Erratum

Helv. Chim. Acta **1987,** *70,* 1897, No. 175: by Maria Cattani-Lorente, Gérald Bernardinelli, and Michel Geoffroy:

Professor *J. D. Dunitz* has pointed out to us that there is an error in the published space group for the phosphochloridate **1**. From a consideration of bond lengths for chemically equivalent bonds, he has suggested that the space group should be *I2/m* and not *I2*. Refinement of **1** in *I2/m* leads to the same *R* value and improved e.s.d.'s of all parameters. In *I2/m*, there is a mirror plane passing through the molecule and, consequently, only 9 atoms in the asymmtric unit instead of 15 in *I2*. Corrected interatomic distances and angles are given in the *new Table 2*[1]).

Table 2. *Interatomic Distances* [Å] *and Relevant Bond Angles* [°] (e.s.d.'s in parentheses)

Cl–P	1.986 (2)	C(1)–C(2)	1.377 (4)
P–O(1)	1.589 (2)	C(2)–C(3)	1.365 (4)
P–O(3)	1.445 (3)	C(3)–C(4)	1.390 (4)
O(1)–C(1)	1.407 (3)	C(4)–C(5)	1.383 (4)
Cl–P–O(1)	104.7 (1)	O(1)–P–O(3)	117.7 (1)
Cl–P–O(3)	111.5 (1)	P–O(1)–C(1)	108.7 (2)
O(1)–P–O(2)	98.8 (1)	O(1)–C(1)–C(2)	111.6 (2)

In the meantime, the program MISSYM [1], which searches for forgotten symmetry operations in crystal structure data, has become available in this laboratory. MISSYM indicated the presence of the missing mirror plane and center of symmetry in our published data. Another indication of the missing symmetry could have been deduced from the value of the absolute-structure parameter *x* [2] obtained from refinement in *I2*. This value was $x = 0.47$ (37). A value close to 0.5 for *x* could either indicate a 50% inversion twin or a centrosymmetric structure refined in a non-centrosymmetric space group. The e.s.d. of *x* for clearly non-centrosymmetric structures of compounds with similar molecular formula [2] [3] is usually very much smaller than that obtained here. The large value of 0.37 is due to the very small non-centrosymmetric contribution of the structure description in *I2*. Refinements using more accurate intensity data would lead to an even smaller non-centrosymmetric contribution and an even larger value for the e.s.d. of *x*. Clearly refinements indicating a value of *x* close to 0.5 with an usually large e.s.d. should be viewed with suspicion.

REFERENCES

[1] Y. Le Page, *J. Appl. Crystallogr.* **1987,** *20,* 264.
[2] G. Bernardinelli, H. D. Flack, *Acta Crystallogr., Sect. A* **1985,** *41,* 500.
[3] G. Müller, *Acta Crystallogr., Sect. B* **1988,** *44,* in press.

[1]) Corrected values of atomic positional and displacement parameters have been deposited with the CCDC, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England, and can be obtained from the *Editorial Office of HCA*.