an early melting fraction of the mantle which is formed primarily from mineral phases having high rubidium-strontium and uranium plus thorium–lead ratios, and if these magmas can be brought to the surface without complete mixing with later derived magmas, the observed isotope differences would result. Second, the inter-island differences may reflect regional variations in the rubidium-strontium and uranium-lead ratios in the mantle. We have already shown that a general increase in the uranium-lead ratio for the last billion years or so in the region of the source of the volcanic rocks on Ascension Island could explain the different Pb^{206} abundance in the two islands. This mechanism requires that the increase in the uranium-lead ratio was not accompanied by a corresponding increase in the thorium-lead ratio. The data for strontium show that the postulated enrichment of uranium with respect to lead would have taken place without enrichment of rubidium with respect to strontium. If correct, this explanation indicates that fractionation of these elements has occurred in the outer mantle in ways that do not follow those commonly observed in magmatic differentiation of plutonic rocks. This is probably more an indication of our ignorance of chemical fractionation processes in sub-crustal regions than an argument against the existence of chemically differentiated regions in the mantle. The work of Shavrova (*18*) and Gottfried *et al.* (*19*) on the thorium and uranium content of a series of circumpacific volcanic rocks gives some support to the high uranium-thorium ratios inferred for the source of the magmas on Ascension Island. Their work shows, first, that the uranium-thorium ratios of 1 : 2 are not uncommon in volcanic rocks and, second, that this ratio does not change with the composition of the rock. The second observation suggests that the observed uranium-thorium ratio is related to that in the source of the rock rather than to a magmatic differentiation process. Gottfried *et al.* (*19*) suggest that the high uranium-thorium ratio is due to assimilation of geosynclinal sediments. This hypothesis, however, implies some change in the uranium-thorium ratio with the changing composition of the volcanic rock, and is thus not entirely consistent with the observations. An alternative hypothesis is that the high uranium-thorium ratio in the volcanic rocks is due to a similar high ratio in some parts of the mantle. It is perhaps more than coincidence that the uranium-thorium ratio in the mantle, inferred from isotope data for Ascension Island, is similar to that inferred from chemical data in the circumpacific region.

It appears that regional chemical heterogeneities in the upper mantle are the most plausible explanation of observed inter-island variations in the isotope composition of lead and strontium. If the uranium-lead ratio in different parts of the mantle has been differentiated at various times in the last 3 to 4 billion years as we have inferred, the existence of terrestrial lead evolved in a chemically closed system formed at the same time as the planet is open to question. Also, if the isotopic variations observed at these two islands are due to chemical processes occurring in the mantle, the initial isotope ratios of lead and strontium in extrusive igneous rocks may not be used in continental regions as unambiguous indicators of contamination with older crustal rocks.

The hypotheses we have listed offer neither a unique nor a complete explanation of the observed variations. We report these measurements because they indicate a parameter which may be useful in investigating magma forming mechanisms, and because they give some indication of the scale on which isotope measurements must be undertaken in order to yield detailed information on the upper mantle.

PAUL W. GAST
Department of Geology and Geophysics, University of Minnesota, Minneapolis
G. R. TILTON
Geophysical Laboratory, Washington, D.C. 20008
CARL HEDGE
U.S. Geological Survey, Washington, D.C. 20005

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Hydrogen Atom Thermal Parameters

Abstract. *Isotropic hydrogen atom thermal parameters for* N,N′*-hexamethylenebispropionamide have been determined. They show a definite trend and vary from approximately the same as the mean thermal parameters for atoms other than hydrogen near the center of the molecule to appreciably greater for atoms near the end. The indicated trend for this compound, along with other results, provides the basis for a possible explanation of the anomolous values that have been obtained for hydrogen atom thermal parameters.*

The techniques of x-ray diffraction have now advanced to the point where hydrogen atom parameters of some significance can be determined for organic molecules in the solid state. Several recent refinements of structures (*1*) have included isotropic thermal parameters for the hydrogen atoms and, in most instances, have led to results where the apparent parameters are less than those of the atoms to which hydrogen is bonded and in some cases even to negative values (*2*).

We now report the results of refining hydrogen atom thermal parameters in *N,N′*-hexamethylenebispropionamide (HMBPA) (Fig. 1) and suggest a possible explanation for the anomolous results that have appeared.

The reported parameters for HMBPA (*3*) were used as the starting point in further refining the structure by full matrix least squares (*4*). In the last stage of refinement, variation of both position and isotropic thermal parameters for hydrogen reduced $R = \Sigma|\Delta F| / \Sigma|F_o|$ to 0.047.

There is considerable variation in the thermal parameters (B) for atoms other than hydrogen in this compound and even wider variation in those for hydrogen atoms. Moreover, there is a pronounced trend in the results with B'_H, the apparent thermal parameter for a hydrogen atom, running from approximately the same as those of the nonhydrogen atoms near the center of the molecule to appreciably greater for atoms near the end. This is best seen from a graph of B'_H plotted against $B_{non\text{-}H}$, the mean thermal parameter of the atom to which the hydrogen atom is bonded (Fig. 2). The plot is approximately linear. None of the points deviates greatly from the solid straight line except that for C_{12}, the terminal atom in the chain.

We have also refined further the structures of 3-benzoylanthranil (*5*) and salicylic acid (*6*). The mean thermal parameters for the hydrogen atoms in these compounds are appreciably smaller than those in HMBPA, and, except for one of the 15 hydrogen atoms, the results fall close to the solid line in Fig. 2. The regularity is surprising considering the possible differences in packing about the hydrogen atoms in these compounds.

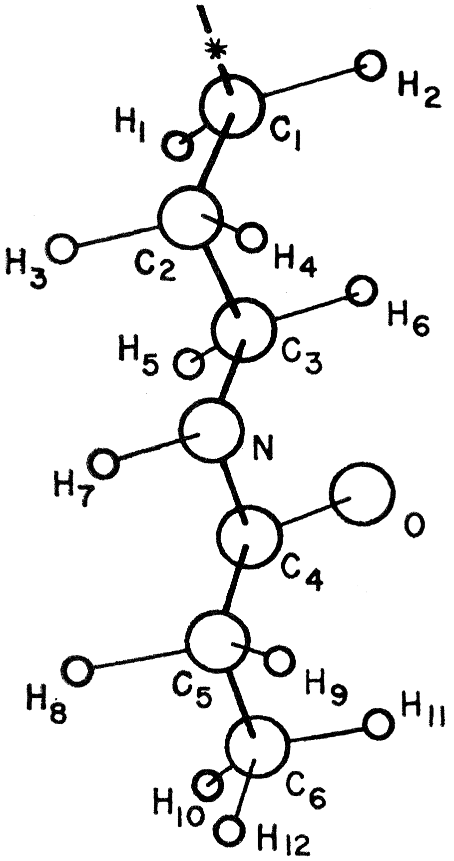

Fig. 1. Numbering of the atoms in *N,N'*-hexamethylenebispropionamide. The half molecule shown is the asymmetric unit in the crystal.

While it is not known how generally the aforementioned results apply, nevertheless it is reasonable to assume similar behavior for compounds with similar packing. The graph indicates that, for such compounds, hydrogen atom thermal parameters can be expected to become negative when B values for atoms other than hydrogen fall below about 2.5 Å^2.

We shall now show that the results in Fig. 2 can be explained in a straightforward way which accounts for the anomolous B'_H in terms of incorrect scattering factors for hydrogen, $f_{H\ free}$, and supports the idea that the actual thermal motion for the hydrogen atoms exceeds that of the heavier atoms.

The equation of the solid straight line in Fig. 2 may be written

$$B'_H = mB_{non\text{-}H} - K \qquad (1)$$

where K is a positive number. The apparent temperature factor (T.F.) for a hydrogen atom then becomes

$$\begin{aligned} \text{T.F.} &= \exp(B'_H \sin^2\theta/\lambda^2) \\ &= \exp[-(mB_{non\text{-}H} - K)\sin^2\theta/\lambda^2] \\ &= \exp(K\sin^2\theta/\lambda^2) \times \\ &\quad \exp[-(mB_{non\text{-}H})\sin^2\theta/\lambda^2]. \qquad (2) \end{aligned}$$

The term $\exp(K\sin^2\theta/\lambda^2)$ in Eq. 2 absorbs in the temperature factors differences between the scattering factors for the free hydrogen atom used in the calculations and those for the bonded hydrogen atoms actually present in the structure. While the exponential can correct only approximately for differences, to this degree of approximation the scattering factor for a bonded hydrogen atom may be written

$$f_{H\ bonded} = (f_{H\ free})\exp(K\sin^2\theta/\lambda^2). \quad (3)$$

The positive value of K indicates that the electron charge cloud is more localized than that in the free atom.

The term $\exp[-(mB_{non\text{-}H})\sin^2\theta/\lambda^2]$ in Eq. 2 represents the actual temperature factor for hydrogen, and we have

$$B_H = mB_{non\text{-}H} \qquad (4)$$

where B_H is the actual thermal parameter. The proportionality between B_H and $B_{non\text{-}H}$ may, at first sight, seem surprising. Indeed, packing in the solid state introduces complexities, and differences in packing probably account for the irregularities in Fig. 2. Nevertheless, thermal parameters for hydrogen atoms, at least on the average, would be expected to exceed those of the heavier atoms not only because of the small mass of the hydrogen atoms but also because of their terminal positions in the molecule.

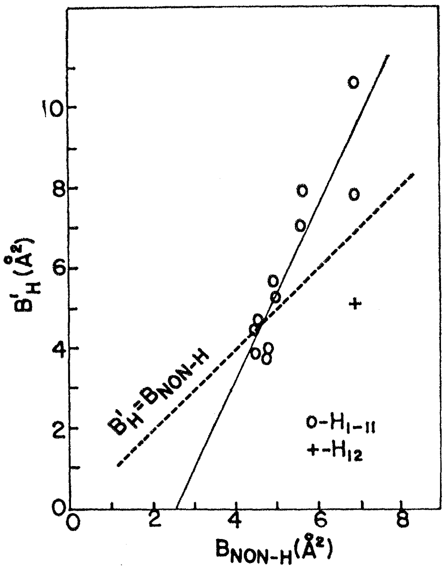

Fig. 2. Graph of B'_H, the apparent thermal parameter of a hydrogen atom, plotted against $B_{non\text{-}H}$, the mean thermal parameter of the atom to which hydrogen is bonded.

Uncertainties due to differences in packing and intermolecular forces in the solid state and limited knowledge of the exact zero point energies make any determination of K by extrapolation in Fig. 2 of questionable validity. These difficulties would be obviated, however, if both neutron and x-ray diffraction data of sufficient precision were available for the same structures. This would allow verification of certain aspects of the foregoing suggestions and a direct determination of the scattering factor for a bonded hydrogen atom.

While it is premature to speculate on the exact magnitude of K, it may be the equivalent of several units in B over the range of CuKα data. If K is so large, it is evident that hydrogen contributes appreciably more to high order reflections than has been considered heretofore.

L. H. JENSEN
M. SUNDARALINGAM
Department of Biological Structure, University of Washington, Seattle

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Acid Phosphatases of Human Red Cells: Predicted Phenotype Conforms to a Genetic Hypothesis

Abstract. *Analysis of data from 80 families and 369 unrelated individuals confirms the hypothesis that human red cell acid phosphatase phenotypes are determined by three codominant alleles at a single autosomal locus. Further confirmation is afforded by the finding of the predicted sixth phenotype.*

Hopkinson, Spencer, and Harris (*1*, *2*) demonstrated that the acid phosphatase of human red cells may occur in different forms which are genetically determined. They proposed that the acid phosphatase phenotypes are determined by three alleles, P^a, P^b, and P^c, at an autosomal locus. They observed five phenotypes, two homozygous (called A and B) and three heterozygous (called BA, CA, and CB) types, and predicted a sixth type, homozygous C (*1*, *2*). We report here data confirming their genetic hypothesis and the discovery of the C homozygote (*3*).

The phenotypes were determined by starch-gel electrophoresis. We followed the procedure of Hopkinson *et al.* (*2*), except that we obtained better separations with an 8 percent starch concentration rather than the 10 percent recommended by the makers (*4*).

Acid phosphatases from the red cells of members of families from a genetic isolate (a religious group—the H sect) composed of people of Swiss and German ancestry, and of members of families of mixed ancestry from Brazil, were studied. The cells obtained from the persons of sect H were fresh (less than 4 days old); the cells of the persons from Brazil had been stored in glycerol at −40°C for at least 6 months before use. No effects of storage were noted.

The family data are presented in Table 1. The samples from family members were not tested in family groups. The data are adequately explained by the hypothesis advanced by Hopkinson *et al.* (*1*, *2*) that the phenotypes are due to three alleles P^a, P^b, P^c, and to that extent confirm it. A significant deficit of BA offspring from matings of B × BA (to a greater degree in set A than in set B) occurs in our sample. Such a deficit does not appear in the data of Hopkinson *et al.* (*1*, *2*). It is possible that experimental errors entered into our determinations of phenotype during the earlier stages of our work (set A and the first part of set B) because the ratios seemed to improve as our work proceeded.

At this point, since we had confirmed the hypothesis of three alleles, we set out to find matings which could have C offspring. Therefore, only samples from the parents of the Brazilian families were tested. Two hundred and sixty-three individuals were examined before we found a mating (CB × CB) with both parents having the P^c allele. These 263 parents, plus those of the 53 Brazilian families tested completely (Table 1), provide a sample of 369 unrelated individuals, which may be used to test the hypothesis of three alleles by comparison with the Hardy-Weinberg equilibrium. The data are presented in Table 2. The agreement between the observed and expected values computed on the basis of the Hardy-Weinberg law is clearly satisfactory. The frequency of allele P^c is essentially the same in this sample as it is in the English sample of Hopkinson *et al.* (*2*) (0.03 compared to 0.04), but there are marked differences between the frequencies of P^a and P^b in the two samples (0.20 compared to 0.36, and 0.77 compared to 0.60, respectively). This suggests that the gene frequencies may vary among different populations as well as among smaller isolates, and thus be useful for population studies.

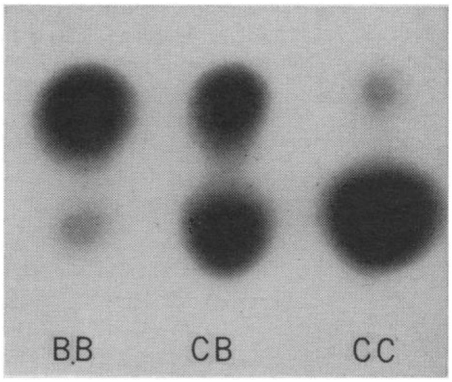

Fig. 1. Starch-gel electrophoretic pattern of acid phosphatase phenotypes of red cells, *BB*, *CB*, and *CC* (from left to right). Insertion is at the base of the figure and migration is toward the anode at the top of the figure. The conditions of electrophoresis and staining are essentially those described by Hopkinson *et al.* (*2*).

The CB × CB mating is of particular interest, because two of the seven children showed a new phenotype, presumably the missing C phenotype, three of the remainder were B, and two were CB. Figure 1 shows one of the homozygous CC samples with a homozygous BB and a CB sample for comparison. It is striking that the CC phenotype is almost the mirror image of the BB phenotype. The starch-gel electrophoretic pattern of each has two zones; in B the faster zone shows greater activity, while in C the slower zone shows more activity. There is much greater activity in the slower zone of C, however, than there is in the faster zone of B. This is in accordance with the prediction of Hopkinson *et al.* (*2*) based on quan-

Table 1. Phenotypes of acid phosphatase in red cells in families from two populations.

Matings		Offspring					
		Total	Phenotypes				
Phenotype*	No.		A	BA	B	CB	CA
		A. An inbred group isolated by religious customs living in the U.S.					
A × BA	5	30	15	15			
A × B	2	14		14			
B × B	2	13			13		
B × BA	11	64		23	41		
BA × BA	7	35	12	13	10		
		B. Families of mixed Caucasian, Negro, and South American Indian ancestry					
A × BA	3	13	6	7			
A × B	3	7		7			
B × B	17	83			83		
B × BA	23	104		47	57		
B × CB	5	24			13	11	
BA × CB	2	8		2	2	1	3

* Matings are listed according to the phenotypes of the parents without regard to sex.