Crystal Structure and Absolute Configuration of Dihydro-*O*-methylcancentrinemethine Hydrobromide, a Derivative of the Alkaloid Cancentrine

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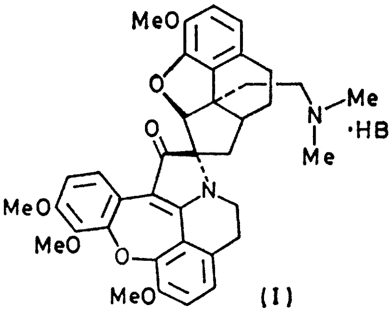
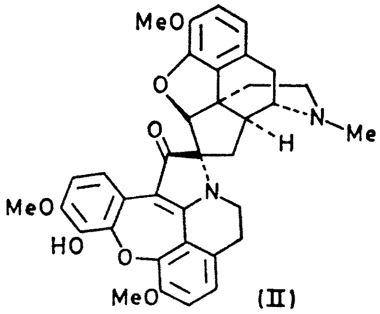
The crystal and molecular structure and the absolute configuration of the title compound has been determined by *X*-ray diffraction methods. The crystals are orthorhombic with cell dimensions: $a = 10{\cdot}639 \pm 0{\cdot}002$, $b = 12{\cdot}036 \pm 0{\cdot}004$, and $c = 26{\cdot}979 \pm 0{\cdot}007$ Å, space group $P2_12_12_1$. $Z = 4$. The structure was solved by the heavy-atom method. After refinement by least-squares methods using anisotropic thermal parameters. R was 0·072 for 2475 observed reflections. The molecule consists of two units derived from morphine and cularine, linked by a spiro-ring junction. The absolute configuration was determined and shows that the morphine-related fragment has the opposite configuration to that found in morphine.

CANCENTRINE (F-22), the yellow alkaloid of *Dicentra canadensis*, was first isolated forty years ago.[1] After all subsequent investigations failed to elucidate the structure, an *X*-ray crystallographic study was undertaken.



(I)



(II)

Unit-cell dimensions and space groups of several derivatives were determined before crystals of the dihydro-*O*-methyl methine hydrobromide (I) salt appeared to be suitable. The subsequent deduction of the structure of the parent alkaloid cancentrine (II) has been outlined in our preliminary report.[2]

EXPERIMENTAL

The compound crystallizes from methanol as pale yellow needles. Preliminary Weissenberg photographs showed the crystals to be orthorhombic.

Crystal Data.—$C_{38}H_{42}N_2O_7$,HBr, $M = 719{\cdot}69$, Orthorhombic, $a = 10{\cdot}639 \pm 0{\cdot}002$, $b = 12{\cdot}036 \pm 0{\cdot}004$, $c = 26{\cdot}979 \pm 0{\cdot}007$ Å, $U = 3454{\cdot}6$ Å^3, D_m (by flotation) $= 1{\cdot}37 \pm 0{\cdot}01$, $Z = 4$, $D_c = 1{\cdot}379 \pm 0{\cdot}001$, $F(000) = 1504$. Cu-K_α radiation, $\lambda(\alpha_1) = 1{\cdot}54051$, $\lambda(\beta) = 1{\cdot}39217$ Å, $\mu(\text{Cu-}K_\alpha) = 22{\cdot}0$ cm^{-1}. Systematic absences: $h00$ for $h = 2n + 1$, $0k0$ for $k = 2n + 1$ and $00l$ for $l = 2n + 1$, indicate space group $P2_12_12_1(D_2^4)$.

The crystal used for the intensity measurements had dimensions $0{\cdot}115 \times 0{\cdot}095 \times 0{\cdot}075$ mm. The intensity data were measured by use of the stationary-crystal–stationary-counter technique, with nickel-filtered Cu-K_α radiation. All the unique reflections with $2\theta \leq 135°$ were measured first and then an additional 6100 of the 6955 reflections in the hemisphere, giving three measurements for most reflections. A correction (maximum 7%) was applied for the decrease in the intensities of the four standard reflections which were measured after every 100 reflections. A total of 3509 independent reflections was obtained after averaging equivalent reflections, of which 2475 having $I \geqslant 1{\cdot}2$ times the respective background counts were considered observed. The remaining 1034 unobserved reflections were entered as 0·1 times the appropriate background count and were flagged with a minus sign. These

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[1] R. H. F. Manske, *Canad. J. Res.*, 1932, **7**, 258.

[2] G. R. Clark, R. H. Manske, G. J. Palenik, R. Rodrigo, D. B. MacLean, L. Baczynskyj, D. E. F. Gracey, and J. K. Saunders, *J. Amer. Chem. Soc.*, 1970, **92**, 4998.

values were then corrected for the $\alpha_1 - \alpha_2$ splitting at 2θ values greater than 80° and then converted to a set of structure amplitudes by standard means.

Structure Analysis.—The position of the bromine atom was determined from a sharpened Patterson function. The bromine atom was close to $z = \frac{1}{4}$ so that the Fourier synthesis phased on only the bromine atom contribution contained many false maxima. Consequently, four Fourier syntheses and one difference Fourier synthesis were required before all the lighter atoms could be located. One full-matrix least-squares cycle was calculated in which all the atoms (except bromine) were treated as carbon atoms. The resulting lower isotropic thermal parameters for the nitrogen and oxygen atoms, in conjunction with chemical evidence, was used to distinguish these atoms from the remaining carbon atoms. Two additional least-squares cycles were computed after all the atoms had been correctly identified and R was reduced to 0·12. All atoms were then assigned anisotropic thermal parameters and subsequent refinements were carried out using a block-diagonal approximation to the matrix. One-half the calculated shift was applied during each cycle. After 10 cycles, the shifts were $<0{\cdot}7\sigma$ and the refinement was terminated; R was 0·072. No attempt was made to locate the 43 hydrogen atoms. The final parameters are given in Table 1. Observed and calculated structure factors are listed in Supplementary Publication No. SUP 20386 (4 pp., 1 microfiche).†

TABLE 1

Final positional and thermal parameters ($\times 10^{-4}$) * with their estimated standard deviations in parentheses

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Br(1)	1770(1)	2155(1)	2410(1)	69	74	29	0	−1	−14
O(1)	1655(6)	7291(5)	3357(2)	51	38	7	6	0	8
O(2)	−2506(6)	10,029(6)	3868(2)	43	53	7	7	−3	5
O(3)	1791(6)	8546(5)	4321(3)	35	56	12	0	−4	2
O(4)	3935(6)	8069(6)	2913(3)	52	61	12	4	10	13
O(5)	−4963(6)	10,277(6)	3822(3)	42	70	24	28	−16	−12
O(6)	−3015(6)	12,121(6)	4194(3)	61	53	14	31	7	−4
O(7)	−1326(8)	13,294(6)	4713(3)	130	28	21	10	−14	−9
N(1)	−0941(6)	6951(6)	4226(3)	30	27	8	3	6	−4
N(2)	−0031(8)	4220(7)	2428(3)	79	67	8	−23	10	−7
C(1)	1309(8)	5406(7)	3649(3)	47	39	6	6	0	4
C(2)	1279(9)	5048(8)	4200(3)	62	36	6	37	0	−6
C(3)	2477(11)	4352(9)	4360(4)	96	55	10	69	−15	3
C(4)	3337(11)	3949(9)	3917(4)	75	64	15	70	14	12
C(5)	3643(9)	4935(8)	3592(4)	63	38	10	32	2	−4
C(6)	2632(8)	5639(8)	3514(3)	43	49	4	7	−5	−5
C(7)	2742(9)	6672(7)	3318(3)	48	30	5	12	−9	−1
C(8)	3894(9)	7030(8)	3123(3)	55	43	8	0	1	−1
C(9)	4911(10)	6320(9)	3176(4)	55	66	9	25	2	−5
C(10)	4797(10)	5296(9)	3419(4)	70	68	9	40	−2	−6
C(11)	0734(8)	6597(7)	3617(3)	37	35	7	3	−2	0
C(12)	0430(8)	6961(8)	4163(3)	42	49	4	6	−4	5
C(13)	1163(10)	6156(8)	4490(4)	69	43	9	8	−2	2
C(14)	0726(7)	8200(7)	4267(3)	18	52	4	−10	0	1
C(15)	−0428(8)	8790(7)	4263(3)	32	43	5	10	1	−9
C(16)	−1371(7)	8003(8)	4225(3)	29	46	5	1	3	3
C(17)	−2745(8)	8173(8)	4202(3)	31	56	8	−16	4	−10
C(18)	−3535(8)	7266(9)	4337(3)	35	66	7	−19	8	−23
C(19)	−2924(9)	6174(8)	4449(4)	60	52	8	−39	17	2
C(20)	−1793(10)	5990(8)	4134(3)	59	38	9	−18	8	−5
C(21)	−4814(9)	7427(10)	4320(4)	43	107	10	−51	0	−25
C(22)	−5324(9)	8428(10)	4158(4)	27	77	12	1	−3	−29
C(23)	−4548(9)	9294(9)	4014(4)	32	70	12	4	0	−26
C(24)	−3253(9)	9155(8)	4059(3)	33	53	9	7	4	−23
C(25)	−0610(8)	9962(8)	4368(3)	31	40	6	−17	9	12
C(26)	−1651(9)	10,525(7)	4208(3)	39	43	6	−17	2	−7
C(27)	−1915(9)	11,635(8)	4325(4)	57	37	10	−3	14	10
C(28)	−1022(10)	12,199(9)	4615(4)	89	39	8	7	3	0
C(29)	0018(10)	11,672(9)	4786(4)	81	40	10	−4	−4	−10
C(30)	0252(10)	10,575(8)	4645(3)	68	38	7	−21	−4	3
C(31)	0628(9)	4569(8)	3317(4)	59	52	7	−9	−8	−7
C(32)	0679(10)	4955(9)	2775(4)	65	54	8	−42	−3	−18
C(33)	−1359(11)	4020(11)	2589(5)	76	93	18	−90	−6	−28
C(34)	−0022(15)	4698(12)	1909(4)	162	101	8	−42	−2	−10
C(35)	5110(12)	8434(11)	2696(5)	88	77	24	−20	39	34
C(36)	−6249(11)	10,335(11)	3667(5)	60	90	24	42	−31	−20
C(37)	−3069(14)	12,507(13)	3702(6)	120	132	22	60	−7	38
C(38)	−0790(16)	13,768(11)	5155(5)	201	64	13	0	−14	−19

* The temperature factor for an atom is of the form $\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - \beta_{12}hk - \beta_{13}hl - \beta_{23}kl)$.

The quantity $\Sigma w(F_o - F_c)^2$ was minimized in the least-squares calculations. The weighting scheme used was $\sqrt{w} = F_o/20$ if $F_o < 20$, $\sqrt{w} = 1$ if $20 < F_o < 40$ and $\sqrt{w} = 40_o/F$ if $F_o > 40$. The scattering factors for bromine[3] were corrected for real dispersion effects. The

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† For details of Supplementary Publications, see Notice to Authors No. 7 in *J. Chem. Soc.* (*A*), Issue No. 20 (items less than 10 pp. will be supplied as full size copies).

[3] H. P. Hanson, F. Herman, J. D. Lea, and S. Skillman, *Acta Cryst.*, 1964, **17**, 1040.

scattering factors for carbon, nitrogen, and oxygen were taken from ref. 4.

Absolute Configuration.—The chirality of the molecule was determined by use of the anomalous dispersion factor of the bromine atom.[5] Eighteen reflections were selected on the basis of their relatively large calculated differences between $I_{\bar{h}\bar{k}\bar{l}}$ and I_{hkl}. Each reflection hkl and its corresponding Friedel partner $\bar{h}\bar{k}\bar{l}$ were measured and the intensities compared with those previously calculated assuming the listed atomic co-ordinates relative to a right-handed axial system (Table 1). The results are outlined in Table 2.

TABLE 2

Friedel Pairs: comparison of integrated intensities and calculated values

			Obs.		Calc.
h	k	l	I_{hkl}	$I_{\bar{h}\bar{k}\bar{l}}$	$I_{hkl} >< I_{\bar{h}\bar{k}\bar{l}}$
1	1	1	1159	756	>
1	3	10	357	311	>
1	3	13	125	97	>
1	4	7	153	188	<
1	5	3	426	372	>
1	5	7	208	145	>
2	1	10	428	528	<
2	3	3	351	303	>
2	5	2	452	414	>
3	4	1	591	499	>
4	1	12	156	186	<
4	3	2	343	388	<
4	3	3	868	927	<
4	3	4	374	410	<
4	3	8	164	199	<
4	5	2	291	238	>
5	1	5	448	360	>
7	3	2	156	113	>

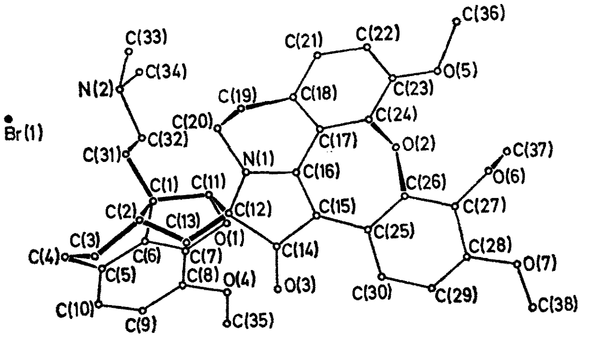
The comparison establishes the absolute configuration of the molecule as being the same as the listed co-ordinates and as illustrated in the diagram. The chirality of the morphine-related segment of the molecule is seen to be the opposite of that of morphine itself,[6] but the same as some other morphine-related alkaloids *e.g.*, (+)-kreysiginine.[7]

DISCUSSION

The overall molecular geometry is illustrated in the Figure. The basic skeleton is composed of two major fragments, modified cularine[8] and morphine, joined by a spiro-ring junction at C(12). The structure of the parent alkaloid cancentrine was deduced from the present derivative and differs mainly in that N(2) is bonded to C(6), forming another heterocyclic ring.

The intramolecular bond distances and angles are listed in Tables 3 and 4, together with their estimated standard deviations. The bond lengths of O(3)–C(14), C(14)–C(15), C(15)–C(16), and C(16)–N(1) indicate an extensive delocalization characteristic of the vinylogous amide grouping. The remaining bond distances appear normal. The mean values for different bond types are: C(Ph)–O(ether) 1·369, O(ether)–C(Me) 1·433, C=C-(aromatic) 1·387, N(sp^3)–C(sp^3) 1·502, and C(sp^3)–C(sp^3) 1·542 Å.

The cularine fragment contains three heterocyclic ring systems. The seven-membered ring defined by atoms O(2), C(15), C(16), C(17), C(24), and C(28) is boat-like, the ring defined by atoms N(1), C(16), C(17), C(18), C(19), and C(20) has a half-boat conformation while the ring N(1), C(12), C(14), C(15), and C(16) is approximately planar. The best-fitting plane through each non-aromatic ring system is given in Table 5, together with selected displacements of other atoms from the plane.



The molecular stereochemistry and atomic numbering. The absolute configuration is that shown in the diagram

TABLE 3

Bond distances (Å) and their estimated standard deviations

Br(1) · · · N(2)	3·140(9)	C(5)–C(6)	1·385(13)
O(1)–C(7)	1·380(11)	C(5)–C(10)	1·383(15)
O(1)–C(11)	1·466(11)	C(6)–C(7)	1·355(13)
O(2)–C(24)	1·414(12)	C(7)–C(8)	1·401(13)
O(2)–C(26)	1·423(11)	C(8)–C(9)	1·385(14)
O(3)–C(14)	1·216(10)	C(9)–C(10)	1·402(15)
O(4)–C(8)	1·374(12)	C(11)–C(12)	1·570(12)
O(4)–C(35)	1·450(15)	C(12)–C(13)	1·525(13)
O(5)–C(23)	1·365(13)	C(12)–C(14)	1·549(13)
O(5)–C(36)	1·433(14)	C(14)–C(15)	1·418(12)
O(6)–C(27)	1·355(12)	C(15)–C(16)	1·383(12)
O(6)–C(37)	1·409(17)	C(15)–C(25)	1·452(13)
O(7)–C(28)	1·382(13)	C(16)–C(17)	1·478(12)
O(7)–C(38)	1·441(16)	C(17)–C(18)	1·425(14)
N(1)–C(12)	1·470(11)	C(17)–C(24)	1·356(14)
N(1)–C(16)	1·346(11)	C(18)–C(19)	1·497(14)
N(1)–C(20)	1·490(12)	C(18)–C(21)	1·375(13)
N(2)–C(32)	1·493(13)	C(19)–C(20)	1·489(14)
N(2)–C(33)	1·498(15)	C(21)–C(22)	1·391(16)
N(2)–C(34)	1·514(15)	C(22)–C(23)	1·385(15)
C(1)–C(2)	1·550(13)	C(23)–C(24)	1·394(14)
C(1)–C(6)	1·481(13)	C(25)–C(26)	1·368(12)
C(1)–C(11)	1·562(13)	C(25)–C(30)	1·394(13)
C(1)–C(31)	1·530(14)	C(26)–C(27)	1·402(13)
C(2)–C(3)	1·584(15)	C(27)–C(28)	1·406(14)
C(2)–C(13)	1·551(14)	C(28)–C(29)	1·356(15)
C(3)–C(4)	1·581(16)	C(29)–C(30)	1·396(14)
C(4)–C(5)	1·512(15)	C(31)–C(32)	1·535(14)

In the morphine-like portion, the stereochemical features are similar to the corresponding segments in

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[4] 'International Tables for *X*-Ray Crystallography,' vol. III, Kynoch Press, Birmingham, 1962, p. 201.

[5] J. M. Bijvoet, A. F. Peerdeman, and A. J. van Bommel, *Nature*, 1951, **168**, 271.

[6] M. Mackay and D. C. Hodgkin, *J. Chem. Soc.*, 1965, 3261.

[7] J. Fridrichsons, A. McL. Mathieson, and M. F. Mackay, *Tetrahedron*, 1970, **26**, 1869.

[8] R. H. F. Manske, *Alkaloids*, 1954, **4**, 249.

morphine.[6] However, as noted, the chirality is opposite to that of morphine.* The atoms O(1), C(1), C(6), C(7), C(11), and C(1), C(2), C(11), C(12), C(13), both define rings which, though puckered, are almost planar. The six-membered ring formed by C(1), C(2), C(3), C(4), C(5), and C(6), is seen to be a slightly flattened boat. In both morphine and the parent alkaloid, N(2) forms another heterocyclic ring system which is opened in forming the present derivative.

TABLE 4

Bond angles (°) and their estimated standard deviations

C(7)–O(1)–C(11)	106·8(0·6)	C(11)–C(12)–C(13)	105·1(0·7)
C(24)–O(2)–C(26)	115·9(0·7)	C(11)–C(12)–C(14)	113·3(0·7)
C(8)–O(4)–C(35)	118·0(0·8)	C(13)–C(12)–C(14)	113·8(0·7)
C(23)–O(5)–C(36)	117·6(0·9)	C(2)–C(13)–C(12)	107·2(0·8)
C(27)–O(6)–C(37)	115·0(0·9)	O(3)–C(14)–C(12)	122·7(0·8)
C(28)–O(7)–C(38)	116·3(0·9)	O(3)–C(14)–C(15)	129·5(0·8)
C(12)–N(1)–C(16)	109·2(0·7)	C(12)–C(14)–C(15)	107·7(0·7)
C(12)–N(1)–C(20)	126·2(0·7)	C(14)–C(15)–C(16)	106·6(0·7)
C(16)–N(1)–C(20)	121·6(0·7)	C(14)–C(15)–C(25)	126·9(0·8)
Br(1) · · · N(2)–C(32)	99·8(0·6)	C(16)–C(15)–C(25)	125·6(0·8)
Br(1) · · · N(2)–C(33)	116·9(0·7)	N(1)–C(16)–C(15)	113·4(0·8)
Br(1) · · · N(2)–C(34)	106·4(0·7)	N(1)–C(16)–C(17)	117·8(0·8)
C(32)–N(2)–C(33)	113·0(0·8)	C(15)–C(16)–C(17)	128·8(0·8)
C(32)–N(2)–C(34)	110·6(0·9)	C(16)–C(17)–C(18)	117·8(0·8)
C(33)–N(2)–C(34)	109·6(0·9)	C(16)–C(17)–C(24)	121·8(0·8)
C(2)–C(1)–C(6)	108·0(0·7)	C(18)–C(17)–C(24)	120·4(0·9)
C(2)–C(1)–C(11)	107·4(0·7)	C(17)–C(18)–C(19)	117·9(0·8)
C(2)–C(1)–C(31)	111·6(0·7)	C(17)–C(18)–C(21)	117·9(0·9)
C(6)–C(1)–C(11)	100·7(0·7)	C(19)–C(18)–C(21)	124·1(0·9)
C(6)–C(1)–C(31)	115·6(0·8)	C(18)–C(19)–C(20)	111·5(0·8)
C(11)–C(1)–C(31)	112·8(0·7)	N(1)–C(20)–C(19)	106·3(0·8)
C(1)–C(2)–C(3)	113·0(0·8)	C(18)–C(21)–C(22)	121·2(1·0)
C(1)–C(2)–C(13)	104·3(0·7)	C(21)–C(22)–C(23)	120·5(1·0)
C(3)–C(2)–C(13)	112·4(0·8)	O(5)–C(23)–C(22)	124·5(0·9)
C(2)–C(3)–C(4)	115·0(0·9)	O(5)–C(23)–C(24)	117·2(0·9)
C(3)–C(4)–C(5)	108·8(0·9)	C(22)–C(23)–C(24)	118·4(0·9)
C(4)–C(5)–C(6)	113·7(0·9)	O(2)–C(24)–C(17)	121·9(0·8)
C(4)–C(5)–C(10)	129·3(0·9)	O(2)–C(24)–C(23)	115·8(0·8)
C(6)–C(5)–C(10)	116·5(0·9)	C(17)–C(24)–C(23)	121·5(0·9)
C(1)–C(6)–C(5)	125·8(0·8)	C(15)–C(25)–C(26)	121·9(0·8)
C(1)–C(6)–C(7)	110·6(0·8)	C(15)–C(25)–C(30)	122·1(0·8)
C(5)–C(6)–C(7)	123·6(0·9)	C(26)–C(25)–C(30)	116·1(0·8)
O(1)–C(7)–C(6)	113·2(0·8)	O(2)–C(26)–C(25)	120·9(0·8)
O(1)–C(7)–C(8)	126·5(0·8)	O(2)–C(26)–C(27)	114·6(0·8)
C(6)–C(7)–C(8)	120·2(0·8)	C(25)–C(26)–C(27)	124·3(0·8)
O(4)–C(8)–C(7)	117·5(0·8)	O(6)–C(27)–C(26)	121·7(0·8)
O(4)–C(8)–C(9)	125·3(0·9)	O(6)–C(27)–C(28)	121·4(0·9)
C(7)–C(8)–C(9)	117·0(0·8)	O(26)–C(27)–C(28)	116·4(0·9)
C(8)–C(9)–C(10)	121·5(1·0)	O(7)–C(28)–C(27)	114·1(0·9)
C(5)–C(10)–C(9)	120·7(1·0)	O(7)–C(28)–C(29)	125·0(0·9)
O(1)–C(11)–C(1)	106·7(0·7)	C(27)–C(28)–C(29)	121·0(0·9)
O(1)–C(11)–C(12)	115·3(0·7)	C(28)–C(29)–C(30)	119·7(1·0)
C(1)–C(11)–C(12)	106·6(0·7)	C(25)–C(30)–C(29)	121·9(0·9)
N(1)–C(12)–C(11)	108·1(0·7)	C(1)–C(31)–C(32)	109·9(0·8)
N(1)–C(12)–C(13)	115·8(0·7)	N(2)–C(32)–C(31)	113·6(0·8)

The distance from the bromide ion to N(2) is 3·140 ± 0·009 Å, shorter than the values (3·17—3·38 Å) found in most other alkaloid hydrobromide derivatives.[9] The possibility of an N–H · · · Br$^-$ hydrogen bond has been discussed and presumably accounts for the observed N · · · Br distance. Although the hydrogen atom on N(2) was not located, the angles C(32)–N(2) · · · Br (99·8°), C(33)–N(2) · · · Br (116·9°), and C(34)–N(2) · · · Br (106·4°), are sufficiently close to the ideal tetrahedral value to suggest that there is an N–H · · · Br hydrogen bond. The range of angles about N(2) is smaller than that found in many other alkaloid hydrobromides but is more irregular than those found in some hydrochlorides.[10]

TABLE 5

Equations of best least-squares planes in the form $AX + BY + CZ = D$ where X, Y, and Z are orthogonal co-ordinates in Å relative to ***a***, ***b***, and ***c***. Deviations (Å × 10^2) of atoms from the planes are given in square brackets

	A	*B*	*C*	*D*
Plane (I):				
C(15)—(17), C(24)—(26), O(2)	−0·279	0·094	0·956	12·33
[C(14) −62, C(15) −22, C(16) −12, C(17) 24, C(18) 72, C(23) 42, C(24) 14, C(25) 24, C(26) 20, C(27) 71, C(30) 77, O(2) 48, N(1) −37]				
Plane (II):				
C(12), C(14)—(16), N(1)	0·006	−0·091	0·996	10·50
[C(11) 151, C(12) −8, C(13) 89, C(4) −6, C(15) −2, C(16) 8, C(17) −13, C(20) −7, C(25) 13, O(3) 18, N(1) 8]				
Plane (III):				
C(16)—(18), N(1)	0·094	0·140	0·986	12·56
[C(12) −8, C(16) 9, C(17) −8, C(18) 4, C(19) 22, C(20) 54, N(1) −5]				
Plane (IV):				
C(1), C(6), C(7), C(11), O(1)	0·288	0·289	0·913	11·35
[C(1) −8, C(2) 114, C(5) 33, C(6) 7, C(7) −2, C(8) −2, C(11) 8, C(12) 145, C(31) −140, O(1) −4]				
Plane (V):				
C(1), C(2), C(11)—(13)	0·928	0·371	−0·030	3·33
[C(1) 7, C(2), −16, C(3) 70, C(6), 149, C(11) 4, C(12) −14, C(13) 19, C(14) 69, C(31), −95, C(31) 128, N(1) −151]				
Plane (VI):				
C(2), C(3), C(5), C(6)	0·387	0·752	0·534	11·19
[C(1) −51, C(2) −5, C(3) 5, C(4) −60, C(5) −5, C(6) 5]				

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* The absolute configuration of morphine was determined as part of the study of (+)-kreysiginine.[7]

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