1,3-Diphenylisoindoles

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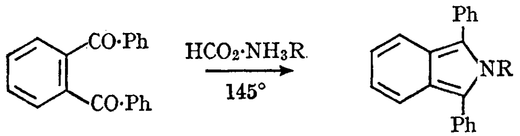
A number of syntheses of *N*-substituted isoindoles are known,[1] but only one synthesis (and isolation) of *N*-unsubstituted isoindoles has been reported.[2] We now report the conversion of *o*-dibenzoylbenzene (I) into 1,3-diphenylisoindole (IIa) or 1,3-diphenyl-2-methylisoindole (IIb) by means of the Leuckart reaction.[3] In addition, we find that (IIa) can also be prepared from the toluene-*p*-sulphonamide (III) using the method suggested by Fenton and Ingold[4] and recently realized[5] for the synthesis of isoindole (which was trapped with a dienophile but not isolated).

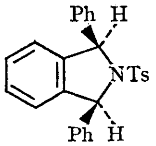
Reaction of (I) with ammonium formate at 145° gave, after chromatography, a 44% yield of (IIa) as pale yellow needles, m.p. 148—150° (decomp.) (oxygen excluded), ν_{max} ($CHCl_3$) 3445 (NH) and 1595 cm.$^{-1}$ (C=C stretching), and λ_{max} (log ϵ) 228 (4·24) (sh.), 237 (4·27), 268 (4·22) (sh.), 273 (4·27), 322 (4·13), 335 (4·16), and 387 mμ (4·37). The nuclear magnetic resonance spectrum (in $CDCl_3$) shows a broad NH peak at τ 0·7 and aromatic protons at τ 2·0—3·2, but no other detectable CH absorption. Thus, little or none of the isoindolenine tautomer can be present.



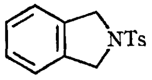
(I)

(IIa); R = H

(IIb); R = Me



(III)



(IV)

Similar reaction of (I) with methylammonium formate gave, after chromatography and recrystallization from ethanol, a 28% yield of (IIb), m.p. 149—150°, previously prepared by Theilacker and Schmidt.[6] The ultraviolet absorption spectrum of (IIb), in ethanol, is similar to that of (IIa) with λ_{max} (log ϵ) 228 (4·47), 268 (4·13) (sh.), 276 (4·20), 332 (4·01), and 371 mμ (4·27).

Solutions of (IIa) lose their blue fluorescence when exposed to air for 24 hr. or more, but the compound can be handled easily under nitrogen. Reduction of (IIa) with zinc in acetic acid gave *cis*-1,3-diphenylisoindoline,[7] m.p. 108—109° (84%). The spectral data were consistent with this structure and in agreement with the data reported by Carpino.[8] Treatment of this dihydroisoindole with toluene-*p*-sulphonyl chloride in pyridine gave the sulphonamide (III), m.p. 238—239° (reported[7] m.p. 255°), which, on reaction with potassium t-butoxide in a dimethyl sulphoxide–benzene solution,[5] gave, after chromatography, a 38% yield of 1,3-diphenylisoindole (IIa), identical with the sample prepared from (I). Thus the failure by Fenton and Ingold[4] to obtain isoindole by treatment of the sulphonamide (IV) with aqueous potassium hydroxide seems to be due to their choice of reagents.

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