

tion that the probability that $\phi_{200} = \pi$ is not insignificant. It seems reasonable to insist that a probabilistic argument be labelled as such, particularly when the probabilities involved cannot be evaluated readily and rough estimates are not overwhelmingly conclusive; the argument presented by Hauptman certainly falls in this category, but no indication of this was given in the original article.

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Comments on Gilardi's paper 'A priori, for estriol, $\phi_{200} = 0$ or π '. By HERBERT HAUPTMAN, *Medical Foundation of Buffalo, Buffalo, New York, U.S.A.*

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Gilardi's thesis [*Acta Cryst.* (1973). **B29**, 1739–1740] is certainly correct. However, his work is based on a misunderstanding of the intent of the earlier paper which it purports to criticize so that it is, in reality, a valid criticism of his misinterpretation.

First, it is surely true that there exist *a priori* acceptable structures with E_{200} large and negative and $E_{100} = 0$, as Gilardi (1973) demonstrates by his example. However, he has misconstrued the essential point of the earlier paper (Hauptman, 1972) which is not that there are no acceptable structures with $\phi_{200} = \pi$ but that such structures are relatively rare. The proof of this contention lies in the comparison (apparently too concise in the earlier paper) of Gilardi's equations (1) and (2). First, since the ε_μ are small, it is clear that the magnitude of each contributor to (1) is, in general, significantly less than the magnitude of the corresponding contributor to (2). Next, 21 of the contributors to (1) are positive and 21 are negative, a distribution of signs most conducive to complete or nearly complete annihilation. A situation as favorable as this is quite unlikely (but admittedly not impossible) in (2) since the ε_μ are, *a priori*, just as likely to be positive as negative so that the probability of equal numbers of positive and negative signs is only 0.1, approximately. (In fact, the probability that the difference between the number of positive contributors to (2) and the number of negative contributors be less than four is still

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only about 0.3. A similar comparison may be made if one chooses to invoke the one-dimensional random walk.) Finally, the numerical factor in (1), $1/\sqrt{84}$, is just half the corresponding factor in (2), $2/\sqrt{84}$. For these three reasons then, while it may not have been 'clear' in the earlier paper, it is nevertheless true that the 'right-hand side of equation (1) is more consistent with a value of zero (for E_{100}) than that of equation (2)', in the probabilistic sense.

In correspondence with Professor David Templeton it has been pointed out that several factors 2π following equation (6) have been lost. This error is most easily corrected by replacing the ε_μ of equations (4) and (5) of the original paper by $\varepsilon_\mu/2\pi$. I wish to thank Professor Templeton for noting this error and also for other constructive criticism.

References

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The crystal structure and X-ray diffraction data for anhydrous gadolinium bromide. By HENRY H. THOMAS, *Goodyear Atomic Corporation, P.O. Box 628, Piketon, Ohio 45661, U.S.A.* and W. A. BAKER JR, *University of Texas, Arlington, Texas, U.S.A.*

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The X-ray diffraction data for GdBr_3 are reported. The crystal structure of GdBr_3 is the monoclinic AlCl_3 type belonging to space group $C2/m$. The unit-cell parameters are: $a = 7.224 \pm 0.005$, $b = 12.512 \pm 0.005$, $c = 6.84 \pm 0.01$ Å, and $\beta = 110.6 \pm 0.2^\circ$. The results of pycnometer density measurements are reported.

Introduction

In the course of a general investigation of the properties of some anhydrous rare-earth halides, an X-ray study of several

of the compounds was carried out and the lattice parameters determined. The result of the X-ray investigation of GdBr_3 is reported herein.

Though nearly all the lanthanide trifluoride, trichloride,