5,5-DISUBSTITUTED 7-OXO-1,2,3,4,6,7-HEXAHYDROCYCLOPENTA[d]PYRIMIDINES

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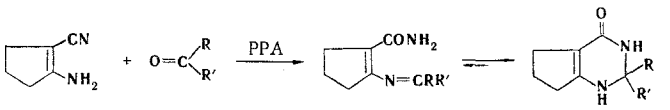
We have developed a new method for the synthesis of 5,5-disubstituted 7-oxo-1,2,3,4,6,7-hexahydrocyclopenta[d]pyrimidines (II-VI, Table 1) by condensation of 1-amino-2-cyano-1-cyclopentene (I) with acyclic and alicyclic ketones in the presence of polyphosphoric acid (PPA) (at 80°C for 5 h).



I II-VI

One might assume the existence of ring-chain tautomerism for II-VI, but the substances that we isolated have a cyclic structure, as confirmed by the IR spectra (ν_{NH} bands of only secondary NH groups for both the solids and solutions in $CHCl_3$), the absence of hydrolysis in hot alkali solutions, and alternative synthesis of the known IV from urea and cyclopentanone. The IR and UV spectra of II, III, V, and VI, which were obtained for the first time in this research, are very characteristic and are similar to the spectra of pyrimidine IV obtained by alternative synthesis. UV spectra: λ_{max} 308-309 m (log ε 3.80-4.01). The IR spectra contain bands in the δ_{NH}, $\nu_{C=C}$, $\nu_{C=O}$, and ν_{NH} regions at 1540-1560, 1605-1615 (very strong), 3060, and 3200-3245 cm^{-1} (very strong). The individuality of the compounds was monitored by thin-layer chromatography on activity II Al_2O_3 in a benzene–methanol system (92.8).

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TABLE 1. 5,5-Disubstituted 7-Oxo-1,2,3,4,6,7-hexahydrocyclopenta[d]pyrimidines

Compound	R	R'	mp, °C	Empirical formula	Found, %			Calculated, %			Yield, %
					C	H	N	C	H	N	
II	CH_3	CH_3	225—227	$C_9H_{14}N_2O$	65,1	8,7	16,8	65,1	8,4	16,9	94
III	CH_3	C_2H_5	194—197	$C_{10}H_{16}N_2O$	66,9	9,0	15,5	66,7	8,9	15,5	53
IV	$(CH_2)_4$		229—230	$C_{11}H_{16}N_2O$	68,7	8,4	14,3	68,7	8,3	14,6	24
V	$(CH_2)_5$		226—227	$C_{12}H_{18}N_2O$	69,9	8,8	12,1	69,9	8,7	13,6	39
VI	$(CH_2)_6$		200—202	$C_{13}H_{20}N_2O$	71,1	9,0	12,6	71,0	9,1	12,7	34

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