Zhang Bin, Chen Xin and Chen Songhua*

Crystal structure of 5,6-diphenyldibenzo[*c, g*]chrysene, C₃₈H₂₄

<https://doi.org/10.1515/ncrs-2020-0112>

Received February 29, 2020; accepted April 6, 2020; available online June 2, 2020

Abstract

C₃₈H₂₄, monoclinic, *C*2/*c* (no. 15), *a* = 37.6829(14) Å, *b* = 7.4695(3) Å, *c* = 17.4881(7) Å, β = 95.269(3)°, *V* = 4901.6(3) Å³, *Z* = 8, *R*_{gt}(*F*) = 0.0472, *wR*_{ref}(*F*²) = 0.1177, *T* = 123(2) K.

CCDC no.: 1977274

The molecular structure is shown in the figure (hydrogen atoms are omitted for clarity). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

*Corresponding author: Chen Songhua, College of Chemistry and Material Science, Longyan University, Longyan Fujian 364012, P.R. China, e-mail: songhua@iccas.ac.cn. <https://orcid.org/0000-0002-0858-3664>

Zhang Bin: School of Biomedical Engineering, XinXiang Medical University, Xinxiang Henan 453003, P.R. China

Chen Xin: National Science Library, Chinese Academy of Sciences, Beijing, 100190, P.R. China

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.20 × 0.05 × 0.01 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.07 mm ⁻¹
Diffraction, scan mode:	Rigaku IP, ω
$\theta_{\max}$, completeness:	30.7°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	33046, 6962, 0.043
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 5151
<i>N</i> (<i>param</i>) _{refined} :	343
Programs:	Olex2 [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	0.62538(3)	0.72504(16)	0.32524(6)	0.0240(3)
C2	0.63409(4)	0.81998(17)	0.25881(7)	0.0283(3)
C3	0.66710(4)	0.78792(18)	0.22985(7)	0.0313(3)
H3	0.673974	0.858193	0.188401	0.038*
C4	0.68945(4)	0.65686(18)	0.26054(7)	0.0302(3)
H4	0.712431	0.643370	0.243015	0.036*
C5	0.67866(3)	0.54153(17)	0.31803(6)	0.0247(3)
C6	0.64643(3)	0.57193(16)	0.34946(6)	0.0221(2)
C7	0.70289(3)	0.38998(17)	0.34326(7)	0.0255(3)
C8	0.73725(3)	0.42797(19)	0.37610(8)	0.0320(3)
H8	0.745041	0.548865	0.379912	0.038*
C9	0.76016(4)	0.2927(2)	0.40318(9)	0.0370(3)
H9	0.783276	0.321274	0.426251	0.044*
C10	0.74938(4)	0.1155(2)	0.39665(8)	0.0346(3)
H10	0.764950	0.022346	0.415589	0.042*
C11	0.71573(4)	0.07527(19)	0.36230(7)	0.0326(3)
H11	0.708480	−0.046182	0.356655	0.039*
C12	0.69253(4)	0.21071(18)	0.33606(7)	0.0290(3)
H12	0.669449	0.181359	0.313037	0.035*
C13	0.63260(3)	0.43937(15)	0.40349(6)	0.0210(2)
C14	0.65229(3)	0.38557(16)	0.47124(7)	0.0237(2)
H14	0.675835	0.429240	0.483000	0.028*
C15	0.63765(4)	0.26886(17)	0.52136(7)	0.0286(3)
H15	0.651134	0.234599	0.567614	0.034*
C16	0.60364(4)	0.20186(17)	0.50474(8)	0.0310(3)
H16	0.593545	0.124177	0.539909	0.037*
C17	0.58439(4)	0.24876(17)	0.43651(8)	0.0289(3)
H17	0.561282	0.200245	0.423971	0.035*
C18	0.59878(3)	0.36650(16)	0.38637(7)	0.0246(3)
H18	0.585364	0.397936	0.339643	0.030*
C19	0.60849(4)	0.93961(18)	0.22071(7)	0.0336(3)
H19	0.614714	1.007106	0.177886	0.040*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C20	0.57573(4)	0.95769(18)	0.24476(7)	0.0344(3)
H20	0.557904	1.021831	0.214064	0.041*
C21	0.56744(3)	0.88080(17)	0.31650(7)	0.0282(3)
C22	0.59435(3)	0.78679(16)	0.36203(7)	0.0238(3)
C23	0.58924(3)	0.76135(15)	0.44195(7)	0.0212(2)
C24	0.55469(3)	0.76778(16)	0.46551(7)	0.0243(3)
C25	0.52672(3)	0.83955(19)	0.41422(8)	0.0312(3)
H25	0.503032	0.841836	0.428661	0.037*
C26	0.53384(4)	0.90496(19)	0.34448(8)	0.0329(3)
H26	0.515783	0.968174	0.314066	0.039*
C27	0.61918(3)	0.74815(15)	0.50130(6)	0.0205(2)
C28	0.65304(3)	0.81587(16)	0.48923(7)	0.0232(2)
H28	0.656661	0.869082	0.441218	0.028*
C29	0.68106(3)	0.80672(17)	0.54545(7)	0.0265(3)
H29	0.703814	0.851680	0.535877	0.032*
C30	0.67589(3)	0.73103(18)	0.61668(7)	0.0285(3)
H30	0.695387	0.719539	0.654842	0.034*
C31	0.64263(3)	0.67334(17)	0.63143(7)	0.0263(3)
H31	0.639226	0.625546	0.680566	0.032*
C32	0.61331(3)	0.68353(15)	0.57502(6)	0.0215(2)
C33	0.57724(3)	0.64003(16)	0.59234(7)	0.0234(2)
C34	0.54817(3)	0.69705(16)	0.54120(7)	0.0246(3)
C35	0.51341(4)	0.6694(2)	0.56204(8)	0.0334(3)
H35	0.493696	0.710996	0.529060	0.040*
C36	0.50736(4)	0.5834(2)	0.62909(8)	0.0380(3)
H36	0.483674	0.567513	0.642325	0.046*
C37	0.53594(4)	0.5194(2)	0.67772(8)	0.0356(3)
H37	0.531732	0.456455	0.723221	0.043*
C38	0.57024(4)	0.54773(18)	0.65961(7)	0.0297(3)
H38	0.589600	0.504217	0.693109	0.036*

Source of materials

The title compound was obtained by Scholl-based cyclodehydrogenation of 3,4,5,6-tetraphenylphenanthrene with equal ratio $FeCl_3$ and the compound was purified through flash column chromatography. Single crystals suitable for X-ray diffraction were obtained by crystallization of the title compound from dichloromethane and *n*-hexane.

Experimental details

The hydrogen atoms were placed with common isotropic displacement factors $U_{iso}(H) = 1.2$ times $U_{eq}(C, \text{aromatic ring})$. The final refinement succeeded using geometrical restraints, with $C-H = 0.95 \text{ \AA}$.

Comment

Helicene and its derivatives are one of the traditional π -conjugated functional molecules due to their steric demands [4–7]. They have been widely utilized materials in the science of supramolecular chemistry and asymmetric synthesis [8]. To date, a series of helicenes derivatives were

synthesized showing specific physical properties and optical properties, especially the excellent luminescent properties. In this paper, we reported the synthesis of the title compound showing chiral optical property by cyclodehydrogenation of phenylphenanthrene using $FeCl_3$ as catalyst [9–11]. A view on the structure of the title molecule is shown in the figure.

Acknowledgements: This work was funded by the research funds of Youth Talented Scholars Plan in Universities of Fujian Province, Young and Middle-aged Teacher in Science Research of Fujian Province (No. JAT190732) and Science and Technology Program of Longyan (No. LY2018LYF8007).

References

- Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.: OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **42** (2009) 339–341.
- Sheldrick, G. M.: Crystal structure refinement with SHELX. *Acta Crystallogr.* **C71** (2015) 3–8.
- Sheldrick, G. M.: Crystal structure refinement with SHELX. *Acta Crystallogr.* **A71** (2015) 3–8.
- Shen, Y.; Chen, C.-F.: Helicenes: synthesis and applications. *Chem. Rev.* **112** (2012) 1463–1535.
- Tinnemans, A. H. A.; Laarhoven, W. H.: Photodehydrocyclizations in stilbene-like compounds. X. rearrangements in the photocyclization of 4,5-diphenyltriphenylene and 4,5-diphenylphenanthrene. *J. Am. Chem. Soc.* **96** (1974) 4617–4622.
- S. Barlow, S.; Marder, S. R.: Chapter 11: nonlinear optical properties of organic materials. In: *Functional organic materials: syntheses, strategies and applications* (Eds. Müller, T. J. J.; Bunz, U. H. F.), p. 393–437. Wiley-VCH, Weinheim (2007).
- Ogawa, N.; Yamaoka, Y.; Takikawa, H.; Takasu, K.: Synthesis of polycyclic spirocarbocycles *via* acid-promoted ring-contraction/dearomative ring-closure cascade of oxapropellanes. *Org. Lett.* **21** (2019) 7563–7567.
- Sharma, B. K. A.; Shaikh, M.; Agarwal, N.; Kamble, R. M.: Synthesis, photophysical and electrochemical studies of acridone-amine based donor-acceptors for hole transport materials. *RSC Adv.* **6** (2016) 17129–17137.
- Hemgesberg, M.; Ohlmann, D. M.; Schmitt, Y.; Wolfe, M. R.; Müller, M. K.; Erb, B.; Sun, Y.; Gooßen, L. J.; Gerhards, M.; Thiel, W. R.: Simple access to sol–gel precursors bearing fluorescent aromatic core units. *Eur. J. Org. Chem.* **2012** (2012) 2142–2151.
- Chen, S.; Li, Y.; Yang, W.; Chen, N.; Liu, H.; Li, Y.: Synthesis and tuning optical nonlinear properties of molecular crystals of benzothiadiazole. *J. Phys. Chem. C* **114** (2010) 15109–15115.
- Carreras, J.; Patil, M.; Thiel, W.; Alcarazo, M.: Exploiting the π -acceptor properties of carbene-stabilized phosphorus centered trications $[L_3P]^3+$: applications in Pt(II) catalysis. *J. Am. Chem. Soc.* **134** (2012) 16753–16758.