

## SYNTHESIS OF 2,4,6-TRIPHENYL-1,3,5-TRIAZINE

V. V. Korshak, T. M. Frunze,  
A. A. Izyneev, and V. G. Samsonova

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The triaryl-S-triazines are known to be chemically and thermally stable compounds, and for this reason they attract the attention of many investigators [1-5]. The existing methods for the preparation of triphenyltriazine are based on the cyclotrimerization of benzonitrile (BN) at high pressure (7500-8500 atm) in the presence of either ammonia or benzamidine at 400-430°, or the cyclotrimerization of benzonitrile in chlorosulfonic acid (CSA) at ~0°C [5]. In the latter case the yield of the desired product is 60%.

We studied the cyclotrimerization of benzonitrile in CSA in order to increase the yield of 2,4,6-triphenyl-1,3,5-triazine (I) and ascertain the optimum conditions for running the synthesis. This reaction is a model reaction for obtaining triazine polymers by the polycyclotrimerization of dinitriles. The results of the cyclotrimerization of BN are given in Table 1.

As the obtained data show, the reaction temperature and time for the cyclotrimerization of BN, and also the CSA:BN molar ratio, have great importance in the process for the formation of (I).

The optimum conditions for the synthesis of (I) are a temperature of 0-5°, a reaction time of 12-24 h, and a CSA:BN molar ratio of 3:1. An increase in the CSA:BN molar ratio leads to a sharp reduction in the yield of (I) (almost to half). A partial sulfochlorination of (I) (S 1.2%, Cl up to 1.0%) occurs when the cyclotrimerization reaction is run at 10°.

## EXPERIMENTAL METHOD

Into a pear-shaped flask was charged 3.4 g of BN (bp 189°) and to it, with cooling, was added in drops the calculated amount of CSA (bp 151-152°) in a predetermined length of time. The rate of adding the CSA was regulated in such a manner that the reaction temperature did not exceed the given temperature. With cooling, the reaction mass was stirred and then poured over ice. The obtained (I) was filtered, and washed in succession with distilled water and alcohol. The product was dried at 105°; mp 223-234; 237-238° (from toluene). From [5]: mp 232°. Found: C 81.58; H 4.84; N 13.63%.  $C_{21}H_{15}N_3$ . Calculated: C 81.53; H 4.88; N 13.58%.

## CONCLUSIONS

A study was made of the cyclotrimerization of benzonitrile in chlorosulfonic acid and the optimum conditions were ascertained for the formation of 2,4,6-triphenyl-1,3,5-triazine.

TABLE 1

T., °C	Time, h	Molar ratio of CSA:BN	Yield of (I), %	T., °C	Time, h	Molar ratio of CSA:BN	Yield of (I), %
0	6	3:1	81,5	5	12	3:1	83,6
0	9	3:1	82,9	10	12	3:1	78,0
0	12	3:1	84,5	0	24	1:1	76,4
0	24	3:1	87,9	0	24	2:1	79,6
0	48	3:1	88,2	0	24	3:1	84,5
-5	12	3:1	76,0	0	24	6:1	76,6
0	12	3:1	82,0	0	24	9:1	59,2
				0	24	12:1	45,6

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