McCarley (1957b). Elemental analyses for C, H, N gave satisfactory agreement with calculated values (in parentheses): PtenCl₃: C 6·8 (6·64), H 2·3 (2·23), N 7·9 (7·75); PtenBr₃: C 5·0 (4·85), H 1·6 (1·63), N 5·9 (5·66); PtenI₃: C 4·1 (3·78), H 1·2 (1·27), N 4·1 (4·41). Single crystals of PtenCl₃ and PtenBr₃ were grown by slowly cooling aqueous solutions (Interrante & Browall, 1974). The resulting crystals had a metallic sheen and were strongly dichroic.

The lattice constants in Table 1 were obtained by a leastsquares analysis of the Debye-Scherrer patterns given in Table 2 (obtained with a 114.6 mm camera radius and Cu K α radiation). Intensities (peak heights) were obtained from densitometer traces. The space group, *Ama*2, was ascertained from X-ray precession photographs of single crystals of PtenBr₃ and PtenCl₃ and is equivalent to that reported for the disordered structure described by Ryan & Rundle (1961).

The lattice constants of PtenBr₃ given by Ryan & Rundle (1961) (after interchanging *a* and *c* to bring the reported space group, C2cm, into the standard setting, Ama2) are $a = 10 \cdot 12$, $b = 14 \cdot 77$, $c = 5 \cdot 60$ Å. Referring to Table 1, the discrepancy between the sets of data is seen to be associated almost entirely with the value of *b*. It is difficult to check on the origin of the discrepancy because of an internal inconsistency in the paper by Ryan & Rundle. The reported X-ray density of $4 \cdot 027$ cm⁻³ does not follow from their (Ryan & Rundle, 1961) unit-cell data, which would correspond to a density of $3 \cdot 93$ g cm⁻³. The measured density is $4 \cdot 03$ g cm⁻³.

On the other hand, our single-crystal data appear to correspond to those of Ryan & Rundle (1961) with respect to systematic absences and in regard to agreement of individual structure factors so that no major difference in the crystal structure is suggested by our results. One difference in the single-crystal results is that we have not been able to observe the streaking between layer lines normal to c^* as described by Ryan & Rundle (1961). Presumably, then, this would imply more complete disorder in the arrangement of the chains that are parallel to c.

It does not appear that a typographical error was responsible for the abnormally large value of b given by Ryan & Rundle (1961), since their interatomic distances follow from their lattice constants. In particular, the molecular plane (non-chain axis) Pt(IV)-Br and Pt(II)-Br distances of 2.51 Å are consistent with the reported b value. On the other hand, the new lattice constants indicate a value of 2.43 Å; this is in better agreement with the corresponding distance of 2.46 (6) Å in the related compound, [Pt(NH₃)₂Br₄] [Pt(NH₃)₂Br₂] (Wallen, Brosset & Vannerberg, 1962). The revised PtenBr₃ values also indicate that the in-plane Br-Br distance is 3.54 Å and the Br-Pt-Br angle is $86^{\circ}24'$.

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References

- INTERRANTE, L. V. & BROWALL, K. W. (1974). Inorg. Chem. In the press.
- INTERRANTE, L. V., BROWALL, K. W. & BUNDY, F. P. (1974). Inorg. Chem. In the press.
- RYAN, T. D. & RUNDLE, R. E. (1961). J. Amer. Chem. Soc. 83, 2814–2816.
- WALLEN, J., BROSSET, C. & VANNERBERG, N. (1962). Ark. Kem. 18, 541-551.
- WATT, G. W. & MCCARLEY, R. E. (1957a). J. Amer. Chem. Soc. 79, 3315-3317.
- WATT, G. W. & MCCARLEY, R. E. (1957b). J. Amer. Chem. Soc. 79, 4585-4589.

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A reinvestigation of the crystal and molecular structure of hexachloroborazine. A correction. By M. S. GOPINA-THAN, M. A. WHITEHEAD, C. A. COULSON,* J. R. CARRUTHERS and J. S. ROLLETT, *Theoretical Chemistry Department*, 1 South Parks Road, Oxford OX1 3TG, England

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In the paper by Gopinathan, Whitehead, Coulson, Carruthers & Rollett [Acta Cryst. (1974). B30, 731–737] Fig. 5 represents the enantiomorph of the structure obtained from the parameters of Table 5 of the same paper.

The parameters resulting from our refinements in Table 5 (Gopinathan, Whitehead, Coulson, Carruthers & Rollett, 1974) have been inverted through a centre of symmetry so that they can be compared with the results of Haasnoot, Verschoor, Romers & Groeneveld (1972). In the preparation of Fig. 5 this inversion was not performed and the

* Deceased.

figure represents the enantiomorph of the structure obtained from the parameters of Table 5.

References

- GOPINATHAN, M. S., WHITEHEAD, M. A., COULSON, C. A., CARRUTHERS, J. R. & ROLLETT, J. S. (1974). *Acta Cryst.* **B30**, 731–737.
- HAASNOOT, J. G., VERSCHOOR, G. C., ROMERS, C. & GROENEVELD, W. L. (1972). Acta Cryst. B28, 2070–2073.