Dr H. M. M. Shearer. Programs, other than diffractometer-control software, were written by WC and Professor G. M. Sheldrick.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1981). B**37**, 1321–1322

Triclinic and orthorhombic barium dihydrogenphosphate: a statistical comparison.

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Abstract

Two independent X-ray structure analyses of triclinic $Ba(H_2PO_4)_2$ are compared by means of half-normal probability-plot analysis. Two independent determinations of orthorhombic $Ba(H_2PO_4)_2$ are likewise compared. The weighted mean coordinates for the triclinic and orthorhombic structures along with the resulting interatomic distances and angles have been deposited. These should be used in place of the results given in the earlier publications.

Two papers on the triclinic $Ba(H_2PO_4)_2$ structure have recently been published independently by Gilbert & Lenhert (1978) (GL) and Durif & Guitel (1978) (DG). Two papers on the orthorhombic form have also appeared [Gilbert, Lenhert & Wilson (1977) and Prelesnik, Herak, Čurić & Krstanović (1978) (GLW and PHCK)]. We have compared the two pairs of coordinate and thermal-parameter sets with the aid of half-normal probability plots (Abrahams & Keve, 1971) using the ranked moduli of Hamilton & Abrahams (1972). Important features of the four X-ray experiments are summarized in Table 1 with each experiment listed under the initials of the authors.

In the course of our analysis we found a small discrepancy between the coordinates, cell parameters and bond distances and angles in the paper by DG. The half-normal probability-plot analysis, however, showed very little systematic difference between the coordinates of DG and GL for the triclinic structures.

The first plot for the orthorhombic coordinates showed clear evidence of systematic differences. The data set for PHCK was obtained and upon repeating the refinement, the

Table 1. *A summary of the four* $Ba(H_2PO_4)_2$ *analyses*

	Triclinic		Orthorhombic	
	GL	DG	GLW	PHCK
Number of reflections measured	13 381	1856	5792	1253
Maximum sin θ/λ (Å^{-1})	0·99	0·69	0·99	0·85
Radiation	Mo $K\alpha$, Nb filtered	Mo $K\beta$, monochromated	Mo $K\alpha$, Nb filtered	Mo $K\alpha$, Zr filtered
Least-squares weights	Statistical	Statistical	Statistical	Unit weights
Absorption correction	Yes	No	Yes	None, sphere
Extinction correction	Yes	No	Yes	Yes
H atoms located	Refined	No	Yes	Refined?

R factor dropped from their value of 0·031 to 0·027 and the systematic differences were virtually eliminated. When modified Hughes weights were used (statistical weights were not available for PHCK) *R* dropped to 0·026 and the slope of the half-normal probability plot was very close to unity.

Comparison of the thermal parameters showed substantial systematic differences for both sets. Large differences are found for the heavy atoms, especially Ba. The systematic differences in the data sets, in particular, the treatment of absorption, weak reflections and the different sin θ/λ limits, may be responsible. For further details, the interested reader should consult the deposited material which includes the improved coordinate sets for both structures.*

* All tables and plots, together with a more detailed discussion of the analysis have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36019 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1981). B**37**, 1322

The modulated structure of the layered perovskite γ-bis(*n*-propylammonium) tetrachloromanganate(II): refinement of the average structure, the possible superspace group and a model for the modulated structure. Erratum.

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Abstract

A printer's error is corrected. In the paper by W. Depmeier [*Acta Cryst.* (1981). B**37**, 330–339] a wrong superspace group is given in the middle of page 336. The superspace group given in the line beginning with '(holohedry)' should read $L^{Cmmm}_{1\,1\,\bar{1}}$ instead of $N^{Cmmm}_{1\,1\,\bar{1}}$.

All relevant information is given in the *Abstract*.

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