

Technical Information Bulletin

BPD IN THE MANUFACTURE OF ACYLPHOSPHINE OXIDE PHOTOINITIATORS

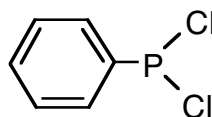
Introduction

BPD (Benzene Phosphorus Dichloride) is a highly reactive molecule that is utilized as an intermediate in the manufacture of acylphosphine oxide (APO) photoinitiators. The chemical composition and high reactivity of the BPD molecule affords a safe and viable cost-effective route to the manufacture of the mono and bisacylphosphine oxide (i.e., MAPO and BAPO) photoinitiator products.

Technology

Photoinitiators are molecules that utilize energy from either ultraviolet or visible light to induce a chemical reaction. In coatings, inks and other applications, photoinitiators are utilized to cure or dry the substrate through the application of light rather than heat. A coating or ink containing a photoinitiator can dry or cure in less than a few seconds. Additionally, drying or curing of materials via photoinitiators reduces volatile solvents and energy requirements.

One principal commercial type of photoinitiators is based on acyl phosphine oxide chemistry. Acylphosphine oxide (APO) photoinitiators are ideal for

Structure**Chemical Name**

Benzene Phosphorus Dichloride or
Phenylphosphorus Dichloride (BPD)

curing either white or highly pigmented, thick coatings. They also exhibit low yellowing tendencies and do not discolor the end coating. Dependent upon the starting raw materials, it is possible to produce both liquid and solid products that exhibit a range of solubility and odor characteristics.

Physical and Chemical Properties

In its purified form at ambient conditions, BPD is a liquid product. The chemical structure, nomenclature, general characteristics and properties of the product are as follows:

Product Sales Specifications:

Assay (GC)	99.0% minimum
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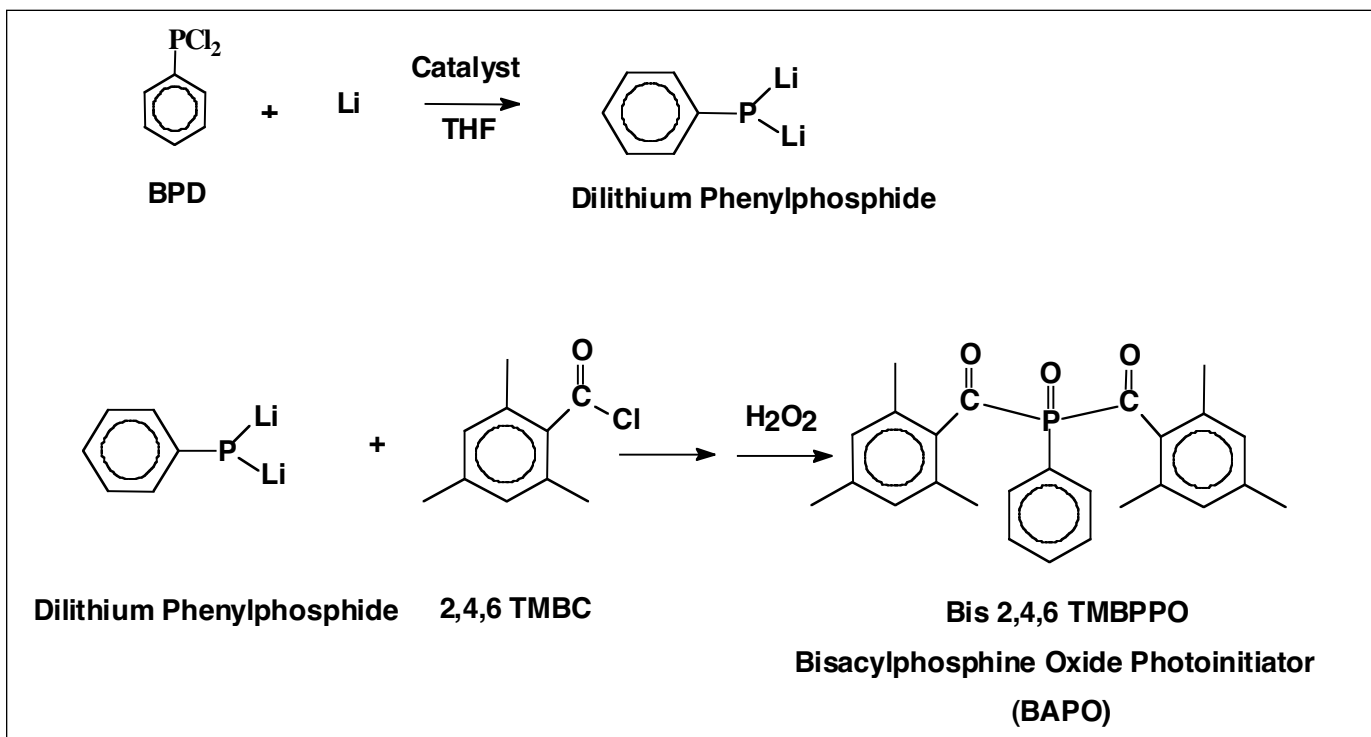
Characteristics and Properties:

Description	Colorless liquid with phosphine-like odor
Empirical Formula	$C_6H_5PCl_2$
Molecular Weight	178.99
Boiling Point	224.6°C
Specific Gravity @ 25°C	1.316-1.320
Vapor Pressure (mm Hg)	10 @ 98°C
Viscosity @ 25°C	1.3 cps
Autoignition Temperature	265°C
Solubility:	Soluble in most aprotic organic solvents Decomposes in water and protic solvents.

APO photoinitiators can be either mono or bisacyl-based, and are typically referred to as either MAPO (i.e., monoacylphosphine oxide) or BAPO (i.e., bisacylphosphine oxide) products. Typical applications for MAPO and BAPO photoinitiators include radiation curable coatings, printing inks, preregs, photoresists, UV curable adhesives and other areas.

Several synthetic routes exist for the production of both MAPO and BAPO photoinitiators, based upon utilizing BPD as a starting raw material. One approach for the synthesis of a BAPO product is disclosed in World Patent WO 00/32612 (see below). In this disclosure, the BPD molecule provides an alternative and simplified synthetic route that offers significant safety, health, environmental and economic advantages over alternative phosphine-based approaches.

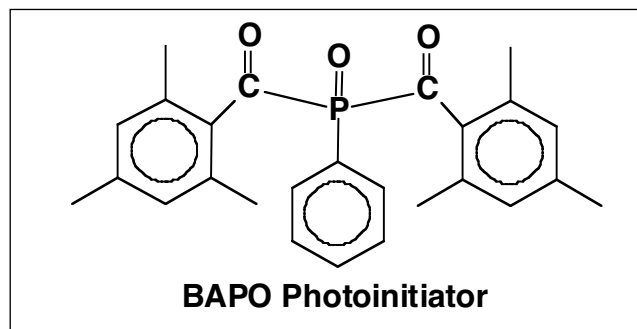
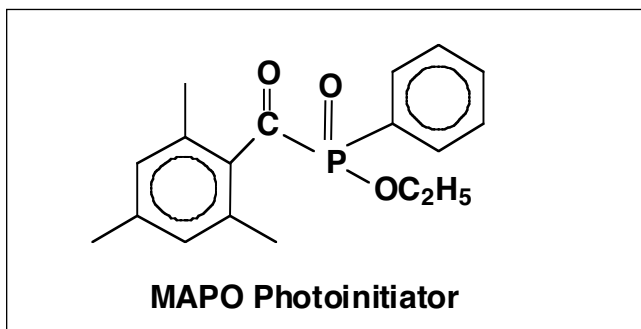
Synthesis of BAPO Photoinitiator



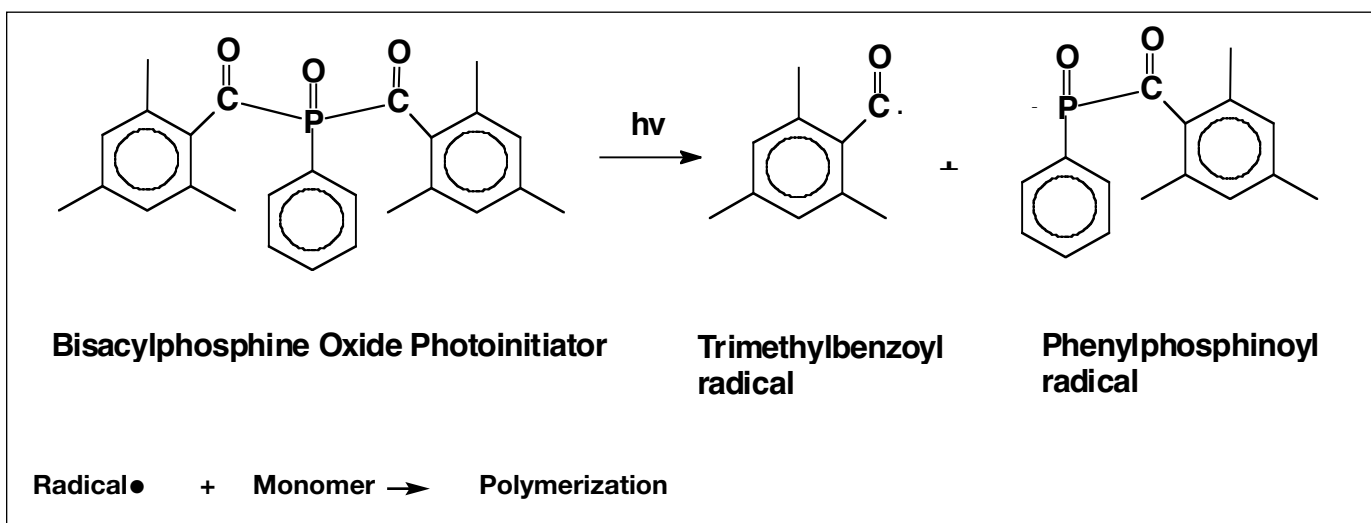
APO photoinitiators (see BPD derived MAPO and BAPO types below) are so called alpha cleavers that form trimethylbenzoyl and phosphinoyl radicals from a photochemically excited singlet state. This excited state is achieved through exposure to UV light. The mechanism for the alpha cleavage of a BAPO molecule into radicals is detailed below. The BAPO products do evidence a higher degree of efficacy than the MAPO products, as they are able to generate more radicals that initiate polymerization. Typically a MAPO

photoinitiator generates two (2) radicals, while a BAPO photoinitiator generates four (4) radicals. All generated radicals can react with monomers to initiate the polymerization reaction. The phosphinoyl radical is very reactive towards olefinic monomers such as acrylic esters, methacrylic esters, acrylonitrile, vinyl acetate and styrene, and it is actually 2 to 3 times more effective when adding to the double bond site of a molecule than the trimethylbenzoyl radical.

MAPO and BAPO Photoinitiators - Derived from BPD



Cleavage of BAPO Photoinitiator



Features and Benefits

The features and benefits of BPD with respect to the manufacture of MAPO and BAPO products are as follows:

Features

1. BPT molecule
2. Cl atom on BPD
3. Phosphorus atom in BPD molecule
4. Aryl moiety on BPD molecule

Benefits

Affords safe and economical route to MAPO and BAPO molecules

Readily reacts with either metals or alcohols to yield phosphine intermediate

Imparts highly reactive carbonyl phosphine oxide site to MAPO or BAPO molecule

Provides site for cleaving of MAPO or BAPO molecule and generation of highly reactive phosphinoyl radical

Contributes high molecular weight to MAPO and BAPO products, yielding both solid and liquid materials that exhibit low volatility

Markets and Recommendations

Manufacturers are encouraged to consider the evaluation of BPD as a starting raw material for the production of MAPO and BAPO and other photoinitiators products.

Safety and Toxicity Information

Please refer to the Material Safety Data Sheet for information on safety and toxicity.

Technical Service Information

Cytec's Phosphine & Phosphorus Specialties group provides technical service assistance for BPD and other products. Samples of BPD are available upon request.

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