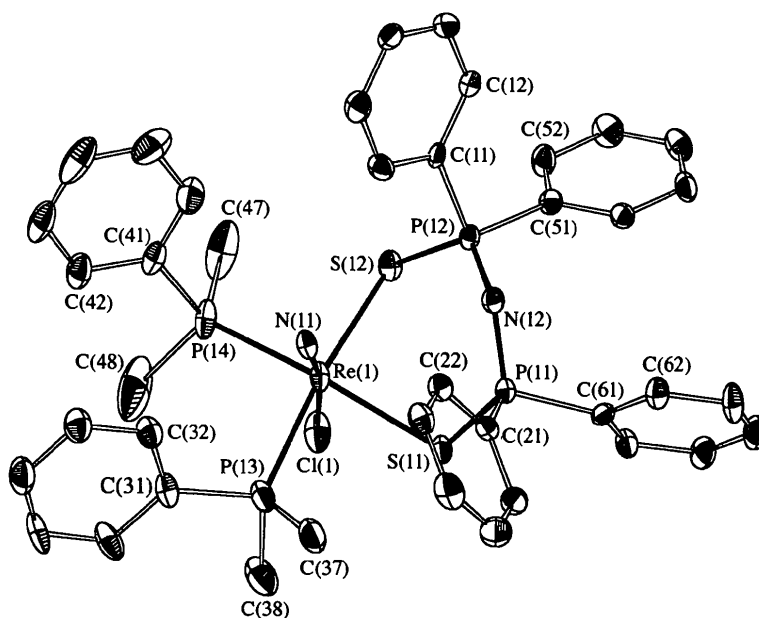


Fig. 1. ZORTEP (Zsolnai, 1994) diagram of one of the two independent molecules of [ReNCl(Me<sub>2</sub>PhP)<sub>2</sub>(SPh<sub>2</sub>PNPPh<sub>2</sub>S)] showing 30% probability displacement ellipsoids. The H atoms have been omitted for clarity.

(Me<sub>2</sub>PhP)<sub>2</sub>(HEt<sub>2</sub>tcb)] (where HEt<sub>2</sub>tcb<sup>-</sup> is *N,N*-diethylthiocarbamoylbenzamidinate) (Abram & Ritter, 1993) and [ReNCl(Me<sub>2</sub>PhP)<sub>2</sub>(Me<sub>2</sub>dtc)] (where Me<sub>2</sub>dtc<sup>-</sup> is dimethyldithiocarbamate) (Ritter & Abram, 1994). An exceptionally long bond distance is found between the Re atom and the chloro ligand, which is coordinated *trans* with respect to the terminal nitrido N atom. This is due to the labilizing *trans* influence of 'N<sup>3-</sup>' and has been discussed previously (Abram & Ritter, 1993; Ritter & Abram, 1994; Forsellini, Casellato, Graziani & Magon, 1982). The formation of a six-coordinate complex is in contrast to the results which were obtained from the reaction of [ReNCl<sub>2</sub>(Ph<sub>3</sub>P)<sub>2</sub>] with Na(SPh<sub>2</sub>PNPPh<sub>2</sub>S), where the five-coordinate [ReNCl(Ph<sub>3</sub>P)(SPh<sub>2</sub>PNPPh<sub>2</sub>S)] is formed. In this complex, chlorine is coordinated in the basal plane of a square pyramid, with an Re—Cl distance of about 2.37 Å (Rossi *et al.*, 1993).

## Experimental

*mer*-[ReNCl<sub>2</sub>(Me<sub>2</sub>PhP)<sub>3</sub>] (68 mg, 0.1 mmol) was dissolved in CH<sub>2</sub>Cl<sub>2</sub> (20 ml) and a solution of Na(SPh<sub>2</sub>PNPPh<sub>2</sub>S) (150 mg, 0.3 mmol) in methanol (20 ml) was added. The resulting mixture was refluxed for 1 h and the precipitated NaCl was removed by filtration. Upon standing, yellow crystals of [ReNCl(Me<sub>2</sub>PhP)<sub>2</sub>(SPh<sub>2</sub>PNPPh<sub>2</sub>S)] were formed. These were filtered off and washed with water and methanol. Yield: 72 mg (75% based on Re).

### Crystal data

[ReNCl(C<sub>24</sub>H<sub>20</sub>NP<sub>2</sub>S<sub>2</sub>)-  
(C<sub>8</sub>H<sub>11</sub>P)<sub>2</sub>]

*M<sub>r</sub>* = 960.41

Triclinic

*P*1̄

*a* = 10.476 (1) Å

*b* = 19.543 (3) Å

*c* = 20.690 (3) Å

α = 74.32 (7)°

β = 89.44 (7)°

γ = 81.22 (6)°

*V* = 4028 (1) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 1.584 Mg m<sup>-3</sup>

*D<sub>m</sub>* not measured

### Data collection

Enraf–Nonius CAD-4  
diffractometer

ω scans

Absorption correction:

semi-empirical ψ scans  
(Frenz, 1983)

*T<sub>min</sub>* = 0.735, *T<sub>max</sub>* = 0.843

18 424 measured reflections

15 722 independent  
reflections

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 25  
reflections

θ = 9.40–14.07°

μ = 3.377 mm<sup>-1</sup>

*T* = 203 (2) K

Needle

0.40 × 0.10 × 0.05 mm

Yellow

11 533 reflections with

*I* > 2σ(*I*)

*R<sub>int</sub>* = 0.0305

θ<sub>max</sub> = 26.02°

*h* = -1 → 12

*k* = -23 → 24

*l* = -25 → 25

3 standard reflections

every 300 reflections

frequency: 60 min

intensity decay: none

### Refinement

Refinement on *F*<sup>2</sup>

*R*(*F*) = 0.044

*wR*(*F*<sup>2</sup>) = 0.105

*S* = 1.12

15 689 reflections

901 parameters

H atoms placed in calculated  
positions

$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 7.9532P]$

where  $P = (F_o^2 + 2F_c^2)/3$

(Δ/*σ*)<sub>max</sub> = -0.001

Δρ<sub>max</sub> = 1.417 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -1.040 e Å<sup>-3</sup>

Extinction correction: none

Scattering factors from

*International Tables for  
Crystallography* (Vol. C)

Table 1. Selected geometric parameters (Å, °) for the first molecule of (I)

Re(1)—N(11)	1.667 (6)	Re(1)—Cl(1)	2.632 (4)
Re(1)—P(13)	2.410 (4)	N(12)—P(11)	1.586 (6)
Re(1)—P(14)	2.418 (5)	N(12)—P(12)	1.588 (6)
Re(1)—S(11)	2.499 (4)	P(11)—S(11)	2.023 (4)
Re(1)—S(12)	2.505 (4)	P(12)—S(12)	2.027 (4)
N(11)—Re(1)—P(13)	86.5 (2)	N(11)—Re(1)—Cl(1)	171.2 (2)
N(11)—Re(1)—P(14)	95.2 (2)	P(13)—Re(1)—Cl(1)	88.42 (14)
P(13)—Re(1)—P(14)	96.61 (15)	P(14)—Re(1)—Cl(1)	78.19 (15)
N(11)—Re(1)—S(11)	106.4 (2)	S(11)—Re(1)—Cl(1)	80.35 (14)
P(13)—Re(1)—S(11)	86.14 (14)	S(12)—Re(1)—Cl(1)	85.23 (14)
P(14)—Re(1)—S(11)	158.27 (8)	P(11)—N(12)—P(12)	132.2 (4)
N(11)—Re(1)—S(12)	100.4 (2)	N(12)—P(11)—S(11)	118.0 (2)
P(13)—Re(1)—S(12)	171.67 (7)	N(12)—P(12)—S(12)	118.0 (2)
P(14)—Re(1)—S(12)	87.38 (15)	P(11)—S(11)—Re(1)	102.91 (14)
S(11)—Re(1)—S(12)	87.48 (14)	P(12)—S(12)—Re(1)	105.3 (2)

Scattering factors, dispersion corrections and absorption coefficients were taken from *International Tables for Crystallography* (Vol. C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *CAD-4 Software*, *SDP* (Frenz, 1983) and *HKL* (Kretschmar, 1994). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ZORTEP* (Zsolnai, 1994). Software used to prepare material for publication: *SHELXL93*.

This work was supported by the Deutsche Forschungsgemeinschaft, the DAAD, the British Council and the Fonds der Chemischen Industrie. UA thanks Professor Joachim Strähle, University of Tübingen, for his kind hospitality and for providing the facilities.

Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: FR1002). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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### *cis*-Di(nitrato-*O, O'*)bis(tricyclohexylphosphine oxide-*O*)nickel(II)

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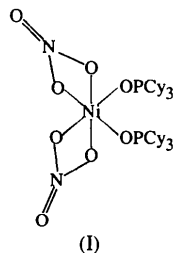
(Received 3 October 1996; accepted 13 November 1996)

#### Abstract

The formal pseudo-octahedral coordination around the Ni<sup>II</sup> atom in the title complex, [Ni(NO<sub>3</sub>)<sub>2</sub>(OPCy<sub>3</sub>)<sub>2</sub>], places the OPCy<sub>3</sub> ligands (C<sub>18</sub>H<sub>33</sub>OP; Cy is cyclohexyl, C<sub>6</sub>H<sub>11</sub>) in an unusual mutually *cis* conformation. This may be rationalized by viewing each bidentate NO<sub>3</sub> group as occupying only one site of a tetrahedral coordination shell.

#### Comment

The ability of stereochemically demanding ligands to stabilize unusual coordination geometries and electronic states has been well documented (Brown & Lee, 1993; Murray, Hope, Hvorslef & Power, 1984). *cis*-[Ni(η<sup>2</sup>-NO<sub>3</sub>)<sub>2</sub>(OPCy<sub>3</sub>)<sub>2</sub>] (I), was obtained during our studies of a series of tricyclohexylphosphine complexes, prepared to help elucidate the nature of this stabilization process.



The coordination geometry about nickel would be conventionally described as octahedral, with six O atoms bound to the metal. Distortion of the octahedron is caused by the intrinsically small bite angles of the bidentate nitrato groups [61.2(1) and 61.6(1)° for O(3)—Ni(1)—O(4) and O(6)—Ni(1)—O(7), respectively]. It has been noted, however, by Cotton & Bergman (1964), that such bidentate ligands may be viewed as occupying one coordination site of a metal. Thus, compound (I) could be described alternatively as having a distorted tetrahedral structure about the Ni(1) atom. This alternative description is supported by the N(1)···Ni(1)···N(2) angle of 108.6(1)° and by consideration of the relative stereochemistry of the OPCy<sub>3</sub> ligands [O(1)—Ni(1)—O(2) 95.3(1) and P(1)···Ni(1)···P(2) 115.92(3)°]. In an octahedral arrangement, these ligands must be viewed as being mutually *cis*. Such a relationship between bulky groups is unexpected. For example, PCy<sub>3</sub> ligands are normally situated *trans* with respect to one another, the *cis* geometry being a rarity (Watson, Woodward, Conole, Kessler & Sykara, 1994; Clark & Hampden-Smith, 1987). Although sterically less demanding than PCy<sub>3</sub>, as defined by the classic cone angle (Tolman, 1977), OPCy<sub>3</sub> is nevertheless a large ligand and it is unusual for such ligands to preferentially adopt a *cis* arrangement. A similar conformation is found in the related complex [Ni(η<sup>2</sup>-NO<sub>3</sub>)<sub>2</sub>(OAsPh<sub>3</sub>)<sub>2</sub>] (Marques & Tomita, 1990) and comparable geometric parameters are in good agreement between the complexes.

The NO<sub>3</sub> ligands are symmetrically bidentate, as classified by Kleywegt *et al.* (1985). The P—O distances of 1.505(3) and 1.502(3) Å are slightly shorter than

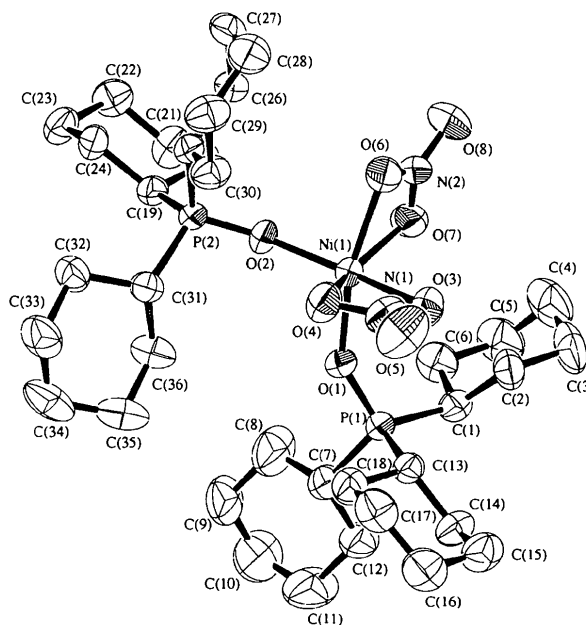


Fig. 1. ORTEP (Johnson, 1976) view of (I) with 50% probability ellipsoids. H atoms have been omitted for clarity.