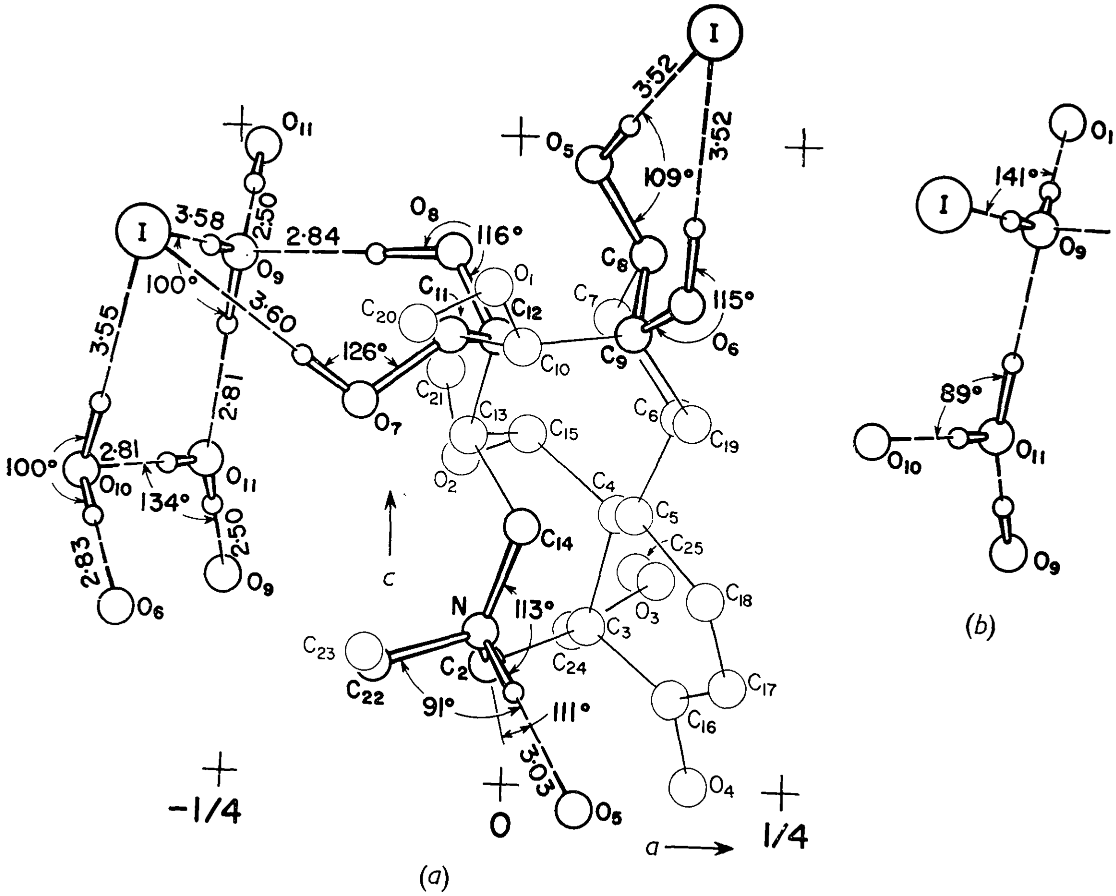

Fig. 1. (*a*) Hydrogen bonding scheme, showing the locations of the hydrogen atoms. (The true positions of these atoms may not correspond to precisely linear hydrogen bonds, as depicted.) (*b*) Alternate, and only slightly less favorable, arrangement of the hydrogen atoms of the water molecules O(9) and O(11).

The present note completes that discussion by including the rest of the hydrogen bond donor and acceptor atoms. It is comforting that in this complicated structure the principles governing hydrogen bond formation (Donohue, 1952) are nicely adhered to. Finally, the 'very low' ionic character in an isolated HI molecule is not germane to this alkaloid salt.

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Powder indexing and lattice constants for ThC_2.

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In the course of studying phase relationships between some metal carbides, it was desirable to have a set of indices for the powder pattern of ThC_2. A single-crystal study carried out by Hunt & Rundle (1951) provided the necessary information to calculate the powder pattern for ThC_2. However, the calculated *d* spacings varied sufficiently from our observed pattern to necessitate successive trial indices. An X-ray pattern was recorded with the use of Cr *Kα* radiation in a 114·6 mm Straumanis-loading Debye-Scherrer camera filled with hydrogen.

Table 1. ThC_2 *powder pattern with* Cr *Kα radiation*

No.	hkℓ	HkL[a]	θ Observed	$\theta_o-\theta_c$ ×100	d(A) Observed	I[b] Calculated	I[c] Observed
1	$11\bar{1}$	012	20.35	-2	3.294	76	30
2	002 200	$20\bar{2}$ 202	20.63		3.252	45 40	40
3	111	210	22.85	1	2.949	100	100
4	$20\bar{2}$	004	25.76	0	2.636	52	50
5	112	$31\bar{1}$	30.46	-2	2.259	10	3
6	020	020	32.87	1	2.111	23	5
7	202	400	33.62	-2	2.069	32	5
8	021	$12\bar{1}$	34.77	2	2.009	24	4
9	$11\bar{3}$	$21\bar{4}$	35.52	5	1.972	57	35
10	$31\bar{1}$	214	35.70	-1	1.963	64	35
11	022 220	$22\bar{2}$ 222	40.28		1.772	36 35	40
12	113	$41\bar{2}$	40.68	-2	1.757	50	20
13	311	412	40.90	-2	1.749	45	20
14	221	321	43.83	6	1.654	12	3
15	$22\bar{2}$	024	43.98	2	1.650	35	3
16	$20\bar{4}$ $31\bar{3}$ 400	$20\bar{6}$ 016 404	44.83		1.625	25 41 28	50
17	$40\bar{2}$	206	45.16	-0	1.615	20	5
18	023	$32\bar{3}$	48.94	-5	1.519	11	4
19	222	420	50.74	-1	1.479	35	30
20	130	131	56.22	-3	1.378	35	10
21	$13\bar{1}$	032	57.25	1	1.362	28	10
22	204 402 131	$60\bar{2}$ 602 230	59.05		1.336	38 36 21	30
23	$40\bar{4}$	008	60.13	3	1.321	37	30
24	313	610	60.80	2	1.312	56	30
25	223 024 $13\bar{2}$	$52\bar{1}$ $42\bar{4}$ $13\bar{3}$	62.25		1.294	32 49 39	50
26	$22\bar{4}$ 420	$22\bar{6}$ 424	62.86		1.287	51 52	30
27	$11\bar{5}$ $42\bar{2}$	$41\bar{6}$ 226	63.13		1.284	77 51	30
28	$51\bar{1}$	416	63.96	-3	1.275	64	20
29	132	$33\bar{1}$	66.66	1	1.248	68	25
30	421	523	69.74	-2	1.221	48	10
31	$31\bar{5}$	$21\bar{8}$	71.27	-1	1.210	102	30
32	$51\bar{3}$	218	72.02	-0	1.204	130	40
33	$13\bar{3}$ $33\bar{1}$	$23\bar{4}$ 234	74.02		1.191	51 45	10
34	330 115	333 $61\bar{4}$	75.92		1.181	116 129	10 10
35	511	614	77.75	2	1.172	167	10

[a] $H = h + \ell$, $L = h - \ell$.

[b] Calculated from Hunt and Rundle's (1951) parameters and cylindrical absorption corrections based on $\mu R = 100$.

[c] Rough visual estimates.

The carbide sample (85·60% Th, 14·25% total carbon, 5·45% free carbon, 228 ppm O_2, 51 ppm N_2, 15 ppm H_2) was loaded into a Lindemann glass capillary in an inert-atmosphere dry box. The lattice constants were refined by a Nelson-Riley analytical extrapolation least-squares program on an IBM 7090.

The observed θ values and the differences between the observed and calculated θ values are listed in Table 1. Two sets of indices are given in the table, one based on the monoclinic cell of Hunt & Rundle and the other derived from the following index transformations: $H = h + l$ and $L = h - l$. Although the latter correspond to an unorthodox set of monoclinic a and c axes, they subtend an angle almost equal to 90°; thus, only small differences in the positions of HkL and $Hk\bar{L}$ lines are seen in Table 1. Kempter & Krikorian (1962), in fact, assumed a 90° β angle in their analysis of the ThC_2 powder pattern, but this resulted in many indexing errors of higher angle lines (*e.g.* $31\bar{5}$ is assigned the indices $42\bar{3}$). Revision of some of their indexing assignments has resulted in the latice constants given in Table 2. These show approximate agreement with our lattice constants, and the small differences may result from the compositions implied by chemical analyses – $ThC_{1\cdot89}$ for Kempter & Krikorian (1962) and $ThC_{1\cdot99}$ for the present work.

Table 2. *Lattice parameters for* ThC_2

Hunt & Rundle (1951)	Present work*
a = 6·53 Å	a = 6·691 ± 0·001 Å
b = 4·24 Å	b = 4·231 ± 0·001 Å
c = 6·56 Å	c = 6·744 ± 0·002 Å
β = 104°	β = 103° 50′ ± 1′
A = 8·05 Å	A = 8·287 ± 0·002 (8·285 ± 0·005†) Å
b = 4·24 Å	b = 4·231 ± 0·001 (4·225 ± 0·002†) Å
C = 10·31 Å	C = 10·575 ± 0·002 (10·585 ± 0·005†) Å
	β' = 90° 28′ ± 1′ (90° 26′ ± 3′†)

* Based on a Cr *Kα* wavelength of 2·2909 Å.

† Calculated from d spacings of Kempter & Krikorian (1962).

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