Addition of Phenols to *NN'*-Dicyclohexylcarbodi-imide

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EXAMPLES of direct addition of phenols to carbodi-imides are very scarce in the chemical literature[1]. Only polynitrated phenols easily give addition products which (owing to the strong withdrawing effect of the nitro-groups) rearrange to *N*-acylureas. In agreement with this, we obtained *NN'*-dicyclohexyl-*N*-(2,4,6-trinitrophenyl)urea [m.p. 208—210°, ν(C=O) st. in a KBr pellet at 1642 cm.$^{-1}$] and *NN'*-dicyclohexyl-*N*-(2-methyl-4,6-dinitrophenyl)urea [m.p. 192—193°, ν(C=O) st. 1639 cm.$^{-1}$], in good yield, by adding benzene solutions of either picric acid or 2-methyl-4,6-dinitrophenol to *NN'*-dicyclohexylcarbodi-imide in the same solvent, but no adducts were obtained from ethyl salicylate, *o*-aminophenol, or 4-hydroxy-3-methoxybenzaldehyde under a variety of conditions. However, *o*-diphenols, such as pyrocatechol and 2,3-dihydroxynaphthalene, gave addition products, to which the following isourea structures were assigned on an infrared spectroscopic basis: *NN'*-dicyclohexyl-*O*-(2-hydroxyphenyl)isourea [m.p. 140—141°, ν(C=N) st. 1667 cm.$^{-1}$] and *NN'*-dicyclohexyl-*O*-(2-hydroxy-4,5-benzophenyl)isourea [m.p. 136·5—137·5°, ν(C=N) st. 1650 cm.$^{-1}$]. The ease of formation of these products must be related to the formation of a hydrogen bridge between the imidic nitrogen and the hydroxylic proton which has a great stabilizing effect.

Attempts to obtain *NN'*-dicyclohexyl-*O*-(2-methylphenyl)isourea from *o*-cresol and *NN'*-dicyclohexylcarbodi-imide in the presence of sodium ethoxide, gave, after recrystallization from hexane, the isourea adduct with one molecule of ethanol and one of water (m.p. 57—58°), as shown by elemental analysis, i.r. spectrum (3571 cm.$^{-1}$ in $CHCl_3$ and 1664 cm.$^{-1}$ in C_2Cl_4), and n.m.r. spectrum which shows the characteristic triplet–quadruplet of the ethyl group.

All the products gave correct elemental analyses.

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