

constants used by Giglio show that configuration *B* is more stable than configuration *A*, in accordance with the experimental evidence. Although the result obtained here is sensitive to the choice of the various parameters, in particular those of repulsive energy, it is certain that the interactions between non-bonded atoms are important in the determination of the geometrical relationship between adjacent TCNQ molecules (Goldstein, Seff & Trueblood, 1968).

As mentioned above, TCNQ molecules are stacked face-to-face to form columns of monadic units of TCNQ. The same monadic unit has also been found in crystals of *N*-methylphenazinium(TCNQ). This fact seems to be closely related to the fact that the cations are planar (aromatic in both cases). It is noteworthy that both salts are among the best electrically conductive organic compounds hitherto reported.

The calculations were performed on the HITAC 5020E computer at the Computer Centre of this University with a universal crystallographic computation program system, *UNICS*, and on the FACOM 270-30 computer at this Institute.

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The Family 24L of ZnS Polytypes

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Twelve new ZnS polytypes of the family 24L have been found in two ZnS needles. Row lines of the X-ray oscillation photographs are shown. Observed and calculated intensities are compared.

Crystals of ZnS were grown from chemically pure ZnS powder in a quartz tube by outgassing for one hour at 650°C and then introducing H₂S at 1 atm pressure and increasing the temperature to 1280°C. This temperature was maintained for 20 hours. Two needle-shaped crystals with a hollow core along the axis containing polytypes of the family 24L were found in one batch.

Specimen 232/51 contains 9 wide (>0.1 mm) polytypic regions, six of which are new polytypes and specimen 232/56 contains 8 wide polytypic regions, six of which are new polytypes. A list of the polytypes found in these two specimens is given in Table 1.

The polytypic regions were photographed by the X-ray oscillation method using Cu K α radiation. The

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Table 1. *A list of the polytypes found in specimens 232/51 and 232/56*

Specimen No.	New polytypes	Other polytypes
232/51	72R (17 7) ₃	24L (21 3)*
	72R (22 2) ₃	72R (14 5 2 3) ₃ *
	72R (9 7 4 4) ₃	36R (7 5) ₃ †
	72R (17 3 2 2) ₃	3C
	72R (7 3 3 5 3 3) ₃	
	72R (8 6 3 2 2 3) ₃	
	72R (7 7 7 3) ₃	24L (7 7 5 5)*
232/56	24L (9 7 3 5)	24L (6 5 3 5 3 2)*
	72R (5 5 3 5 3 3) ₃	
	24L (6 5 3 3 3 4)	
	24L (7 3 3 7 2 2)	
	72R (7 5 4 2 3 3) ₃	

* Previously reported (Kiflawi & Mardix, 1969).

† Previously reported (Mardix, Kiflawi & Kalman, 1969).

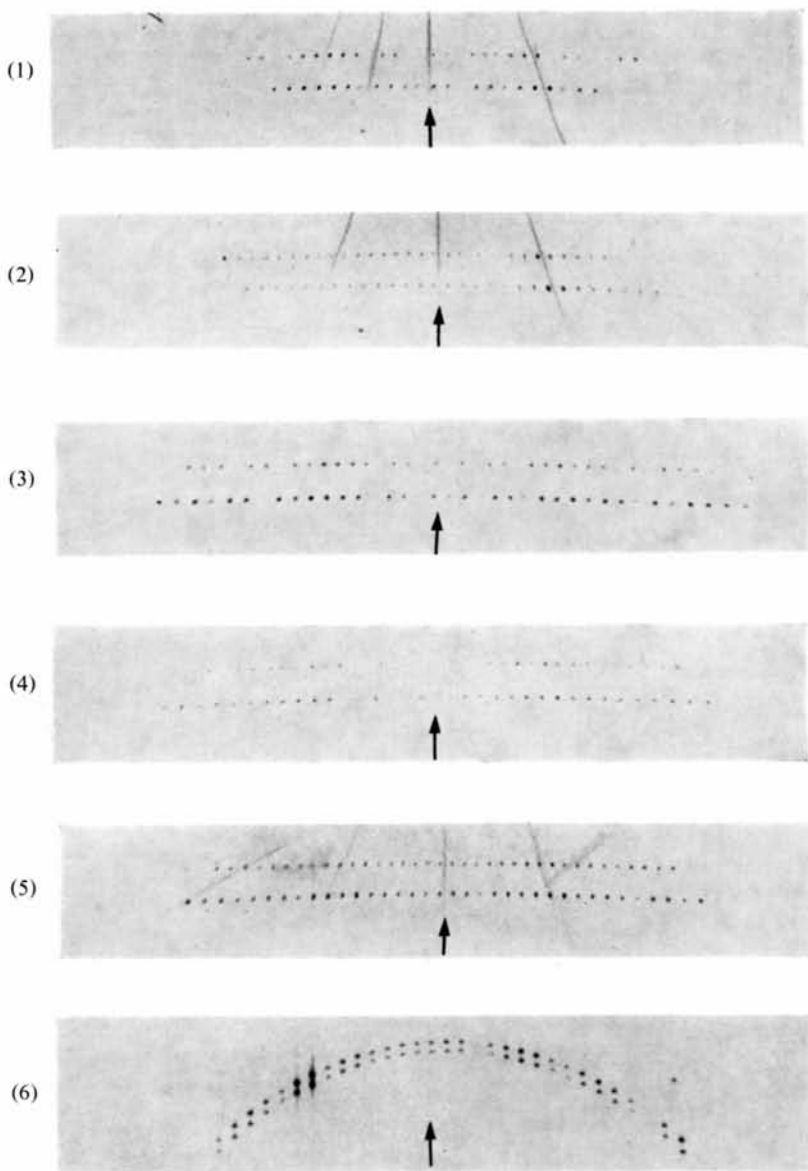


Fig. 1. Row lines of 15° oscillation X-ray photographs of the new polytypes. Cu K radiation, 60 mm diameter camera. Magnification $\times 3$. The zero line is indicated by an arrow. (6) is the photograph of the (40. l) row line. All the others are photographs of the (10. l) row lines. (1) $72R(17\ 7)_3$; (2) $72R(22\ 2)_3$; (3) $72R(7\ 7\ 7\ 3)_3$; (4) $72R(9\ 7\ 3\ 5)_3$; (5) $72R(9\ 7\ 4\ 4)_3$; (6) $72R(17\ 3\ 22)_3$;

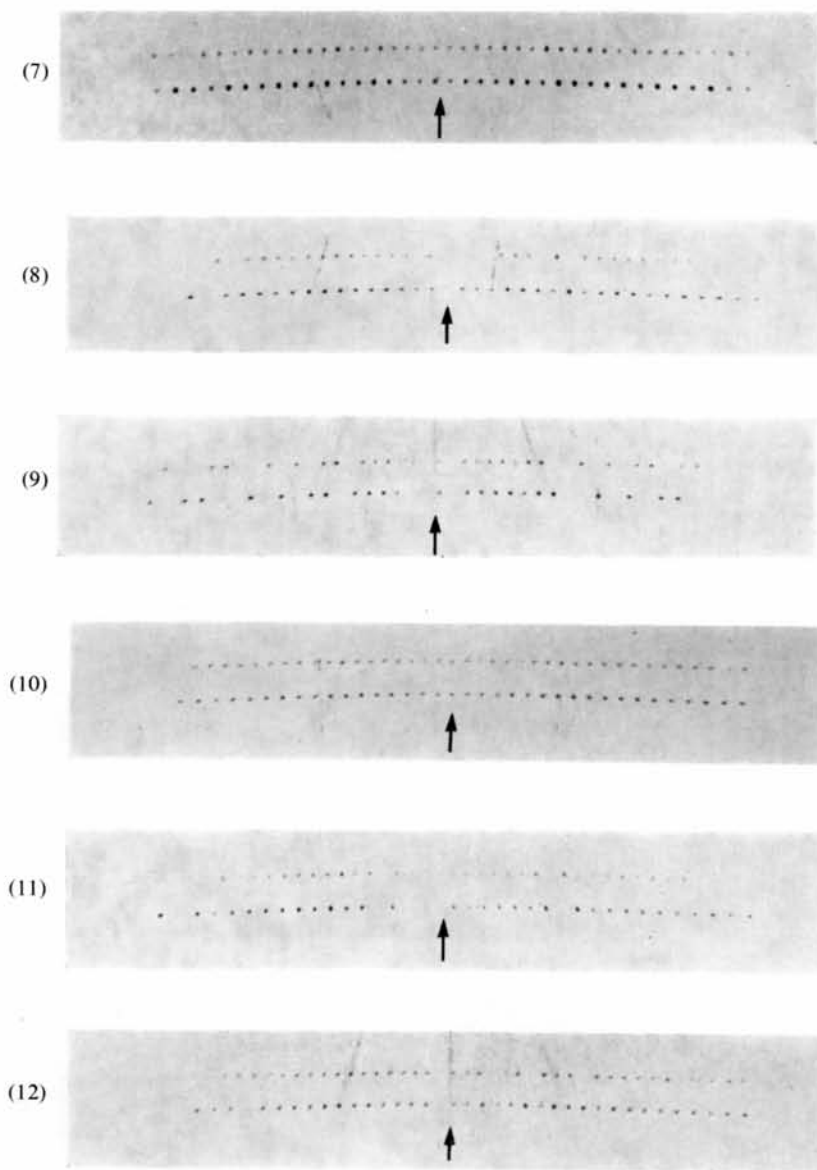


Fig. 1 (cont.) (7) $72R (5\ 5\ 3\ 5\ 3\ 3)_3$; (8) $24L (6\ 5\ 3\ 3\ 3\ 4)$; (9) $72R (7\ 3\ 3\ 5\ 3\ 3)_3$; (10) $24L (7\ 3\ 3\ 7\ 2\ 2)$; (11) $72R (7\ 5\ 4\ 2\ 3\ 3)_3$; (12) $72R (8\ 6\ 3\ 2\ 2\ 3)_3$.

10.1 or 40.1 row lines of these photographs are shown in Fig. 1.

The polytypes were identified by the elimination method (Mardix, Kalman & Steinberger, 1970). The observed and calculated intensities of the reflexion spots of the new polytypes are compared in Table 2.

Table 2. Comparison of the observed and calculated intensities of the new polytypes

<i>l</i>	Obs.	Calc.
72R (17 7) ₃		
1	<i>vw</i> (1 > 4)	1.05
4	<i>vw</i>	0.68
7	<i>a</i>	0.003
10	<i>vw</i>	1.13
13	<i>w</i>	2.17
16	<i>vvw</i>	0.47
19	<i>w</i> (19 > 13)	2.75
22	<i>vs</i>	55.89
25	<i>vvs</i>	100.00
28	<i>vvw</i>	0.42
31	<i>w</i> (31 > 19)	3.74
34	<i>w</i> (34 ~ 19)	2.16
-2	<i>vvw</i>	0.20
-5	<i>vvw</i>	0.26
-8	<i>vw</i>	1.38
-11	<i>vw</i>	1.01
-14	<i>a</i>	0.02
-17	<i>w</i>	3.65
-20	<i>s</i>	12.88
-23	<i>s</i> (-23 > -26)	20.11
-26	<i>s</i>	17.99
-29	<i>m</i>	8.92
-32	<i>vw</i>	1.55
-35	<i>a</i>	0.11
72R (22 2) ₃		
1	<i>vw</i>	0.60
4	<i>w</i>	0.76
7	<i>w</i>	0.89
10	<i>w</i>	1.00
13	<i>w</i>	1.07
16	<i>w</i> (16 > 13)	1.12
19	<i>w</i> (19 > 16)	1.14
22	<i>w</i> (22 > 25)	1.14
25	<i>w</i>	1.11
28	<i>w</i>	1.08
31	<i>w</i>	1.05
34	<i>w</i>	1.03
-2	<i>vw</i> (-2 > -5)	0.44
-5	<i>vw</i>	0.27
-8	<i>vvw</i>	0.11
-11	<i>a</i>	0.01
-14	<i>vvw</i>	0.06
-17	<i>vw</i>	0.61
-20	<i>s</i>	4.04
-23	<i>vvs</i>	100.00
-26	<i>vs</i>	32.34
-29	<i>s</i> (-29 > -20)	5.94
-32	<i>m</i>	2.44
-35	<i>w</i>	1.28
72R (7 7 7 3) ₃		
1	<i>w</i>	2.06
4	<i>vvw</i>	0.13
7	<i>vw</i> (7 > -2)	1.15
10	<i>m</i> (10 > 16)	8.24
13	<i>a</i>	0.01
16	<i>m</i>	9.08
19	<i>s</i>	19.25

Table 2 (cont.)

<i>l</i>	Obs.	Calc.
22	<i>vs</i>	47.05
25	<i>vvs</i>	100.00
28	<i>w</i>	2.26
31	<i>s</i>	20.61
34	<i>a</i>	0.01
-2	<i>vw</i>	0.79
-5	<i>w</i>	2.12
-8	<i>a</i>	0.03
-11	<i>m</i>	8.55
-14	<i>w</i> (-14 > -5)	4.73
-17	<i>a</i>	0.02
-20	<i>vs</i>	46.43
-23	<i>m</i>	9.90
-26	<i>vs</i> (-26 > -20)	58.19
-29	<i>w</i>	2.09
-32	<i>m</i>	13.12
-35	<i>w</i> (-35 > -29)	5.16
24L (9 7 3 5)		
0	<i>a</i>	0.001
1	<i>w</i> (1 > 2)	2.21
2	<i>w</i>	2.10
3	<i>w</i> (3 ~ 4)	3.02
4	<i>w</i> (4 > 1)	3.46
5	<i>m</i>	8.22
6	<i>s</i> (6 > 7)	20.98
7	<i>s</i>	13.35
8	<i>vvs</i>	100.00
9	<i>s</i> (9 ~ 7)	12.78
10	<i>s</i> (10 ~ 6)	19.51
11	<i>m</i>	7.66
12	<i>w</i>	3.45
-1	<i>w</i>	2.81
-2	<i>vvw</i>	0.28
-3	<i>vw</i>	0.81
-4	<i>s</i> (-4 > -10)	13.84
-5	<i>vw</i> (-5 > -3)	1.74
-6	<i>vw</i>	1.51
-7	<i>vs</i> (-7 > -8)	63.16
-8	<i>vs</i>	43.75
-9	<i>vs</i> (-9 ~ -8)	47.69
-10	<i>s</i>	10.45
-11	<i>m</i>	6.04
-12	<i>w</i>	3.45
72R (9 7 4 4) ₃		
1	<i>w</i>	3.22
4	<i>vvw</i> (4 > -8)	0.52
7	<i>vw</i> (7 > 10)	2.46
10	<i>vw</i>	2.11
13	<i>w</i>	3.39
16	<i>vw</i>	2.82
19	<i>vs</i>	50.13
22	<i>s</i>	11.84
25	<i>vs</i> (25 > 28)	56.18
28	<i>vs</i>	39.78
31	<i>vw</i>	2.06
34	<i>m</i>	5.08
-2	<i>w</i>	3.35
-5	<i>vvw</i>	1.28
-8	<i>vvw</i>	0.28
-11	<i>w</i>	3.94
-14	<i>m</i>	5.20
-17	<i>m</i>	5.12
-20	<i>vs</i>	62.16
-23	<i>s</i>	16.82
-26	<i>vvs</i>	100.00
-29	<i>m</i>	4.78
-32	<i>m</i> (-32 > -29)	6.14
-35	<i>m</i> (-35 > -32)	7.67

Table 2 (cont.)

<i>l</i>	Obs.	Calc.
72R (17 3 2 2) ₃		
1	<i>vw</i>	0.98
4	<i>w</i>	2.09
7	<i>vw</i>	1.64
10	<i>a</i>	0.09
13	<i>vw</i>	1.38
16	<i>m</i>	6.04
19	<i>m</i> (19 > 22)	8.77
22	<i>m</i>	5.88
25	<i>vw</i>	1.25
28	<i>vw</i>	0.85
31	<i>m</i>	4.44
34	<i>m</i> (34 > 31)	6.79
-2	<i>vvw</i>	0.73
-5	<i>vw</i>	1.46
-8	<i>vw</i>	1.44
-11	<i>vw</i>	1.43
-14	<i>w</i>	3.10
-17	<i>w</i> (-17 > -14)	3.99
-20	<i>vw</i>	1.35
-23	<i>vvs</i>	100.00
-26	<i>vs</i>	39.07
-29	<i>vw</i>	1.24
-32	<i>w</i>	2.82
-35	<i>m</i>	5.82
72R (5 5 3 5 3 3) ₃		
1	<i>w</i>	2.37
4	<i>vvw</i> (4 > -2)	0.89
7	<i>vw</i>	1.56
10	<i>m</i> (10 > 19)	6.04
13	<i>s</i>	28.37
16	<i>m</i>	3.77
19	<i>m</i> (19 > 16)	5.31
22	<i>vs</i>	70.69
25	<i>s</i>	16.43
28	<i>s</i> (28 > 25)	24.71
31	<i>s</i> (31 ~ 28)	25.99
34	<i>m</i>	4.71
-2	<i>vvw</i>	0.62
-5	<i>w</i>	2.91
-8	<i>m</i>	4.95
-11	<i>w</i>	2.71
-14	<i>s</i>	31.97
-17	<i>m</i> (-17 > -8)	7.31
-20	<i>w</i> (-20 > -11)	3.15
-23	<i>vvs</i>	100.00
-26	<i>s</i>	37.52
-29	<i>m</i> (-29 ~ -17)	7.14
-32	<i>s</i>	25.09
-35	<i>m</i> (-35 > -29)	12.43
24L (6 5 3 3 3 4)		
0	<i>a</i>	0.00
1	<i>vw</i> (1 > 2)	2.36
2	<i>vw</i> (2 > 3)	2.10
3	<i>vw</i>	1.89
4	<i>m</i> (4 > 6)	13.84
5	<i>s</i>	21.44
6	<i>m</i>	11.24
7	<i>vvw</i>	1.44
8	<i>vvs</i>	100.00
9	<i>vvw</i>	1.37
10	<i>m</i> (10 ~ 6)	10.45
11	<i>s</i>	19.99
12	<i>m</i> (12 ~ 4)	13.79
-1	<i>vw</i> (-1 ~ 2)	2.04
-2	<i>vw</i> (-2 ~ 2)	2.10
-3	<i>w</i>	5.01
-4	<i>m</i> (-4 > -5)	13.84
-5	<i>m</i> (-5 ~ -6)	10.77

Table 2 (cont.)

<i>l</i>	Obs.	Calc.
-6	<i>m</i>	11.24
-7	<i>vs</i>	45.72
-8	<i>s</i>	25.00
-9	<i>vs</i>	50.75
-10	<i>m</i>	10.45
-11	<i>w</i>	3.79
-12	<i>m</i> (-12 > -10)	13.79
72R (7 3 3 5 3 3) ₃		
1	<i>vw</i>	0.98
4	<i>w</i>	2.09
7	<i>vw</i>	1.64
10	<i>a</i>	0.09
13	<i>vw</i>	1.38
16	<i>m</i>	6.04
19	<i>m</i> (19 > 22)	8.77
22	<i>m</i>	5.88
25	<i>vw</i>	1.25
28	<i>vw</i>	0.85
31	<i>m</i>	4.44
34	<i>m</i> (34 > 31)	6.71
-2	<i>vvw</i>	0.73
-5	<i>vw</i>	1.46
-8	<i>vw</i>	1.44
-11	<i>vw</i>	1.43
-14	<i>w</i>	3.10
-17	<i>w</i> (-17 > -14)	3.99
-20	<i>vw</i>	1.35
-23	<i>vvs</i>	100.00
-26	<i>vs</i>	39.07
-29	<i>vw</i>	1.24
-32	<i>w</i>	2.82
-35	<i>m</i>	5.82
24L (7 3 3 7 2 2)*		
0	<i>m</i>	6.98
1	<i>w</i>	4.50
2	<i>vw</i>	3.59
3	<i>w</i>	4.82
4	<i>s</i> (4 ~ 9)	23.72
5	<i>vw</i>	3.52
6	<i>s</i> (6 > 9)	33.73
7	<i>vs</i>	64.44
8	<i>vvs</i>	100.00
9	<i>s</i> (9 > 10)	27.40
10	<i>s</i>	17.00
11	<i>s</i> (11 ~ 9)	29.17
12	<i>s</i> (12 ~ 10)	19.21
72R (7 5 4 2 3 3) ₃		
1	<i>vvw</i>	0.09
4	<i>vw</i>	0.30
7	<i>w</i>	1.05
10	<i>m</i>	11.75
13	<i>vvw</i> (13 > 1)	0.12
16	<i>s</i>	23.46
19	<i>m</i>	8.11
22	<i>vvs</i>	100.00
25	<i>s</i>	21.38
28	<i>vs</i>	31.17
31	<i>s</i> (31 > 34)	20.70
34	<i>s</i>	16.67
-2	<i>m</i>	6.27
-5	<i>w</i> (-5 > 7)	3.10
-8	<i>w</i> (-8 ~ -5)	3.38
-11	<i>m</i>	10.48
-14	<i>m</i> (-14 > -17)	11.86
-17	<i>m</i>	7.41

* The observed intensities are symmetrical with respect to the zero line (*l*=0).

Table 2 (cont.)

<i>l</i>	Obs.	Calc.
-20	<i>vs</i>	39.58
-23	<i>vw</i>	0.20
-26	<i>vs</i> (-26 > -20)	61.62
-29	<i>w</i> (-29 > -8)	4.12
-32	<i>m</i>	8.64
-35	<i>m</i>	10.59
72 <i>R</i> (8 6 3 2 2 3) ₃		
1	<i>vw</i>	2.31
4	<i>vw</i>	1.50
7	<i>s</i>	11.86
10	<i>vvw</i>	0.41
13	<i>w</i>	3.05
16	<i>vs</i>	31.93
19	<i>vvw</i>	0.57
22	<i>vvs</i>	74.96
25	<i>s</i> (25 > 7)	18.24
28	<i>vs</i>	32.57
31	<i>vvw</i>	0.74
34	<i>vs</i>	24.52
-2	<i>vvw</i>	0.31
-5	<i>m</i>	7.36
-8	<i>w</i> (-8 > -11)	5.82
-11	<i>w</i> (-11 > 13)	3.38
-14	<i>m</i>	7.49
-17	<i>vs</i>	29.53
-20	<i>m</i> (-20 > -14)	10.36
-23	<i>vvs</i> (-23 > 22)	100.00
-26	<i>vs</i>	34.03
-29	<i>s</i>	13.56
-32	<i>s</i>	15.04
-35	<i>s</i>	15.42

One of the polytypic regions of specimen 232/51 is 36*R*(7 5)₃ with 12 layers in its elementary stacking sequence while those of all the other polytypes in the same specimen contain 24 layers. At first sight this seems to be a case where there is a change in the Burgers vector of the screw dislocation around which the crystal grew (Mardix & Kiflawi, 1970). However, since the polytypic region 36*R*(7 5)₃ is located between regions of the family 24*L* it follows that during the growth of the crystal two changes in the dimension of

the Burgers vector *b* of the screw dislocation must have occurred – a change from 24 *C*₀ to 12 *C*₀ and back to 24 *C*₀, where *C*₀ is the interplanar distance between the (00.1) planes. Such a change (by 75 Å) is unlikely to occur, and still more unlikely to occur twice. Thus we may presume that this is a case of ‘degeneracy’ where the stacking sequence of 24 consecutive layers is 7 5 7 5. The unit cell of such a sequence happens to be 36*R*(7 5)₃. Similar cases have already been found (Mardix & Kiflawi, 1970).

Two peculiarities of the 24-layer polytypes should be noted:

(a) The number of known 24*L* polytypes is greater than the known number of any other family. 33 different 24-layer polytypes are now known in comparison with 25 and 13 polytypes respectively of the next most frequent families 20*L* and 16*L*.

(b) Each specimen that was found to belong to the family 24*L* contains a relatively large number of different polytypes in wide regions. All 33 known 24*L* polytypes were found in only 4 specimens: 232/51 and 232/56 which are reported here; 220/58 (Mardix & Brafman, 1968) and 106/34 (Kiflawi & Mardix, 1969). No other specimens investigated in this laboratory were found to contain 24-layer polytypes.

A ZnS crystal containing several kinds of 24-layer polytypes was reported by Farkas-Jahnke (1965).

It is clear that property (a) might be a consequence of property (b).

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Refinement of the Structure of (-)-Ephedrine Hydrochloride

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A previous structure determination from two projections of ephedrine hydrochloride has now been refined to *R* = 0.054 using a full set of three-dimensional diffractometer data. The mean standard deviation in bond length has been improved from 0.033 to 0.006 Å.

Introduction

Previous work by Phillips (1954) on the crystal and molecular structure of ephedrine hydrochloride was

carried out in projection on (010) and (001) with Weissenberg data. The mean standard deviation of the bond lengths was estimated to be 0.033 Å. The positional atomic coordinates given by Phillips were used for a