

## A C<sub>66</sub> Polycyclic Aromatic Hydrocarbon with Six Azulene Units and NIR-II Absorption: Toward Azulene-Based Carbon Allotropes

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### Rok wydania

2026

### Czasopismo

Journal of the American  
Chemical Society

### Numer woluminu

148

### Strony

17469-17480

### DOI

10.1021/jacs.6c04336

### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

The development of small-molecule dyes with strong and tunable absorption in the near-infrared II (NIR-II, 1000–1700 nm) window remains a central challenge for optoelectronic and biomedical applications, motivating the exploration of unconventional  $\pi$ -conjugated frameworks. In this context, nonalternant polycyclic aromatic hydrocarbons (PAHs) have emerged as promising candidates, with azulene-embedded architectures offering access to small electronic gaps. However, the lack of efficient synthetic strategies has largely restricted the use of such systems, reducing systematic structure–property relationships and limiting their use as functional NIR-active materials. Here, we report the synthesis of **2-diMes**, a C<sub>66</sub> PAH that represents the first nonalternant PAH incorporating six azulene subunits within a fully conjugated framework. This purely hydrocarbon, closed-shell analogue of hexabenzoperylene (HBP) exhibits an exceptionally small HOMO–LUMO gap, among the smallest reported for neutral closed-shell  $\pi$ -conjugated hydrocarbons. The nonalternant topology of **2-diMes** gives rise to intense near-infrared absorption with an onset extending to 1450 nm (0.85 eV) and a small electrochemical gap of 1.13 V. Notably, **2-diMes** functions as a highly photostable NIR-II photoacoustic dye, combining a strong photoacoustic response with excellent solubility in common organic solvents. Spectroelectrochemical and titration studies revealed further red-shifted absorption upon oxidation, with the radical cation [**2-diMes**]<sup>•+</sup> absorbing beyond 3200 nm (0.39 eV) and the dication [**2-diMes**]<sup>2+</sup> absorbing up to 2600 nm (0.48 eV). These results highlight nonalternant azulene-rich PAHs as a powerful and underexplored platform for the rational design of next-generation NIR-II dyes and functional organic materials.

#### Słowa kluczowe

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Absorption, Aromatic compounds, Cations, Hydrocarbons, Oxidation

#### Adres publiczny

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<http://dx.doi.org/10.1021/jacs.6c04336>

#### Strona internetowa wydawcy

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<https://www.acs.org/content/acs/en.html>

Plik został wygenerowany dnia 2026-10-29 07:55:40

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