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Remarks on 'improved' atomic form factors. By JAMES A. IBERS, *Shell Development Company, Emeryville, California, U.S.A.*

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Recently Hurst, Miller & Matsen (1958) (hereafter abbreviated HM&M) calculated atomic form factors for the two-electron systems H^{-1} through C^{+4} using the radial-correlated analytic wave functions of the Hylleraas-Eckart type with parameters of Shull & Löwdin (1956). HM&M note that these wave functions lead to lower total energies for the two-electron systems than do other approximations, and on this basis state that the form factors derived from Hylleraas-Eckart wave functions may represent an improvement on those based on self-consistent fields. A wave function is regarded as better than another within the framework of the variation principle if it leads to a lower energy for the whole atomic system. Experience has shown that the energy criterion is a generally useful one, but it is by no means true that a wave function yielding a lower energy is necessarily better than another in the sense of better representing the true wave function reliably over a large region of space. Thus, Bartlett (1955) has shown that there are serious defects in Hylleraas's best approximations for the helium atom in some regions of r . Moreover, Green *et al.* (1954) indicate that relatively good energies can be obtained from relatively poor wave functions. As a function of scattering angle the atomic form factor is a complicated function of the wave functions, and it does not follow, as HM&M imply, that those wave functions yielding the lowest energy will *a priori* yield the most reliable atomic form factors. In view of this, an important point, and one which HM&M failed to infer from their results, partly because of their rather unfortunate choice of James & Brindley (1931) form factors for comparison, is that the atomic form factors, even for the very light two-electron atoms and ions, are relatively insensitive to the wave functions used. Insensitivity, from the point of view of present experimental detectability, to radial correlation effects for the slightly heavier atom beryllium had already been established (Ibers, 1957), and a comparison of the radial correlated and uncorrelated (Slater wave function) results of

HM&M indicates that except, of course, for H^{-1} , this is true also for the two-electron systems. Of more interest is the direct comparison of the results of HM&M with Hartree-Fock calculations. Freeman (1958) has computed the atomic form factors for Li^+ and for C^{+4} from the single-configuration Hartree-Fock wave functions of Fock & Petrashen (1935) and Jucys (1939), respectively. Freeman's results are in remarkable agreement with the radial-correlated results of HM&M, the maximum deviations being only 0.003 electrons for C^{+4} and 0.005 electrons for Li^+ . Other comparisons can be made in the region $\sin \theta/\lambda > 0.4$ of the results of HM&M with those for the neutral atoms Be and B (Ibers, 1957; Hartree-Fock, multiple configuration): here the agreement is within about 2%. Such excellent agreement is, of course, most fortunate, for insensitivity of atomic form factors of even the very light atoms to refinements in the calculations of atomic wave functions and to their reliability on an energy criterion, makes immensely simpler the task of obtaining reliable atomic form factors.

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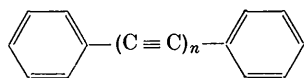
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The crystal structures of α , ω -diphenyl-poly-ynes. I. Crystal data. By T. WATANABÉ, I. TAGUCHI and N. MASAKI, *Faculty of Science, Osaka University, Osaka, Japan*

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In order to elucidate the physical and chemical properties of substances having the conjugated triple bonds, it is of primary importance to determine the detailed molecular and crystal structure of compounds having these.

For this purpose, the series of α, ω -diphenyl-poly-ynes



was chosen, because homologous members with $n =$

1, 2, 3, 4, 5, 6 and 8 are now available (Nakagawa, 1950a, 1950b; Jones *et al.*, 1951; Schlubach & Franzen, 1951; Nakagawa & Inui, 1952). While the crystal structure of tolane ($n = 1$) has been reported by Robertson & Woodward (1938), and of diphenyl-diacetylene ($n = 2$) by Wiebenga (1940), other members of the homologous series remained yet to be explored.

We have determined the unit-cell dimensions and space groups of these members with $n = 3, 4$ and 5. Single crystals of α, ω -diphenyl-1,3,5-hexatriyne ($n = 3$) were obtained from methanol solution. α, ω -diphenyl-1,3,5,7-