which can only appear if the repeat of the electron density pattern is 18·6 Å (or a multiple of this length). This implies that consecutive hydrogen-bonded sheets appear different as in poly(β-n-propyl L-aspartate) (Bradbury *et al.*, 1960) and in poly(S-carbobenzoxy-L-cysteine) (Elliott, Fraser, McRae, Stapleton & Suzuki, 1964), where it has been suggested that the side chains are highly ordered and alternate sheets have different side-chain conformations. There are no reflections requiring a to be doubled, but it does not necessarily follow that the parallel-chain type is appropriate. For instance, the molecular model indicates that the length of a single antiparallel chain of a protected hexapeptide with fully-extended end groups is about 3 Å but it is possible to show by means of CPK space-filling components that the closest packing is obtained when: (1) the t-Boc and -OMe groups are bent with respect to the backbone direction (Fig. 2a) and (2) the chain axes of a sheet are displaced by $a/2$ with respect to the first neighboring sheets (Fig. 2b). This lattice, which is in agreement with the experimental data, in particular with the very high intensity of the 101 reflection and with the absence of the 100 reflection, would be favored by the relatively bulky isopropyl side-chain groups too.

The calculated crystal density is $D_c = n \times 0.266$ Mg m^{-3}, where n is the number of peptide chains in the pseudo-orthorhombic cell. The comparison with the observed density, D_o $= 1.08$ Mg m^{-3}, indicates that such a cell is crossed by four β chains.

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The crystal structure of Li₃ThF₇.

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Abstract

It is pointed out that the unusual coordination polyhedron for the ThF₉ group reported by Cousson, Pagès & Chevalier [*Acta Cryst.* (1978), B34, 1776–1778] for Li₃ThF₇, a tetragonal antiprism with a pyramid on one of the square faces, is one of three best arrangements of nine sp^3d^5 bond orbitals found by consideration of the strengths (concentration in the bond directions) of the hybrid bond orbitals. Theoretical considerations and comparison with other structures indicate that the lithium atoms are not in the positions assigned to them in this crystal.

Cousson, Pagès & Chevalier (1978) have reported for the tetragonal crystal Li₃ThF₇, a structure containing ThF₉ groups with the tetragonal antiprism with a cap (a pyramid) on one of the square faces as the coordination polyhedron. They describe this polyhedron as unusual for complex actinide fluorides; the usually occurring polyhedron is the trigonal prism with three lateral caps, as found, for example, in (NH₄)₃ThF₇ (Penneman, Ryan & Kressin, 1971) and RbThF₁₃ (Brunton, 1971). It is, however, not surprising that both of these coordination polyhedra have been observed, and a third might also be found for these fluorides.

A search for the best set of nine hybrid sp^3d^5 bond orbitals was made by McClure (1970), with the criterion that the sum of the bond strengths (the values of the angular part of the orbital function in the bond directions) be a maximum. The set that he found, the McClure polyhedron, has a mirror plane as its only symmetry element. Two other sets have essentially the same value of the sum of the bond strengths; they are the tetragonal antiprism with one axial cap and the trigonal prism with three lateral caps (Pauling, 1975, 1978). The last of these three has been found in many crystals and molecules and the second in a few, including Li₃ThF₇.

There is little doubt that the reported structure of the ThF₉ group in Li₃ThF₇ is essentially correct, but the positions assigned to the lithium atoms are surely wrong; at least those of two of the three atoms. These two lithium atoms were assigned positions in the same plane as the four F(3) atoms of the complex, at the center of fluorine triangles with a shared edge. They are only 2·03 Å from one another, less than the smallest reported Li$\cdots$Li distance in any compound: 2·31 Å in Li₂O (2·84 Å in LiF). Moreover, the electrostatic-valence rule (Pauling, 1929) indicates that the axial fluorine atom F(1) and the four F(2) atoms, rather than the two F(3) atoms (which are shared between Th polyhedra), should be involved in most of the bonds to lithium. For ionic valence +4 for Th each of the nine bonds has electrostatic valence $\frac{4}{9}$. Two such bonds nearly saturate the F(3) atoms, whereas each of the F(1) and F(2) atoms

requires about two bonds from tetrahedrally or trigonally coordinated lithium to saturate it. I have not succeeded in finding a satisfactory arrangement for the lithium atoms compatible with the assigned space group; perhaps the space-group assignment is wrong or the lithium atoms occupy a larger number of equivalent positions with some randomness. Thus in the plane $z = 0$ there are ten fluorine tetrahedra that might be occupied by lithium atoms; possibly Li(1) atoms occupy two of them, as in the reported structure, with Li(2) atoms in half of the other eight. The total electrostatic bond strengths would then be 0·94 for F(1), 1·07 for F(2), and 0·89 for F(3), in satisfactory agreement with the rule.

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Acta Cryst. (1979). B35, 1536

(+)-Lupanine perchlorate monohydrate: erratum.

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Abstract

In Table 2 of Małuszyńska, Hoser & Kaluski [*Acta Cryst.* (1979), B35, 970–973] the coefficient of Y in the equation for plane 3 should read 0·9657.

All relevant information is contained in the *Abstract.*

Acta Cryst. (1979). B35, 1536

The ethyl carbonate of 1-isoquinolyl(phenyl)methanol.

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Abstract

A printer's error is corrected. In Skrzypczak-Jankun & Kaluski [*Acta Cryst.* (1977), B33, 3921–3923] the first two lines in the right-hand column of text on p. 3922 should read:
  'isoquinolyl)pyrazole (King & Reimlinger, 1971), and 3-methylisoquinoline (Ribár, Divjaković, Janić, Argay,'

All relevant information is contained in the *Abstract.*

Acta Cryst. (1979). B35, 1536–1537

The crystal structure of $BaCaLu_2F_{10}$.

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Abstract

The compound $BaCaLu_2F_{10}$ is isostructural with KY_3F_{10}. The unit cell is cubic with $a = 11·366$ (2) Å. The space group is $Fm3m$, $D_m = 6·40$ (5), $D_x = 6·45$ Mg m^{-3}, $Z = 8$. The structure was solved by conventional methods; of the 617 reflections recorded using an automated four-circle diffractometer 163 which had positive peak intensities were used in the refinement of the model to an R value of 4·1%. There is no ordering between the Ca and Lu atoms, which are statistically distributed in sites 24(*e*).