

TECHNICAL
REPORT

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**Plastics — Basic materials for
polyurethanes — Determination of the
amounts of 2,4- and 2,6-isomers in
toluenediisocyanate by infrared
spectroscopy**

*Plastiques — Matières de base pour polyuréthannes — Détermination
des teneurs en isomères 2,4 et 2,6 du toluylène diisocyanate par
spectroscopie infrarouge*



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Foreword

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Plastics — Basic materials for polyurethanes — Determination of the amounts of 2,4- and 2,6-isomers in toluenediisocyanate by infrared spectroscopy

WARNING — SAFETY PRECAUTIONS

Handle isocyanates with care, and limit inhalation as much as possible. The operator should wear safety glasses and disposable gloves. The workplace should be well ventilated.

1 Scope

This Technical Report describes the determination of toluene-2,4-diisocyanate (2,4-isomer) and toluene-2,6-diisocyanate (2,6-isomer) in toluenediisocyanate.

This method is applicable to mixtures containing 5 % to 95 % of the 2,4-isomer.

NOTES

1 The method does not take into account the presence of other isomers. Purified toluenediisocyanates may contain trace amounts of the 2,5-isomer. This isomer interferes slightly in the determination of the 2,4-isomer at 810 cm^{-1} . For example, 1 % of the 2,5-isomer exhibits approximately the same absorbance as 0,5 % of 2,4-isomer at 810 cm^{-1} .

2 This note does not concern the English text.

2 Principle

Preparation of a cyclohexane solution of the sample to be analysed.

Measurement of the absorbance for the 810 cm^{-1} and 782 cm^{-1} bands which are characteristic of the 1,2,4- and 1,2,6-positions on the aromatic ring.

Calculation of the absorbance ratio (5.3).

Conversion of the absorbance ratio into a ratio of the percentages by mass of the 2,4- and 2,6-isomers (5.1.2). For this, a calibration is carried out using standard solutions. The calibration is checked before each analysis series by means of a reference solution.

3 Reagents

3.1 Cyclohexane, spectroscopy grade.

3.2 Toluene-2,4-diisocyanate, to the following specifications (see note 3):

Crystallization temperature (°C)	21,95
Refractive index (at 20 °C)	1,567 8
Density at 23 °C (kg/m^3)	1 218,6

3.3 Toluene-2,6-diisocyanate, to the following specifications (see note 3):

Crystallization temperature (°C)	18,15
Refractive index (at 20 °C)	1,571 1
Density at 23 °C (kg/m^3)	1 227,0

NOTE 3 In the absence of a pure toluene-2,6-diisocyanate (or toluene-2,4-diisocyanate) sample, a sample as pure as possible, with a known concentration of toluene-2,6-diisocyanate (or toluene-2,4-diisocyanate), and exhibiting no interfering impurity at the measurement wavelengths, should be selected as reference toluene-2,6-diisocyanate (or toluene-2,4-diisocyanate).

3.4 Reference sample (see note 4).

Commercial toluenediisocyanate containing $X \pm 1,5\%$ (m/m) of the 2,4-isomer. The concentration of the 2,4-isomer in this reference sample shall have been measured 10 times by means of the method described in this Technical Report just after calibration of the spectrometer. (X is the assumed concentration of the 2,4-isomer in the sample) of toluene-diisocyanate to be analysed. This value of X must be known or determined by preliminary tests.)