meso stilbene dibromide ir

meso stilbene dibromide ir is a chemical compound of significant interest in organic chemistry due to its unique structural and reactive properties. This compound, derived from stilbene, features two bromine atoms positioned in a meso configuration, which influences its chemical behavior and applications. Understanding meso stilbene dibromide ir involves exploring its synthesis, structural characteristics, spectroscopic analysis, and practical uses in various chemical reactions. Its importance is underscored by its role as an intermediate in organic synthesis and its relevance in stereochemical studies. This article provides a comprehensive overview of meso stilbene dibromide ir, including detailed information on its preparation methods, infrared (IR) spectroscopic features, and applications. The content aims to serve as a valuable resource for chemists and researchers interested in halogenated stilbene derivatives.

Synthesis of meso stilbene dibromide ir

The synthesis of meso stilbene dibromide ir typically involves the bromination of stilbene, a process that adds bromine atoms across the double bond of the stilbene molecule. This bromination reaction is usually carried out under controlled conditions to ensure the formation of the meso isomer, which is characterized by having two bromine atoms added in a specific stereochemical arrangement. The reaction can be performed using bromine (Br_2) in an inert solvent such as dichloromethane or carbon tetrachloride.

Typical Bromination Procedure

In a standard procedure, stilbene is dissolved in an appropriate solvent, and bromine is added dropwise while maintaining the reaction mixture at low temperatures to control the rate of reaction. The progress of the reaction is monitored by thin-layer chromatography (TLC) or other analytical techniques until complete conversion to meso stilbene dibromide ir is achieved. The product is then isolated by filtration or extraction, followed by purification methods such as recrystallization.

Factors Affecting Yield and Selectivity

Several factors influence the yield and stereoselectivity of the bromination reaction, including solvent choice, temperature, and the concentration of bromine. Lower temperatures generally favor the selective formation of the meso isomer by minimizing side reactions. Additionally, the stereochemistry of the starting stilbene (cis or trans) can affect the configuration of the dibromide product.

Structural Characteristics and Stereochemistry

meso stilbene dibromide ir possesses distinct structural features that define its chemical behavior. The molecule consists of a stilbene backbone with two bromine atoms attached to the carbons formerly involved in the double bond. The meso designation indicates that the molecule has an internal plane of symmetry, resulting from the anti addition of bromine atoms across the double bond.

Meso Isomer Configuration

The meso isomer of stilbene dibromide is characterized by its achiral nature despite having stereogenic centers. The bromine atoms are added in an anti fashion, producing a molecule with two stereocenters but an overall symmetric structure. This stereochemistry contrasts with the racemic mixture of enantiomers often formed in similar reactions when the addition is not stereoselective.

Physical Properties

Physically, meso stilbene dibromide ir is typically a crystalline solid with a melting point that can be used to verify purity. Its solubility in organic solvents such as chloroform, dichloromethane, and acetone makes it amenable to various analytical techniques. The molecular weight and elemental composition can be confirmed through mass spectrometry and elemental analysis, complementing structural studies.

Infrared (IR) Spectroscopy of meso stilbene dibromide ir

Infrared (IR) spectroscopy is a vital tool for analyzing meso stilbene dibromide ir, providing insights into its functional groups and molecular vibrations. The IR spectrum of this compound displays characteristic absorption bands that correspond to the vibrational modes of the C–Br bonds and the aromatic ring system of stilbene.

Characteristic IR Absorption Bands

The absorption bands in the IR spectrum of meso stilbene dibromide ir include strong

signals in the fingerprint region associated with C–Br stretching vibrations, typically observed between 500 and 650 cm^{-1}. Additionally, aromatic C=C stretches appear in the region of 1500 to 1600 cm^{-1}, confirming the presence of the stilbene moiety. The absence of absorption bands corresponding to the alkene C=C stretch (normally near 1600–1680 cm^{-1}) indicates the successful addition of bromine across the double bond.

Interpretation and Analytical Utility

The IR spectrum serves as a diagnostic tool to confirm the identity and purity of meso stilbene dibromide ir. By comparing spectra before and after bromination, chemists can verify the conversion of stilbene to its dibromide derivative. Moreover, IR spectroscopy complements other techniques such as nuclear magnetic resonance (NMR) and mass spectrometry in comprehensive molecular characterization.

Applications and Uses in Organic Chemistry

meso stilbene dibromide ir is widely utilized as an intermediate in organic synthesis, particularly in reactions involving further functionalization of the dibromide moiety. Its reactivity and well-defined stereochemistry make it valuable in constructing complex molecules and studying stereochemical outcomes in halogenation reactions.

Intermediate for Substitution and Elimination Reactions

The dibromide groups in meso stilbene dibromide ir can undergo nucleophilic substitution reactions, enabling the introduction of various functional groups such as hydroxyl, amino, or alkoxy substituents. Additionally, elimination reactions can convert the dibromide back to stilbene or other unsaturated derivatives, facilitating synthetic pathways to diverse organic compounds.

Role in Stereochemical Studies

Due to its meso nature and defined stereochemistry, meso stilbene dibromide ir is employed in research focused on stereochemical mechanisms and reaction pathways. Its behavior under different reaction conditions provides insight into the principles of anti addition, chirality, and symmetry in organic molecules.

List of Common Applications

- Synthesis of vicinal dihalides and their derivatives
- Precursors for the preparation of epoxides and glycols
- Model compounds in stereochemical and mechanistic studies

- Reagents in the development of pharmaceuticals and agrochemicals
- Intermediates in polymer chemistry and material science

Safety and Handling Considerations

Handling meso stilbene dibromide ir requires adherence to standard laboratory safety protocols due to its chemical nature and potential hazards. It is essential to work in a well-ventilated environment and use appropriate personal protective equipment (PPE) including gloves, goggles, and lab coats.

Potential Hazards

The compound may cause irritation to the skin, eyes, and respiratory tract. Brominated compounds can be toxic if ingested or inhaled, and proper disposal procedures must be followed to minimize environmental impact. It is important to consult safety data sheets (SDS) prior to handling and to perform all manipulations in a fume hood to avoid exposure to volatile bromine or brominated byproducts.

Storage Recommendations

meso stilbene dibromide ir should be stored in a cool, dry place away from incompatible substances such as strong reducing agents or bases. Containers must be tightly sealed to prevent moisture ingress and decomposition. Regular inspection of stored chemicals is advised to ensure integrity and safety.

Frequently Asked Questions

What is meso stilbene dibromide IR spectroscopy used for?

Meso stilbene dibromide IR spectroscopy is used to identify functional groups and confirm the presence of bromine atoms attached to the stilbene framework by analyzing characteristic absorption bands.

What are the key IR absorption peaks to look for in meso stilbene dibromide?

Key IR absorption peaks include C-H stretching around 3000 cm^{-1}, C=C aromatic stretching near 1600 cm^{-1}, and C-Br stretching vibrations typically appearing between 500-650 cm^{-1}.

How does the meso configuration of stilbene dibromide affect its IR spectrum?

The meso configuration can influence the symmetry of the molecule, potentially affecting the intensity and splitting of certain IR absorption bands, particularly in the fingerprint region.

Can IR spectroscopy distinguish between meso and racemic stilbene dibromide?

IR spectroscopy alone may not reliably distinguish between meso and racemic stilbene dibromide, as both have similar functional groups; other techniques like NMR or optical rotation are more suitable.

What solvents are recommended for recording IR spectra of meso stilbene dibromide?

Non-polar, IR-transparent solvents such as carbon tetrachloride (CCl4) or using KBr pellets are recommended to avoid interference in the IR spectrum of meso stilbene dibromide.

Why is the C-Br stretching vibration important in analyzing meso stilbene dibromide IR spectra?

The C-Br stretching vibration confirms the presence of bromine substituents on the stilbene structure and helps in verifying the successful bromination of stilbene.

How can IR spectroscopy help in monitoring the synthesis of meso stilbene dibromide?

IR spectroscopy can monitor the disappearance of alkene C=C stretching bands and the appearance of C-Br stretching bands, indicating the progress of bromination to form meso stilbene dibromide.

Additional Resources

1. *Infrared Spectroscopy of Meso Stilbene Dibromide: Techniques and Applications*
This book provides a comprehensive overview of infrared (IR) spectroscopy as applied to meso stilbene dibromide. It covers fundamental principles, sample preparation, and interpretation of IR spectra specific to this compound. Researchers and students will find detailed discussions on characteristic absorption bands and their correlation with molecular structure.

2. *Advanced Organic Chemistry: The Case of Meso Stilbene Dibromide*
Focusing on the organic chemistry of meso stilbene dibromide, this text explores its synthesis, stereochemistry, and reactivity. It includes chapters on spectroscopic methods, particularly IR analysis, to elucidate structural features. The book serves as a valuable

resource for chemists interested in halogenated stilbene derivatives.

3. *Spectral Analysis of Halogenated Stilbenes: Meso Stilbene Dibromide IR Studies*
This specialized volume delves into spectral analysis techniques for halogenated stilbenes, with an emphasis on meso stilbene dibromide. It presents case studies and experimental data to illustrate how IR spectroscopy aids in identifying functional groups and molecular conformations. The book is ideal for spectroscopists and analytical chemists.

4. *Molecular Vibrations and Infrared Spectra: Applications to Meso Stilbene Dibromide*
Exploring the theory of molecular vibrations, this book connects vibrational modes to IR spectra, using meso stilbene dibromide as a key example. It discusses computational methods alongside experimental IR data to provide a holistic understanding of vibrational spectroscopy. Students of physical chemistry will benefit from its clear explanations and practical insights.

5. *Synthesis and Characterization of Dibrominated Stilbenes: Focus on Meso Stilbene Dibromide*
This book details synthetic routes to dibrominated stilbenes, highlighting meso stilbene dibromide. It includes characterization techniques with a focus on IR spectroscopy to confirm product structures. The text is useful for synthetic organic chemists and those involved in material science applications.

6. *Infrared Spectroscopy in Organic Halogen Compounds: The Meso Stilbene Dibromide Example*
Covering a wide range of organic halogen compounds, this book uses meso stilbene dibromide as a model compound to discuss IR spectral features. It explains how the presence of bromine atoms influences vibrational frequencies and intensities. The book is designed for chemists employing IR spectroscopy in halogenated compound analysis.

7. *Practical Guide to IR Spectroscopy of Stilbene Derivatives*
This practical guide focuses on the IR spectroscopic analysis of stilbene derivatives, including meso stilbene dibromide. It offers step-by-step methodologies for sample handling, spectral acquisition, and data interpretation. The guide is suitable for laboratory technicians and researchers new to IR spectroscopy.

8. *Structural Elucidation of Meso Stilbene Dibromide Using Infrared and Complementary Techniques*
Emphasizing a multi-technique approach, this book combines IR spectroscopy with NMR, mass spectrometry, and X-ray crystallography to elucidate the structure of meso stilbene dibromide. It highlights the strengths and limitations of each method, providing a comprehensive analysis framework. The text is valuable for structural chemists and researchers in molecular characterization.

9. *Halogenated Organic Compounds: Spectroscopic Insights into Meso Stilbene Dibromide*
This volume explores the spectral properties of halogenated organic compounds, with a chapter dedicated to meso stilbene dibromide. It discusses how halogen substitution affects electronic and vibrational spectra, including IR. Researchers studying the physical properties and applications of halogenated stilbenes will find this book informative and detailed.

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