Intermediates

2,6-Naphthalene dicarboxylic acid (HNDAC)
BASF’s high-purity 2,6-naphthalene dicarboxylic acid (HNDA) is a key monomer for the production of high-performance polyester, polyamide and liquid crystal polymers. Naphthalate-based polymers made from HNDA are known for their dimensional stability and strength at high temperatures as well as excellent vapor barrier properties. These enhanced polymer properties have led to the growth of HNDA use in applications including electronics, food and beverage packaging and films.

Unique product
HNDA is a unique naphthalene-based dicarboxylic acid, which is produced by BASF as a white free-flowing powder. BASF’s HNDA is manufactured through a unique process to hydrolyze dimethyl-2,6-naphthalene dicarboxylate (NDC), resulting in the high-purity product. The double ring structure of HNDA contributes to the higher performance of resulting polymers. Unlike NDC, polymerization of HNDA occurs through a methanol-free process, removing the need for additional process and safety controls.

Reliable partner
BASF is the global leader in production of HNDA with more than 15 years of experience. HNDA is available from BASF with the highest product purity and excellent product quality ensured by our unique process technology. BASF supplies HNDA through a global distribution network and regional sales contacts.
HNDA is a key co-monomer in the production of liquid crystal polymers for high-temperature and high-performance applications, such as electronics.
HNDA for high-performance polyester resins

HNDA can polymerize with polyalcohols to give different types of polyesters, including polyethylene naphthalate (PEN) and polybutylene naphthalate (PBN), which incorporate the naphthalate structure of HNDA. For example, HNDA polymerizes with ethylene glycol to form PEN, similar to the preparation of polyethylene terephthalate (PET) from terephthalic acid and ethylene glycol. Naphthalate-based polyesters have significantly improved thermal, mechanical and vapor barrier properties over their terephthalate counterparts and can be used as copolymers or blends with other polyesters to provide improved performance. These superior polymer properties have led to the use of HNDA-containing polyesters in applications including food and beverage packaging, high-performance films, heat sterilizable medical devices and high-temperature cookware.

Polyesters based on HNDA

<table>
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<tr>
<th>Diacid</th>
<th>Polyalcohol</th>
<th>Polyester</th>
</tr>
</thead>
<tbody>
<tr>
<td>HNDA</td>
<td>Ethylene glycol</td>
<td>Polyethylene naphthalate (PEN)</td>
</tr>
<tr>
<td>HNDA</td>
<td>1,4-Butanediol</td>
<td>Polybutylene naphthalate (PBN)</td>
</tr>
<tr>
<td>HNDA</td>
<td>1,3-Propanediol</td>
<td>Polymethylpropylene naphthalate (PTN)</td>
</tr>
</tbody>
</table>

Enhanced properties in PEN resins

HNDA-based PEN resins show many significant improvements over PET in mechanical, thermal, and barrier properties, as well as better chemical resistance and UV absorbance. Similar trends also exist with other naphthalate-based polyesters. Moderate enhancements can be achieved through copolymerization of HNDA in PET processes.

Comparative properties of PET and PEN resins

With superior attribute values on the outer edge of the figure

- CO₂ permeation [cm³ · mm / (m² · day · atm)]
- O₂ permeation [cm³ · mm / (m² · day · atm)]
- Water vapor transmission [g · mm / (m² · day · atm)]
- Glass transition temperature [°C]
- Mechanical continuous use temperature [°C]
- Hydrolysis resistance [hr]
- Tensile strength [MPa]
- UV absorbance [%] (360 nm)

Polymerization of HNDA with EG to form PEN resin

Ethylene glycol (EG) + HNDA → Poly(ethylene naphthalate) (PEN)
HNDA in polyester copolymers and blends

For many applications, the full performance benefits of PEN resins may not be required. In these cases, PEN can be combined with established terephthalic acid-based polyesters such as PET as a copolymer or blend to enhance the polymer properties. One method to incorporate naphthalene into terephthalic acid-based PET manufacturing processes is copolymerization through replacement of some terephthalic acid with HNDA. In such facilities, HNDA can be used as a direct substitute for terephthalic acid without modification of the polymerization equipment or process.

Properties of naphthalate copolymers

The properties of PET/PEN copolymers and blends will vary based on the HNDA content. For example, both glass transition temperature and vapor barrier properties are directly proportional to the PET/PEN ratio. In addition, copolymers with HNDA can achieve crystallinity at ratios of up to 15% or over 85% naphthalate content while producing a polyester with significant physical property advantages over PET. Therefore, the properties of copolymer and blend formulations can be cost-effectively tuned to meet the needs of any application through the addition of HNDA.

Glass transition temperature as a function of copolymer or blend composition

Methanol-free polyester manufacturing from HNDA

Similar to terephthalic acid, the use of HNDA does not result in the production of methanol, thereby eliminating the need for supplemental control systems and methanol recovery equipment. Polymerization of HNDA with diols releases water during the condensation, rather than methanol as in the transesterification reaction of dimethyl-2,6-naphthalene dicarboxylate (NDC). HNDA, therefore, is a drop-in solution for the production of PET/PEN copolymers in existing PET plants where terephthalic acid is used as a feedstock.

HNDA in polyester food packaging

HNDA-based polyester resins can be used in a variety of rigid or flexible packaging applications to give increased thermal stability, higher strength, and improved vapor barrier properties. By varying the naphthalate content in the polyester, the final product can be optimized for cost versus required performance properties. The addition of HNDA to PET packaging extends the potential applications of polyester to include hot-fill and heat-sterilized bottles, plastic beer bottles, and packaging for sensitive food products. Furthermore, PET homopolymers and PET/PEN copolymers and blends containing HNDA at levels from zero to 100 percent are FDA-approved in the United States for food-contact applications.

UV absorbing properties of HNDA-containing polyesters

In addition to boosting the mechanical, thermal, and barrier properties of polyesters, the use of HNDA also provides a barrier to ultraviolet (UV) radiation. Furthermore, PEN resins remain transparent to visible light, resulting in polyester containers that can protect contents from harmful UV rays while maintaining visible transparency. PET and other visibly transparent materials do not successfully block UV radiation. Even at levels of less than 1 weight percent, HNDA-based polyesters offer a very cost-effective solution to UV protection in food and beverage packaging applications. These UV-blocking properties help to maintain product stability, extend shelf life, and protect against product color loss.

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HNDA in specialty polyamide applications

BASF’s HNDA can be used to make specialty polyamide resins, either as part of a homopolymer system or as a partial replacement for another dicarboxylic acid in nylon-type systems. Polyamides containing HNDA offer improved thermal and hydrolytic stability as well as better chemical resistance and vapor barrier properties. Applications for naphthalate-based polyamides include automotive parts and other engineering plastics.

High-performance polyamide homopolymers based on HNDA
HNDA is used, in combination with various diamines, to produce polyamides with excellent heat resistance and mechanical properties. Utilizing the high chemical resistance of HNDA-based polyamides, these polymers have found significant usage in the automotive industry for fuel hoses and other engineering plastics.

Naphthalate-modified polyamide copolymers
HNDA can replace adipic acid in nylon-type polyamide compositions to improve the polymer thermal and hydrolytic stability while decreasing the required processing temperature. Similar improvements in polymer properties can also be seen in other HNDA-modified polyamide systems. Since naphthalate-based polyamides also see improved UV blocking ability, they find numerous applications in outdoor uses, where high weatherability is important.

Product Properties

<table>
<thead>
<tr>
<th>CAS number</th>
<th>1141-38-4</th>
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<tbody>
<tr>
<td>Synonyms</td>
<td>2,6-Naphthalic acid, 2,6-NDA</td>
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<tr>
<td>Empirical formula</td>
<td>( C_{12}H_8O_4 )</td>
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<tr>
<td>Molecular weight [g/mol]</td>
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<tr>
<td>Organic purity [% min]</td>
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<tr>
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<tr>
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<tr>
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<td>Nickel content [ppm]</td>
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<td>Appearance – visual</td>
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<tr>
<td>Solubility in water at 25°C</td>
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</tr>
</tbody>
</table>

HNDA properties and handling recommendations

HNDA is not classified as a hazardous substance according to GHS or OSHA and does not contain substances with occupational exposure limit values. In general, HNDA can be handled safely following conventional best available practices for non-toxic solid chemicals in powder form that prevent contact with personnel. Standard precautions such as minimal exposure to moisture or oxygen apply for both quality and safety reasons. As with most combustible solids, measures should be taken to avoid static charge buildup, to minimize dust concentration and to control oxygen levels. As HNDA may cause skin and eye irritation, protective gloves and clothing as well as eye protection should always be worn. For further safety data, please refer to the material safety data sheets.

BASF offers HNDA in supersacks as well as 100 kilogram and 25 kilogram fiber drums.
The data contained in this publication is based on our current knowledge and experience. In view of the many factors that may affect processing and application of our product, the data does not relieve processors from carrying out their own investigations and tests; neither does the data imply any guarantees of certain properties, nor the suitability of the product for a specific purpose. Any descriptions, drawings, photographs, data, proportions, weights etc. given herein may change without prior information and do not constitute the agreed contractual quality of the product. It is the responsibility of the recipient of our products to ensure that any proprietary rights and existing laws and legislation are observed. The safety data given in this publication is for information purposes only and does not constitute a legally binding Material Safety Data Sheet (MSDS). The relevant MSDS can be obtained upon request from your supplier or you may contact BASF directly at info.intermediates@basf.com. 2013 edition