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Crystal structure of tetracene-5,12-dione, C\textsubscript{18}H\textsubscript{10}O\textsubscript{2}

Abstract

C\textsubscript{18}H\textsubscript{10}O\textsubscript{2}, orthorhombic, P\textsuperscript{2}\textsubscript{1}2\textsubscript{1}2\textsubscript{1} (no. 19), a = 3.95660(10) Å, b = 12.2859(3) Å, c = 24.5014(6) Å, V = 1191.02(5) Å\textsuperscript{3}, Z = 4, R\textsubscript{gt} (F) = 0.0609, wR\textsubscript{ref} (F\textsuperscript{2}) = 0.1660, T = 302(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

To 1.0 g (5.5 mmol) of (2-(dimethoxymethyl)phenyl)methanol were added 50 mL of glacial acetic acid, 10 mL of water, and 3 g (19 mmol) of 1,4-naphthoquinone. After the mixture was heated 12 h at 100 °C, the precipitate was filtered from the reaction mixture and recrystallized from glacial acetic acid, amounted to 1.05 g (74 %) of a yellow solid.

2 Experimental details

All hydrogen atoms were placed in idealized positions. Their U\textsubscript{iso} values were set to 1.2 U\textsubscript{eq} of the parent atoms.

3 Comment

Oxygenated polycyclic aromatic hydrocarbons (OPAHs) in environmental matrices have been slowly increasing in recent years. Tetracene-5,12-dione, as a typical OPAH, is one of ubiquitous pollutants in urban air that may pose risks to human health [4, 5]. Besides, tetracene-5,12-dione is proved to be a widely used intermediate for organic electronic materials [6, 7]. Therefore, more and more chemists are interested in the analyzation and development of tetracene-5,12-dione and its analogs.

The crystal structure of tetracene-5,12-dione is shown in the above figure. The bond lengths of C4=O1 and C15=O2 in the title molecule are 1.229 and 1.226 Å, respectively, which are similar with its analogs [8, 9]. The angle between the six-membered benzene-ring consisting of (C1, C2, C3, C12, C13, C14) and ten-membered naphthalene-ring consisting of (C5, C6, C7, C8, C9, C10, C11, C16, C17, C18) is 121°. Besides, the distance between two adjacent molecules in parallel arrangement is 3.526 Å, shorter than

Table 1: Data collection and handling.

| Crystal: | Yellow needle |
| Size: | 0.41 × 0.11 × 0.08 mm |
| Wavelength: | Cu Kα radiation (1.54178 Å) |
| μ: | 0.75 mm\textsuperscript{-1} |
| Diffractometer, scan mode: | Bruker APEX-II, φ and ω |
| θ\textsubscript{max}, Completeness: | 68.2°, >99 % |
| N(hkl)\textsubscript{measured}, N(hkl)\textsubscript{unique}, R\textsubscript{int}: | 11233, 2172, 0.053 |
| Criterion for I\textsubscript{obs}, N(hkl)\textsubscript{refined}: | I\textsubscript{obs} > 2σ(I\textsubscript{obs}), 1643 |
| Programs: | Bruker [1], SHELX [2, 3] |

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3.80 Å, indicating π−π stacking interaction between the aromatic cycles [8]. The bond lengths and angles are all in the expected ranges [9, 10].

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