This was the first time we had attempted to use the *FC* link for this purpose. Previously the comparison had been done after refinement by *ORFLS* (in X-RAY 63) or *CRYLSQ* (in X-RAY 70). We have checked that each of these, though in different ways, correctly allows for dispersion, so none of our previous assignments need revision. (*ORFLS* on X-RAY 70 will only refine if not required to allow for dispersion.) Two reruns, using four cycles of *CRYLSQ* (in X-RAY 70) on all the non-zonal reflexions of lycopodine hydrochloride with $\Delta f' = 0{\cdot}33$ and $\Delta f'' = \pm 0{\cdot}72$, produced trifling shifts of all parameters, but gave a very different result, $[R(+) = 0{\cdot}059$, $R(-) = 0{\cdot}077]$ which represents a most emphatic confirmation of the chirality (I).

It is disconcerting to discover that an erroneous program could produce a strongly and *wrongly* biased result, and it is clear that crystallographers must avoid using the *FC* link in X-RAY 63 or 70 for this purpose. They should also check to see whether any chiralities they may have published were based on these versions of *FC*, or on some program that they have not personally checked rigorously.

References

ANET, F. A. L. (1960). *Tetrahedron Lett.* **20**, 13–17.

AYER, W. A., ALTENKIRK, B., BURNELL, R. H. & MOINAS, M. (1969). *Canad. J. Chem.* **47**, 449–455.

BURNELL, R. H. & TAYLOR, D. R. (1961). *Tetrahedron*, **15**, 173–182.

HAMILTON, W. C. (1965). *Acta Cryst.* **18**, 502–510.

HARRISON, W. A. & MACLEAN, D. B. (1960). *Chem. Ind.* pp. 261–262 and references therein.

MANSKE, R. H. F. & MARION, L. (1946). *Canad. J. Res.* (*B*), **24**, 57–62.

STEWART, J. M., KUNDELL, F. A. & BALDWIN, J. C. (1963–1972). Compilers of various editions of the X-RAY Library System of Crystallographic Programs, Univ. of Maryland. *FC* occurs in the 63, 70 and 72 versions; *ORFLS* in 63 and 70; *CRYLSQ* in 70 and 72.

WIESNER, K., FRANCIS, J. E., FINDLAY, A. J. & VALENTE, Z. (1961). *Tetrahedron Lett.* **5**, 187–196.

Acta Cryst. (1974). B**30**, 553

On the crystal structures of $C_5H_{12}N^+HS^-$ and $C_5H_{11}N.HCl$.

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Crystal structures of piperidinium hydrogen sulphide and piperidine hydrochloride are found to be isomorphous.

Recently a paper has been published (Smail & Sheldrick, 1973) on the crystal and molecular structure of piperidinium hydrogen sulphide, $C_5H_{12}N^+HS^-$. A comparison of this structure with the piperidine hydrochloride structure, determined by Dattagupta & Saha (1970) and Rérat (1960), shows that they are isomorphous. Cell dimensions, space groups, fractional coordinates *etc.* of the two reported structures are given in Table 1 for easy comparison. Transformations to be made in one structure for comparison with the other are obvious.

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In both structures the molecules are linked by N–H···S (N–H···Cl) type hydrogen bonds to form infinite chains, and the piperidine ring has a chair conformation with a crystallographic mirror plane through atoms S (Cl), N and C(3).

References

DATTAGUPTA, J. K. & SAHA, N. N. (1970). *Indian J. Phys.* **44**, 561–564.

RÉRAT, C. (1960). *Acta Cryst.* **13**, 72–80.

SMAIL, E. J. & SHELDRICK, G. M. (1973). *Acta Cryst.* B**29**, 2027–2028.

Table 1. *Data relating to the two structures*

	Piperidinium hydrogen sulphide (Smail & Sheldrick, 1973) $C_5H_{12}N^+HS^-$			Piperidine hydrochloride (Dattagupta & Saha, 1970) $C_5H_{11}N.HCl$			
Crystal system	Orthorhombic			Orthorhombic			
Space group	*Pmab*			*Pbcm*			
Cell dimensions	$a = 9{\cdot}77$ Å			$a = 9{\cdot}68$ Å			
	$b = 7{\cdot}30$			$b = 7{\cdot}30$			
	$c = 9{\cdot}84$			$c = 9{\cdot}67$			
Density	$D = 1{\cdot}13$ g cm^{-3}			$D = 1{\cdot}14$ g cm^{-3}			
	$Z = 4$			$Z = 4$			
	10^4x	10^4y	10^4z		10^4x	10^4y	10^4z
S	2500	9632	3269	Cl	1733	363	2500
N	2500	5472	3645	N	1430	4572	2500
C(1)	3753	4641	3046	C(1)	1929	5404	1201
C(2)	3758	4901	1541	C(2)	3469	4967	1155
C(3)	2500	4140	905	C(3)	4081	5851	2500

In both structures the molecules are linked by N–H···S (N–H···Cl) type hydrogen bonds to form infinite chains, and the piperidine ring has a chair conformation with a crystallographic mirror plane through atoms S(Cl), N and C(3).