refinement matrix kept by *RESLSQ* are those relating bonded and next-nearest neighbors.) Final $R(F)$ and $wR = 0.037$ and 0.039 for all data, max. shift in final least-squares cycle 0.019 Å for a hydrogen atom, $S = 1.72$, final difference Fourier excursions 0.30 and -0.18 e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Table 1 lists the coordinates and B_{eq} values for the non-H atoms of ISOE.* Fig. 1 shows the conformation of ISOE. The chirality shown in Fig. 1 was chosen to conform to the absolute configuration of verrucarin A (McPhail & Sim, 1966). As in RORA the C(5)–C(6) bond is somewhat long [1.579 (6) Å in RORA and 1.595 (4) Å in ISOE] and the external CCC angles of the epoxide ring [C(2)–C(12)–C(13) = 125.2 (4) and C(5)–C(12)–C(13) = 128.2 (3)°] are significantly larger than the external CCO angles [C(5)–C(12)–O(2) = 117.6 (3) and C(2)–C(12)–O(2) = 115.6 (3)°]. In RORA these values were 125.6 (4), 126.0 (4), 117.1 (4) and 115.2 (4)° respectively. The conformation of the trichothecene ring system is also similar to that found for RORA. In RORA the configuration at both C(6′) and C(13′) was '*R*' while in ISOE the configuration at both these atoms is '*S*'. In ISOE there is only one intermolecular hydrogen bond. The hydrogen on O(8) is the donor to the ether oxygen O(4) with an O–H distance of 1.89 Å and an O···O distance of 2.89 Å and an O–H···O angle of 172.4°. The only other intermolecular approaches less than van der Waals separations are an O(2)···C(16) approach of 3.01 Å and C(14)···C(14′) approach of 3.53 Å.

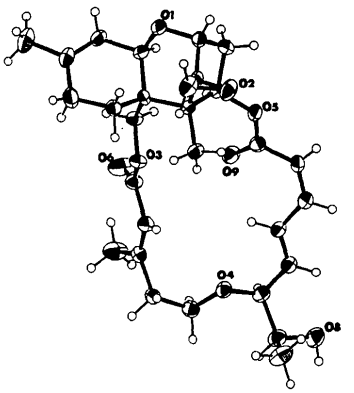

Fig. 1. *ORTEP* (Johnson, 1965) drawing of ISOE. The thermal parameters are drawn at the 50% probability level.

* Lists of structure factors, bond lengths and angles, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42938 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Neurotoxins Producing Parkinson's Syndrome

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Abstract. 1-Methyl-4-phenyl-1,2,5,6-tetrahydropyridinium chloride (I), $C_{12}H_{16}N^+.Cl^-$, $M_r = 209.72$, monoclinic, $P2_1$, $a = 7.014$ (2), $b = 6.634$ (1), $c = 12.248$ (3) Å, $\beta = 96.78$ (2)°, $V = 565.9$ (2) Å^3, $Z = 2$, $D_x = 1.23$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.54178 Å, $\mu = 2.69$ mm^{-1}, $F(000) = 224$, $T = 295$ K, $R = 0.041$ for 1512 observed reflections. 1,3-Dimethyl-4-phenyl-1,2,5,6-tetrahydropyridine–borane complex (II), $C_{13}H_{20}BN$, $M_r = 201.12$, monoclinic, $P2_1/c$, $a = 11.480$ (3), $b = 22.809$ (5), $c = 10.226$ (2) Å, $\beta = 107.76$ (2)°, $V = 2549.7$ (10) Å^3, $Z = 8$, $D_x = 1.05$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.54178 Å, $\mu = 0.412$ mm^{-1}, $F(000) = 880$, $T = 295$ K, final $R = 0.052$ for 2718 observed reflections. 4-(3-Methoxy-4-hydroxyphenyl)-1,2,5,6-tetrahydro-1-pyridinecarbaldehyde (III), $C_{13}H_{15}NO_3$, $M_r = 233.27$, orthorhombic, *Pbca*, $a = 6.563$ (2), $b = 21.964$ (9), $c = 16.016$ (6) Å, $V = 2308$ (1) Å^3, $Z = 8$, $D_x = 1.34$ Mg m^{-3},

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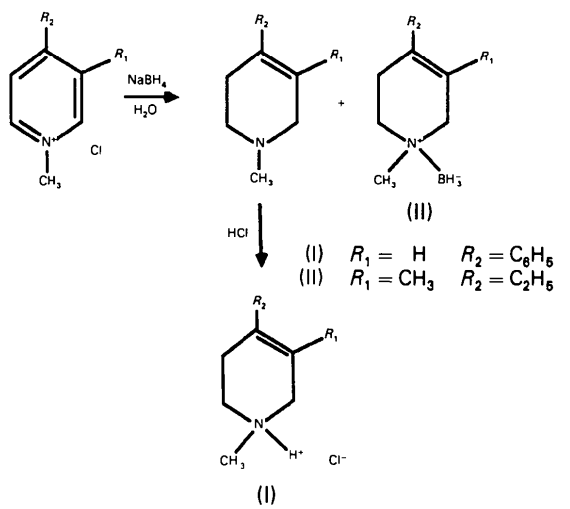
λ(Mo $K\alpha$) = 0·71069 Å, μ = 0·089 mm^{-1}, $F(000)$ = 992, T = 295 K, R = 0·008 for 938 observed reflections. It was recently discovered that (I), also known as MPTP, produces irreversible brain damage similar to that caused by Parkinson's disease. Compounds (II) and (III) were subsequently produced in studies on the synthesis and metabolism of (I). In both (I) and (III) the phenyl ring is essentially coplanar with the tetrahydropyridine ring while in (II) the two rings are rotated with respect to one another. X-ray results also show that the borane group in (II) is covalently bonded to the N atom. The two molecules in the asymmetric unit of (II) are essentially identical in their conformation.

Introduction. 1-Methyl-4-phenyl-1,2,5,6-tetrahydropyridine (MPTP) has been found to be highly neurotoxic in man and in certain animal species, causing effects similar to those observed in Parkinson's disease (Gessner, Brossi, Shen, Fritz & Abell, 1984). This family of compounds is often prepared by reduction of *N*-alkylpyridinium salts with $NaBH_4$. However, such reduction carried out in water also yielded substantial amounts of amine–borane complexes such as (II) as well as the tetrahydropyridines, while reduction in methanol yielded almost no amine–boranes (Gessner & Brossi, 1985). Metabolites of MPTP have also been found to have neurotoxic properties, perhaps many times more potent than MPTP itself. (III) was synthesized in a study of these metabolites (Gessner, Brossi, Shen & Abell, 1985). This paper reports the structures of the neurotoxin MPTP.HCl (I), one of the borane complexes (II), and one of the metabolites (III). The work was done to compare the stereochemistry of the three compounds and to determine the point of attachment of the borane group in (II). All materials were provided by Dr A. Brossi of the National Institutes of Health (Bethesda, Maryland).



Experimental. (I): Crystal size 0·40 × 0·20 × 0·20 mm, unit-cell parameters from a least-squares analysis of 25 reflections with 2θ from 50 to 70°, $P2_1$ derived from systematic absences, 1559 independent reflections with $2\theta_{max}$ = 116°, range of hkl: $h(-7\rightarrow7)$, $k(0\rightarrow7)$, $l(0\rightarrow13)$ plus Friedel equivalents; three standard reflections (400, 040, 009) measured after every 60 new reflections showed an average random variation of 2·0%. D_m not determined, Nicolet R3M diffractometer with graphite monochromator on incident beam, θ–2θ scanning mode with variable scan speed, Lorentz–polarization and absorption (empirical ellipsoidal correction, max. trans. = 0·64, min. trans. = 0·41) corrections. Structure solved by direct methods (Karle & Karle, 1966). Full-matrix least squares, H atoms calculated, C—H = 0·96 Å, H—C—X angles constrained to approach 109·7 or 120°, as appropriate, as closely as was geometrically possible. $\sum w(|F_o|-|F_c|)^2$ minimized where $w = 1/[\sigma^2|F_o| + g(F_o^2)]$ and $g(F_o)^2$ is included to account for random instrumental error (g estimated to be 0·0005). 165 parameters refined: atomic coordinates, anisotropic temperature factors for all non-H atoms, H atoms riding (coordinate shifts of C applied to attached H atoms); disordered phenyl rings refined as two rigid bodies, *i.e.* all distances and angles held fixed, group rotation and translation parameters refined. A maximum of 103 parameters refined each cycle with remaining coordinates fixed which effectively fixed the $P2_1$ y axis origin. R = 0·041, wR = 0·062 for 1512 observed reflections [$F_o > 3\sigma(F_o)$], S = 2·2, $(\Delta/\sigma)_{max}$ = 0·08. Final difference Fourier excursions 0·28 and −0·30 e Å^{-3}.

(II): Crystal size 0·75 × 0·35 × 0·70 mm, unit-cell parameters from least-squares fit of 15 reflections with 2θ from 45 to 51°. $P2_1/c$ from systematic absences, 3626 independent reflections with $2\theta_{max}$ = 116°, range of hkl: $h(0\rightarrow11)$, $k(0\rightarrow24)$, $l(-10\rightarrow10)$, three standards (032, 120, 1,11,1), showed same variation as for (I), same experimental conditions as (I) for data collection and corrections, extinction correction also made. Structure solution as for (I). Full-matrix least squares, H atoms located in difference maps, g = 0·0004, 432 parameters: atomic coordinates for all atoms, anisotropic for non-H atoms, isotropic for H atoms. R = 0·052 and wR = 0·062 for 2718 observed reflections [$F_o > 3\sigma(F_o)$], S = 1·7, (Δ/σ_{max}) = 0·21, final difference Fourier excursions 0·15 and −0·13 e Å^{-3}.

(III): Crystal size 0·35 × 0·35 × 0·05 mm, unit-cell parameters from 24 reflections with 2θ from 10 to 25°, *Pbca* from systematic absences, 1497 independent reflections with $2\theta_{max}$ = 45°, range of hkl: $h(0\rightarrow5)$, $k(0\rightarrow22)$, $l(0\rightarrow17)$, three standards (140, 040, 004) showed same variation as for (I). Structure solved as for (I). Full-matrix least squares, H atoms calculated (as in I), g = 0·0002, 170 parameters, coordinates and anisotropic temperature factors for all non-H atoms,

H atoms riding (shifted along with bonded neighbor atom). Data (from best of three examined crystals) were weak [for 514 of 1497 reflections, $F_o < 3\sigma(|F_o|)$] and of generally poor quality, $R = 0.088$ and $wR = 0.060$ for 983 observed reflections [$F_o > 3\sigma(F_o)$], $S = 1.65$, $(\Delta/\sigma)_{max} = 0.012$, final difference Fourier excursions 0·30 and −0·35 e Å^{-3}. All calculations for all three molecules done using the *SHELXTL* system of programs (Sheldrick, 1980). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Tables 1, 2 and 3 list the refined coordinates and equivalent isotropic U_{eq} values for molecules (I), (II) and (III) respectively.* Bond lengths for the three molecules can be compared in Table 4. The results of the X-ray studies are illustrated in Figs. 1–3. In (I) the heterocyclic ring has an envelope conformation with N(1) being the out-of-plane atom. In (II) and (III) this ring has a flattened half-chair conformation, twisted such that C(6) is slightly below and N(1) is above the plane formed by C(2), C(3), C(4) and C(5). Molecule (I) was found to be disordered with two distinct positions appearing in the electron density maps for each atom of the phenyl ring. The two images of the benzene ring are approximately related to each other by a 21° pivot about an axis passing through C(4) which is perpendicular to the C(2)–C(3)–C(4)–C(5) plane of the dihydropyridine ring. From this experiment, it is not known whether this large excursion is dynamic (a low-frequency lattice vibration) or static ('disorder' from cell to cell). Both images of the benzene ring are shown in Fig. 4, which is a view of the packing of (I) down the *a* axis of the cell. (In Fig. 4, the two molecules within the outlined cell are separated by *ca* 3·5 Å in the viewing direction.) It is possible (in fact, likely) that the molecule actually pivots about an axis closer to the pyridine N atom than C(4); if so, more atoms should be included in the disorder. In view of the agreement factor and our particular interest in the structure, this approach was not pursued further. Some consideration was given to the idea that the 'disorder' was actually an artefact caused by missing a weaker set of layers between the collected layers. However, photographs taken of the diffraction pattern showed no indication of this, and refinement of such a subset of data usually leads to a whole-molecule disorder; this molecule is well behaved in the pyridinium chloride regions of the cell. Each of the disordered rings is twisted very slightly, in opposite directions, out of the plane formed by C(2), C(3), C(4), C(5) and C(6) of the pyridine ring [C(8)–C(7)–C(4)–C(3) = 7·1 and C(8*a*)–C(7*a*)–C(4)–C(3) = −10·5°]. The occupancy ratio for the

Table 1. *Molecule* (I). *Fractional coordinates and equivalent isotropic thermal parameters*

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

	x	y	z	$U_{eq}(\times 10^2)$Å^2
Cl	1·1710 (1)	0·2275 (5)	0·8963 (1)	7·4 (1)
N(1)	0·7383 (2)	0·2268 (8)	0·8814 (1)	5·0 (1)
C(2)	0·6537 (7)	0·0443 (7)	0·8238 (3)	6·1 (1)
C(3)	0·7014 (8)	0·0499 (9)	0·7054 (4)	8·2 (2)
C(4)	0·7133 (3)	0·2354 (12)	0·6487 (2)	5·9 (1)
C(5)	0·7106 (9)	0·4167 (10)	0·7077 (4)	8·2 (2)
C(6)	0·6720 (4)	0·4087 (4)	0·8207 (2)	6·7 (1)
C(7)	0·7371 (12)	0·2693 (8)	0·5269 (4)	5·8 (3)
C(8)	0·7265 (12)	0·0986 (8)	0·4600 (4)	6·1 (3)
C(9)	0·7569 (12)	0·1155 (8)	0·3498 (4)	10·2 (5)
C(10)	0·7978 (12)	0·3031 (8)	0·3066 (4)	8·0 (4)
C(11)	0·8083 (12)	0·4738 (8)	0·3736 (4)	8·8 (4)
C(12)	0·7779 (12)	0·4569 (8)	0·4837 (4)	7·8 (4)
C(13)	0·6967 (3)	0·2272 (12)	0·9982 (2)	6·7 (1)
C(7*a*)†	0·7413 (11)	0·1846 (12)	0·5296 (5)	5·6 (3)
C(8*a*)	0·7822 (11)	−0·0020 (12)	0·4853 (5)	7·5 (4)
C(9*a*)	0·8192 (11)	−0·0155 (12)	0·3761 (5)	10·0 (4)
C(10*a*)	0·8154 (11)	0·1577 (12)	0·3113 (5)	8·8 (4)
C(11*a*)	0·7745 (11)	0·3443 (12)	0·3556 (5)	6·9 (3)
C(12*a*)	0·7375 (11)	0·3577 (12)	0·4648 (5)	8·3 (4)

† Atoms C(7*a*)–C(12*a*) are the disordered atoms [occupancy factor = 0·49 (1)].

Table 2. *Molecule* (II). *Fractional coordinates and equivalent isotropic thermal parameters*

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

	x	y	z	$U_{eq}(\times 10^2)$Å^2
Molecule 1				
N(1)	0·5603 (2)	0·2114 (1)	0·3070 (2)	6·3 (1)
B	0·5905 (4)	0·2791 (1)	0·2810 (3)	9·5 (2)
C(2)	0·5331 (2)	0·1779 (1)	0·1761 (2)	6·2 (1)
C(3)	0·4761 (2)	0·1186 (1)	0·1773 (2)	5·4 (1)
C(4)	0·4258 (2)	0·1032 (1)	0·2736 (2)	5·3 (1)
C(5)	0·4181 (3)	0·1466 (1)	0·3818 (3)	7·2 (1)
C(6)	0·4485 (2)	0·2079 (1)	0·3531 (2)	7·3 (1)
C(7)	0·3771 (2)	0·0436 (1)	0·2850 (2)	5·6 (1)
C(8)	0·4454 (2)	−0·0059 (1)	0·2766 (3)	7·1 (1)
C(9)	0·4024 (2)	−0·0619 (1)	0·2866 (3)	8·5 (1)
C(10)	0·2931 (2)	−0·0696 (1)	0·3077 (3)	8·7 (1)
C(11)	0·2238 (2)	−0·0219 (1)	0·3196 (3)	8·3 (1)
C(12)	0·2656 (2)	0·0347 (1)	0·3075 (2)	7·0 (1)
C(13)	0·6664 (3)	0·1851 (1)	0·4114 (3)	8·4 (1)
C(14)	0·4785 (2)	0·0824 (1)	0·0556 (3)	6·9 (1)
Molecule 2				
N(1′)	0·0974 (2)	0·1926 (1)	0·8667 (2)	6·3 (1)
B′	0·1270 (3)	0·2598 (1)	0·9172 (3)	8·9 (2)
C(2′)	0·1855 (2)	0·1724 (1)	0·7950 (3)	7·1 (1)
C(3′)	0·1869 (2)	0·1079 (1)	0·7704 (2)	6·4 (1)
C(4′)	0·1410 (2)	0·0689 (1)	0·8393 (2)	5·9 (1)
C(5′)	0·0835 (2)	0·0898 (1)	0·9458 (2)	6·9 (1)
C(6′)	0·1106 (3)	0·1530 (1)	0·9868 (3)	7·6 (1)
C(7′)	0·1394 (2)	0·0043 (1)	0·8185 (2)	6·4 (1)
C(8′)	0·1814 (2)	−0·0332 (1)	0·9277 (2)	7·0 (1)
C(9′)	0·1760 (3)	−0·0935 (1)	0·9106 (3)	8·4 (1)
C(10′)	0·1256 (3)	−0·1167 (1)	0·7826 (4)	10·0 (2)
C(11′)	0·0842 (3)	−0·0800 (1)	0·6714 (3)	11·9 (2)
C(12′)	0·0913 (3)	−0·0201 (1)	0·6888 (3)	9·7 (1)
C(13′)	−0·0292 (2)	0·1899 (1)	0·7700 (3)	8·7 (1)
C(14′)	0·2522 (3)	0·0930 (2)	0·6676 (3)	9·3 (1)

* Lists of structure factors, bond angles, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42954 (36 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

two positions refined to be 51:49. There is an N^+—H···Cl hydrogen bond in (I) with the N—H distance at 1·01 Å, the N···Cl distance at 3·02 Å, the H···Cl distance at 2·01 Å and the N—H···Cl angle at 169·7°.

The asymmetric unit of (II) contains two molecules; since both show the same conformation, only one is shown in Fig. 2. In (I) and (III) the two rings are essentially coplanar [average C(8)–C(7)–C(4)–C(3) torsion for the disordered structure in (I) is 8·8°; in (III) this angle is 5·8°]; however, in (II) the two rings are rotated with respect to one another [C(8)–C(7)–C(4)–C(3) = 46·8 and C(8′)–C(7′)–C(4′)–C(3′) = −52·5°]. This twist about the C(7)–C(4) bond is probably due to the presence of the methyl group on C(3) in (II) as opposed to an H atom on C(3) in (I) and

Table 3. *Molecule* (III). *Fractional coordinates and equivalent isotropic thermal parameters*

$$U_{eq} = \tfrac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{eq}(\times 10^2)$Å^2
N(1)	−0·2746 (7)	0·6241 (2)	0·3807 (3)	3·9 (2)
C(2)	−0·3536 (9)	0·5790 (2)	0·4380 (4)	4·8 (2)
C(3)	−0·2555 (11)	0·5180 (3)	0·4230 (4)	5·8 (3)
C(4)	−0·0781 (8)	0·5106 (2)	0·3803 (3)	3·7 (2)
C(5)	0·0203 (9)	0·5629 (2)	0·3431 (4)	6·2 (3)
C(6)	−0·0555 (8)	0·6244 (2)	0·3711 (4)	4·6 (2)
C(7)	0·0203 (8)	0·4491 (2)	0·3686 (3)	3·2 (2)
C(8)	−0·0862 (9)	0·3962 (2)	0·3964 (3)	4·0 (2)
C(9)	−0·0018 (8)	0·3389 (2)	0·3856 (3)	3·6 (2)
O(9)	−0·0912 (7)	0·2855 (2)	0·4111 (3)	4·9 (2)
C(10)	0·1824 (8)	0·3318 (3)	0·3455 (3)	3·8 (2)
O(10)	0·2698 (6)	0·2761 (1)	0·3312 (2)	5·0 (1)
C(11)	0·2879 (9)	0·3835 (2)	0·3182 (3)	4·3 (2)
C(12)	0·2016 (9)	0·4410 (3)	0·3302 (3)	4·1 (2)
C(13)	−0·3968 (9)	0·6627 (2)	0·3394 (3)	4·5 (2)
O(13)	−0·5835 (7)	0·6639 (2)	0·3463 (3)	5·6 (2)
C(15)	−0·2884 (9)	0·2878 (2)	0·4472 (3)	6·0 (3)

Table 4. *Bond lengths* (Å)

	Molecule (I)	Molecule (II)		Molecule (III)
		Molecule 1	Molecule 2	
N(1)–C(2)	1·489 (6)	1·489 (3)	1·491 (4)	1·477 (7)
N(1)–C(6)	1·464 (5)	1·499 (4)	1·494 (3)	1·447 (7)
N(1)–C(13)	1·493 (2)	1·480 (3)	1·488 (3)	1·342 (7)
N(1)–B		1·622 (3)	1·620 (3)	
C(2)–C(3)	1·527 (7)	1·504 (3)	1·494 (3)	1·506 (8)
C(3)–C(4)	1·420 (9)	1·331 (3)	1·338 (3)	1·361 (9)
C(4)–C(5)	1·404 (9)	1·507 (3)	1·511 (4)	1·447 (8)
C(4)–C(7)	1·537 (6)	1·490 (3)	1·488 (3)	1·508 (7)
C(4*a*)–C(7*a*)	1·532 (7)			
C(5)–C(6)	1·442 (6)	1·492 (3)	1·508 (3)	1·508 (7)
C(7)–C(8)	1·395*	1·390 (3)	1·373 (3)	1·428 (7)
C(7)–C(12)	1·395	1·384 (4)	1·388 (3)	1·352 (8)
C(8)–C(9)	1·395	1·385 (3)	1·385 (3)	1·386 (7)
C(9)–C(10)	1·395	1·349 (3)	1·366 (4)	1·378 (8)
C(9)–O(9)				1·374 (6)
C(10)–O(10)				1·371 (6)
C(10)–C(11)	1·395	1·376 (4)	1·373 (4)	1·401 (8)
C(11)–C(12)	1·395	1·395 (4)	1·379 (4)	1·396 (8)
C(3)–C(14)		1·501 (13)	1·505 (4)	
O(9)–C(15)				1·418 (7)
O(13)–C(13)				1·231 (8)

* Disordered phenyl rings were refined as rigid bodies.

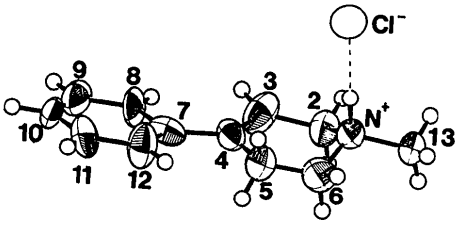


Fig. 1. *ORTEP* (Johnson, 1965) drawing of (I) showing the numbering used. Thermal ellipsoids are drawn at the 50% probability level.

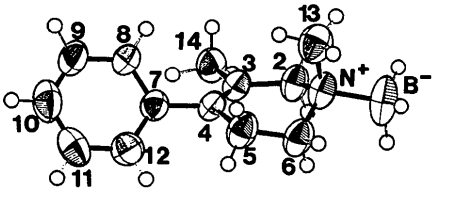


Fig. 2. *ORTEP* drawing of the structural results for molecule (II) showing one of the two molecules in the asymmetric unit. Thermal ellipsoids are drawn at the 50% probability level.

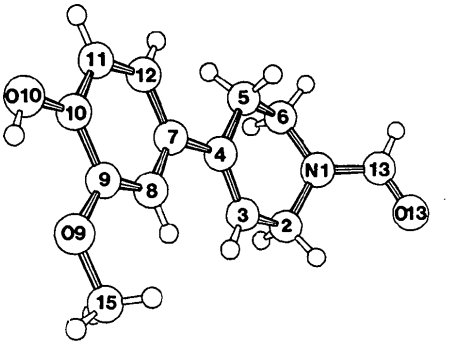


Fig. 3. *ORTEP* drawing of (III) with arbitrary thermal parameters. The numbering used in the discussion is also shown.

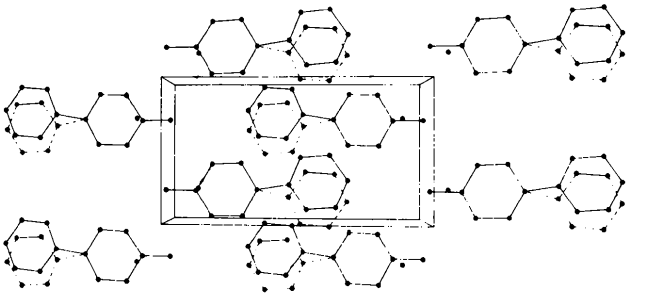


Fig. 4. The contents of the unit cell for molecule (I) illustrating the disordered phenyl ring. The view is shown looking down the *a* axis with *b* vertical and *c* horizontal.

(III). In (I) and (III) where the pseudo bi-aryl conformation allows resonance overlap between the rings there is still inter-ring steric hindrance. In (I), the H(3)···H(8) separation is 2·19 Å [H(3)···H(8a) = 1·82 Å] and in (III) the distance is 1·97 Å, compared to the usual van der Waals H···H contact range of 2·2–2·4 Å. In (III) the formyl group on N(1) is coplanar with the pyridyl N and its adjacent atoms. It is interesting to note that in (I) the CH_3 group on N(1) is equatorial and the H atom is axial while in (II) the CH_3 group on N(1) is axial and the BH_3 moiety is equatorial. In (II), which has a density of only 1·05 Mg m^{-3}, there are no intermolecular approaches less than van der Waals radii. Molecules of (III) form hydrogen-bonded chains in the crystal with the hydroxyl H bonding to the carbonyl of the next molecule [O···O = 2·76 (1) Å, O–H···O = 158 (3)°].

Note added in proof: An independent determination of (I) at 100 K was recently published (Klein, Borne & Stevens, 1985).

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Structure of *trans*-*N*-(1-Benzyl-4-methyl-3-pyrrolidinyl)-5-chloro-2-methoxy-4-methylaminobenzamide Hydrochloride*

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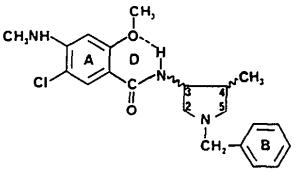
Abstract. $C_{21}H_{27}ClN_3O_2^+Cl^-$, $M_r = 424·37$, monoclinic, $P2_1/c$, $a = 15·863$ (1), $b = 12·660$ (1), $c = 11·264$ (1) Å, $\beta = 106·47$ (1)°, $V = 2169·3$ (3) Å^3, $D_x = 1·299$ g cm^{-3}, $Z = 4$, room temperature, $F(000) = 896$, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 28·6$ cm^{-1}, $R = 0·057$ for 2261 observed reflections with $|F_o| > 3\sigma(|F_o|)$. An intramolecular hydrogen bond between the amide N and the methoxy O is observed. The distance between the tertiary N and the center of the benzene ring is 6·91 Å, and the deviation of the N from the plane of the benzene ring is 1·75 Å.

Introduction. The crystal structure determination of the title compound (1) was undertaken as part of serial studies for finding new potent neuroleptic drugs in the benzamide derivatives. The previous papers (Furuya, Iwanami, Takenaka & Sasada, 1982; Furuya, Iwanami, Takenaka & Sasada, 1986) have reported the crystal structures of the benzamide derivatives having a methyl group at the 2-position of the pyrrolidine ring. The present compound has a methyl group at the 4-position of the ring and it has intermediate activity.



(1) Title compound; (3*R*, 4*S*) and (3*S*, 4*R*).

cf.

(2) YM-09151-2; Methyl group at 2-position [(2*R*, 3*R*) and (2*S*, 3*S*)]

(3) YM-09151-1; Methyl group at 2-position [(2*R*, 3*S*) and (2*S*, 3*R*)]

* New Potent Neuroleptic Drugs of Benzamide Derivatives. V.

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