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Synthesis, crystal structure and photoluminescence of 2,6-dimethylanthracene and its pseudo-triptycene derivatives

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1. Introduction

Polycyclic aromatic hydrocarbons (PAHs), such as anthracene are fused ring aromatic compounds. They are one of key compounds for optical materials with a UV-vis light emission due to the delocalized π electron in the aromatic system and have been investigated as electroluminescence (EL) devices [1,2], fluorescence materials [3,4] and chemosensors [5]. Alkyl group is electron-donating group, and alkyl-substituted anthracenes have attracted researchers' interests due to its inductive and hyperconjugative effects. The hyperconjugative effect is defined as the conjugation of alkyl groups with a multiple bond [6-8]. On the basis of molecular orbital theory, the methyl group, due to its higher π symmetry, can conjugate more effectively with the π orbitals of multiple bonds than other alkyl groups, and this combination allows a flow of electrons between the methyl group and the aromatic ring. So it is expected that methyl-substituted anthracenes, such as 2,6-dimethylanthracene, and their derivatives to exhibit good fluorescence properties. However, so far, the synthesis of 2,6-dimethylanthracene is complicated and usually involved multi-step reactions [9-17], and some reactions are involved poisonous chemicals [18] and much side products.

Triptycene [19,20], which is a class of compounds with a unique propeller-like three dimensional (3D) rigid structure and electron-

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ABSTRACT

A simple one-step synthesis of 2,6-dimethylanthracene, **1**, in high yield is reported utilizing the easily accessible benzyl alcohol as the starting material. Based on 2,6-dimethylanthracene, two pseudo-tripty-cene compounds, cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinic anhydride, **2**, and cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinyl amine, **3**, are firstly synthesized in high yield and they are characterized by single crystal X-ray diffraction. Compound **2** crystallizes in triclinic $P\overline{1}$ space group and compound **3** crystallizes in monoclinic $P2_1/c$ space group. Both compound **2** and **3** exhibit cis-configurations and endo-conformations. Compound **1** exhibits very intense photoluminescence property due to the delocalized electron in the whole molecule, whereas fluorescence quench happens to some extents due to the destruction of the conjugated structure in compound **2**.

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rich property, has been found to be a useful building block for the construction of novel receptors and porous structures [21-25]. The constrained 120° angle between the phenyl rings and the shape of triptycene hinders itself packing into dense structures. So this type of compounds exhibit high chemical and thermal stability and can be used to remove organic impurities from contaminated water (such asparaquat derivatives) and has potential application in environmental protection. However, pseudo-triptycene, 9,10-dihydroanthracene-9,10-α,β-succinic compound with similar 3D structure and unique flexible C-C framework, is rarely explored. Herein, we firstly report the syntheses and crystal structures of two novel pseudo-triptycene compounds, cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo-α,β-succinic anhydride, and cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinyl amine in high yield, utilizing 2,6-dimethylanthracene as starting material. Compounds 2 and 3 are characterized by single crystal X-ray diffraction. The photoluminescence property has been reported.

2. Experimental

2.1. Synthesis and characterization

All chemicals purchased were of reagent grade and used without further purification. C, H, N elemental analyses were performed on Perkin-Elmer 240c elemental analyzer. Infrared spectra were recorded as KBr pellets on a Nicolet 170SXFT/IR spectrometer. Excitation and emission spectra were obtained on a Spex FL-2T2 spectrofluorometer equipped with a 450 W xenon lamp as the





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excitation source. The melting point was determined using an uncorrected X-4 melting point apparatus of Beijing Kaifu Company. ¹H spectra were recorded on a Bruker 500 MHz apparatus with tetramethylsilane (TMS) as internal standard. All measurements were performed at room temperature.

2.2. Synthesis of 2,6-dimethylanthracene, 1

To dry toluene (240 mL), benzyl alcohol (14 g, 0.14 mol) was added dropwise in an ice-bath while stirring. AlCl₃ (51.98 g, 0.385 mol) was then added in one lot. The reaction mixture was heated on an oil-bath at 110 °C for 3 h. Then it was cooled, decomposed with crushed ice (45 g), water (100 mL) and concentrated HCl (65 mL). The mixture was filtered and the residual was washed with water (3× 90 mL), ethyl acetate (3× 40 mL), saturated NAH-CO₃ solution (2× 40 mL) and water (3× 90 mL) and dried at 80 °C in vacuum for 2 h (yield: ca. 60% based on benzyl alcohol). Elemental Anal. Calcd. for C₁₆H₁₄: C, 93.20; H, 6.80%. Found: C, 93.59; H, 6.68%. ¹H NMR (in CDCl₃): δ , 2.52 (s, 6H), 7.26 (d, 2H, *J* = 8.5 Hz), 7.71 (s, 2H), 7.87 (d, 2H, *J* = 8.5 Hz), 8.25 (s, 2H). Melting point (241–242 °C). IR (cm⁻¹): 2909(s), 1633(s), 1539(m), 1455(s), 1376(m), 1307(m), 1272(w), 1171(w), 1036(w), 962(s), 916(m), 894(s), 790(s), 767(w), 742(w), 599(w), 476(s).

2.3. Synthesis of cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinic anhydride, **2**

A solution of 3.227 g (0.0157 mol) of 2,6-dimethylanthracene and 5.451 g (0.0471 mol) of maleic acid in 50 mL of dioxane was refluxed for 30 h. The dioxane was removed in a current of air on a steam-bath and the residue was shaken for 2 h at room temperature with excess, dilute sodium bicarbonate (this treatment had

Table 1

Crystal data and structure refinements for compounds 2 and 3.

been shown to have no effect on the anhydride). The mixture was filtered and the bicarbonate-insoluble residue (the anhydride) was washed with water (3×100 mL). Colorless block crystals were obtained when recrystallized from benzene (yield: ca. 98% based on 2,6-dimethylanthracene). Elemental Anal. Calcd. for C₄₆H₃₈O₆: C, 80.45; H, 5.58%. Found: C, 80.29; H, 5.10%. ¹H NMR (in DMSO-d₆): δ , 2.24 (s, 6H), 3.61 (d, 2H, *J* = 3.0 Hz), 4.75 (d, 2H, *J* = 3.0 Hz), 6.97 (t, 2H, *J* = 7.0 Hz), 7.18 (d, 2H, *J* = 7.5 Hz), 7.32 (d, 2H, *J* = 7.5 Hz). Melting point (170–171 °C). IR (cm⁻¹): 3855(w), 3650(w), 2960(s), 2369(w), 1863(m), 1778(s), 1618(w), 1484(m), 1459(w), 1381(w), 1324(w), 1290(w), 1225(s), 1204(m), 1190 (m), 1135(w), 1073(s), 976(m), 952(s), 931(s), 920(s), 841(w), 814(m), 791(m), 767(w), 741(w), 624(m), 533(s).

2.4. Synthesis of cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinyl amine, **3**

An aqueous solution (10 mL) of compound **2** (0.05 mmol, 0.014 g) was adjusted to pH 6 by 2 N aqueous ammonia solution, then transferred into a Teflon-lined autoclave. The reaction mixture was heated at 120 °C for 2 h, then followed by slow cooling to room temperature. The resulting colorless crystals were filtered off and washed with distilled water (yield: ca. 98% based on cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinic anhydride). Elemental Anal. Calcd. for C₂₀H₁₇O₂N: C, 79.19; H, 5.65; N, 4.61%. Found: C, 79.45; H, 5.33; N, 4.63%. ¹H NMR (in CDCl₃): δ , 2.28 (s, 6H), 3.23 (d, 2H, *J* = 3.0 Hz), 4.67 (d, 2H, *J* = 3.0 Hz), 6.95 (t, 2H, *J* = 7.0 Hz), 7.17 (d, 2H, *J* = 7.5 Hz), 7.22 (d, 2H, *J* = 7.5 Hz), 7.35 (s, 1H). Melting point (180–181 °C). IR (cm⁻¹): 3272(m), 1779(m), 1721(s), 1699(s), 1483(m), 1358(m), 1167(m), 994(m), 825(m), 812(m), 631(m), 616(m), 535(m), 418(w).

Compound	2	3
Empirical formula	$C_{43}H_{32}O_6$	$C_{20}H_{16}NO_2$
Formula weight	644.69	302.34
Temperature (K)	298(2)	298(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Monoclinic
Space group	ΡĪ	$P2_1/c$
a (Å)	9.4720(10)	12.7619(18)
b (Å)	12.8081(14)	9.4138(14)
<i>c</i> (Å)	14.2639(17)	13.688(2)
α (°)	89.475(2)	90
β (°)	85.0550(10)	104.862(2)
γ(°)	86.1960(10)	90
Volume (Å ³)	1720.2(3)	1589.4(4)
Z	2	4
$ ho_{ m calc} (m mgm^{-3})$	1.245	1.263
Absorption coefficient (mm ⁻¹)	0.082	0.082
F(000)	676	636
Crystal size (mm ³)	$0.29\times0.30\times0.42$	$0.42 \times 0.21 \times 0.12$
θ range (°)	2.60-25.01	1.65-25.02
Limiting indices	$-10 \leqslant h \leqslant 11, -15 \leqslant k \leqslant 15, -14 \leqslant l \leqslant 16$	$-13 \leqslant h \leqslant 15, -11 \leqslant k \leqslant 7, -16 \leqslant l \leqslant 16$
Reflections collected	8764	7672
Independent reflections	5756	2803
Absorption correction	ψ -scan	ψ -scan
Max. and min. transmission	0.977 and 0.971	0.990 and 0.980
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F^2
Data, restraints, parameters	5756, 0, 499	2803, 0, 221
Goodness-of-fit on F^2	0.945	1.052
Final <i>R</i> indices $[I > 2\sigma(I)]$	$R_1 = 0.0988,$	$R_1 = 0.0637$,
	$wR_2 = 0.2072$	$wR_2 = 0.1644$
R indices (all data)	$R_1 = 0.2344,$	$R_1 = 0.1440,$
	$wR_2 = 0.2641$	$wR_2 = 0.2215$
Largest diff. peak and hole	0.324 and -0.253	0.429 and -0.223

 $R_1 = \Sigma ||F_0| - |F_c|| / \Sigma |F_0|; \ wR_2 = \sum [w(F_0^2 - F_c^2)^2] / \sum [w(F_0^2)]^2]^{1/2}.$

2.5. X-ray crystallography

Single crystals of dimensions $0.29 \times 0.30 \times 0.42 \text{ mm}^3$ for compound **2**, $0.42 \times 0.21 \times 0.12 \text{ mm}^3$ for compound **3** were used for structure determination. XRD data of compounds 2 and 3 were collected on a Bruker-AXS CCD area detector-equipped diffractometer with graphite-monochromatized Mo Ka (λ = 0.71073 Å) radiation at room temperature. A total of 8764 (5756 unique, $R_{int} = 0.0978$) reflections of compound **2** $(-10 \le h \le 11, -15 \le k)$ ≤ 15. $-14 \le l \le 16$, 2.60 < θ < 25.01) and a total of 7672 (2803 unique, $R_{\text{int}} = 0.0582$) reflections of compound **3** (-13 $\leq h \leq 15$, -11 $\leq k$ \leq 7, $-16 \leq l \leq 16$, 1.65 < θ < 25.02) were measured. An empirical absorption correction from ψ -scan was applied. All the structure was solved by direct methods and expanded using Fourier techniques. The nonhydrogen atoms were refined anisotropically. Hydrogen atoms were added in their calculated positions. All calculations were performed using the SHELXTL-97 program [26-27]. The CCDC reference numbers are the following: 721286 for 2 and 721767 for 3. Crystal data and structure refinements for compounds 2 and 3 are listed in Table 1.

3. Results and discussion

3.1. Synthesis

The synthetic routine for compounds **1–3** are shown in Scheme 1. The synthesis of 2,6-dimethylanthracene, **1**, is a Friedel–Crafts reaction, in which AlCl₃ acts as catalyst and the possible mechanism for the ring-closure reaction is expected (Scheme 2) [18]. As shown in Scheme 2, in the reaction, toluene plays important role in the preparation of compound **1**, it is not only a solvent, but also a starting material [18], which is proved by the parallel experiments: Under similar conditions, we replace toluene with p-xylene, the yield of compound **1** will be decreased dramatically; when m-xylene is used instead, no product can be obtained. The amount of toluene is not necessarily very precise, as long as it is excessive. The synthesis is sensitive to the reaction temperature. When the temperature is lower (such as 80 °C, 95 °C) or higher (such as 140 °C), the yield will be decreased. The reaction time is also important. When the reaction time is longer than 10 h, no products and a lot of unidentified black tar will be obtained. In the present work, it is found that the optimal condition is to reflux at 110 °C for 3–5 h.

The synthesis of compound **2** is a Diels–Alder reaction, in which compound **1**, 2,6-dimethylanthracene, acts as diene and maleic acid acts as dienophile. As known, Diels–Alder reaction works best when there is a marked difference between the electron densities in the diene and the alkene with which it reacts, the dienophile. Usually the dienophile has electron-attracting groups attached to it, e.g., electron-attracting carboxylic group, while the diene is electron rich, e.g., electron-donating methyl group. So the reaction of 2,6-dimethylanthracene with maleic acid is easy to proceed and the yield of compound **2** is higher than 95%.

Diels–Alder reaction is a concerted reaction, in which several bonds in the transition state are simultaneously made and broken.



Scheme 1. The synthetic routine for compounds 1-3.



Scheme 2. The possible mechanism for the formation of compound 2.

When a cyclic diene and a cyclic dienophile react with each other in the present reaction, more than one stereoisomer may be formed. Usually two stereoisomers, endo- and exo-conformations will be obtained. However, the isomer that predominates is the endo-conformation which involves maximum overlap of π electrons in the transition state. Compound **2** is obtained by recrystallizing from benzene. The crystal structure of compound **2** proves the product is the endo-isomer.

The synthesis of compound **3** is a typical formation reaction of acyl amine and the reaction is not sensitive to reaction conditions. Compound **3** can be obtained in high yield without changing the conformation of reactant. The crystal structure of compound **3** indicates that the acyl amine is also the endo-isomer.

3.2. Structure description

Compound **2** crystallizes in triclinic $P\bar{1}$ space group with two cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo-α,β-succinic anhydride molecules and one solvent molecule, benzene in the asymmetric unit. As shown in Fig. 1, in one crystallographically unique 2,6-dimethyl-9,10-dihydroanthracene-9,10-endo-α,β-succinic anhydride, the substituted methyl group has two positions owing to the crystallographic disorder of C(13) and C(13)'. Each of them has 50% occupancy over the two positions. Two phenyl rings 1, 2 and one five-membered ring 3 are composed of C atoms from C14 to C19, C7 to C12, and C1, C2, C3, C4, O1, respectively. The dihedral angles between rings 1 and 2, 1 and 3, 2 and 3 are 122.3°, 177.0° and 60.7°, respectively. Ring 3 is apart from ring 1, indicating it is an endo-isomer. Strong edge-to-face π - π stacking interactions exist between five-membered ring 3 and benzene ring 4, for example, the dihedral angle between planes 3 and 4 is 115.9 °C and the distance between C41A and plane 4 is 4.391 Å (atom with additional label A refers to the symmetry operation: 1 - x, 2 - y, 2 - z), which indicates that solvent molecule, benzene plays important in the separation of the endo-isomer from the endo- and exo-mixtures. The H(2)-C(2)-C(1) and H(3)-C(3)-C(4) bond angles are 109.4° and 110.1°, respectively, indicating the molecule exhibits a cis-configuration. In another crystallographically unique 2,6-dimethyl-9,10dihydroanthracene-9,10-endo- α , β -succinic anhydride, C(33) and

C(33') are disordered over two locations, C(40) and C(40') are disordered over two locations. Each site of them is half-occupied. Two phenyl rings 5, 6 and one five-membered ring 7 are composed of C atoms from C27 to C32, C34 to C39, and C21, C22, C23, C24, O4, respectively. The dihedral angles between rings 5 and 6, 5 and 7, 6 and 7 are 121.7°, 176.0° and 58.8°, respectively. Ring 7 is apart from ring 5, indicating the molecule is also an endo-isomer. Strong C-H···C H-bonds are observed between the molecule and solvent benzene molecule, for example, the H43...C40B and C43...C40B distances are 3.338 and 4.206 Å, respectively, the C43–H43…C40B angle is 133.5° (atom with additional label B refers to the symmetry operation: 1 - x, 2 - y, 1 - z), indicating recrystallization from benzene is effective for the separation of the endo-isomer. The H(22)-C(22)-C(21) and H(23)-C(23)-C(24) bond angles are 110.2° and 110.0°, respectively, indicating the molecule also exhibits a cis-configuration.

Because compound 2 is obtained utilizing compound 1 as starting material, the crystal structure of compound 2 proves the synthesis of methyl-substituted anthracene is accurate and Friedel–Crafts reaction is an effective routine to get polycyclic aromatic hydrocarbons. Due to the disorder of methyl group in



Fig. 2. ORTEP drawing of compound 3 with the atomic numbering scheme and displacement ellipsoids at the 30% probability level (H atoms omitted for clarity).



Fig. 1. ORTEP drawing of compound 2 with the atomic numbering scheme and displacement ellipsoids at the 30% probability level (H atoms omitted for clarity).



Scheme 3. Chiral cis-2,7-dimethyl-9,10-dihydroanthracene-9,10-endo-α,β-succinyl amine (a) and nonchiral cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo-α,β-succinyl amine (b), asterisk indicating the chiral centers.

the crystal structure of compound **2**, the position of the methyl group cannot be determined. In order to make sure the two methyl groups are in 2,6-positions or 2,7-positions, we use compound **2** as starting material and obtain the crystal structure of compound **3**.

Compound **3** is obtained using compound **2** as starting material. Compound **3** crystallizes in monoclinic $P2_1/c$ space group with one dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinyl amine molecule in the asymmetric unit. As shown in Fig. 2, C(20) and C(20') are disordered over two locations and each site of them is half-occupied. Two phenyl rings 1, 2 and one five-membered ring 3 are composed of C atoms from C7 to C12, C14 to C19, and C1, C2, C3, C4, N1, respectively. The dihedral angles between rings 1 and 2, 1 and 3, 2 and 3 are 119.6°, 178.0° and 62.3°, respectively. The H(3)–C(3)–C(2) and H(4)–C(4)–C(1) bond angles are 110.2° and 109.5°, respectively, indicating compound **3** has the endo-conformation and it exhibits the cis-configuration.

As mentioned above, compound **3** crystallizes in nonchiral $P2_1/c$ space group. As we know, the Diels-Alder reaction has been used extensively in the synthesis of natural products because it is regioselective and a number of chiral centers can be formed in the reaction. Both Diels-Alder reaction and the synthesis of acyl amine from acid anhydride do not change the position of methyl groups of the starting material. So if compound **1** is 2,7-dimethylanthracene, as shown in Scheme 3a, compound 3 would be cis-2,7-dimethyl-9,10-dihydroanthracene-9,10-endo-α,β-succinyl amine. which is a chiral compound, and compound **3** would crystallize in a chiral space group, it is inconsistence with the $P2_1/c$ space group. If compound 1 is 2,6-dimethylanthracene, as shown in Scheme 3b, compound 3 would be cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinyl amine, which is a nonchiral compound, and compound **3** would crystallized in a nonchiral space group, it is consistence with our experimental result. The data proves that the positions of the methyl groups in compounds 1-3 are 2,6-positions. It is indicated that the synthesis of compound 1 is accurate and the mechanism for the formation of compound 1 is possible.

3.3. IR spectra

As shown in Scheme 1, compound **1** is a planar aromatic structure and compound **2** is a 3D structure. The IR spectra of compounds **1** and **2** are different. Compound **1** shows characteristic bands of anthracene in the 894–1633 cm⁻¹ range. Compound **2** shows characteristic bands of carboxyl groups at 1863 and 1778 cm⁻¹. Due to the destruction of the conjugated structure of anthracene in compound **2**, the characteristic peaks of phenyl rings in the 920–1618 cm⁻¹ range shift obviously.

3.4. UV-visible spectra

In the solid state, the UV-visible spectrum of compound **1** exhibits one strong peak at 404 nm ascribed to $\pi \rightarrow \pi^*$ transition [28]. Compound **2** exhibits a strong absorption peak at 280 nm in its UV spectrum. The obvious hypsochromic shift of absorption peak in the UV spectrum of compound **2** is attributed to the destruction of the conjugated structure of anthracene. Electron cannot be delocalized over the whole molecule and more energy is needed for the $\pi \rightarrow \pi^*$ transition.

3.5. Photoluminescence property

In the solid state, compound **1** exhibits very intense emission in the 413–816 nm range when excitation at 268 nm at room temperature (see Fig. 3a), which is attributable to the $\pi^* \rightarrow n$ transition [29]. Whereas compound **2** exhibits weak emission in the same range when excitation at 268 nm (Fig. 3b). The emission intensity of compound **2** is much lower than that of compound **1**, indicating fluorescence quench happens to some extents due to the destruction of the conjugated structure of anthracene and undelocalized electron in compound **2**.



Fig. 3. Solid-state emission spectra of compounds $1 \ (a)$ and $2 \ (b)$ at room temperature.

4. Conclusion

In summary, in the present paper, utilizing the easily accessible benzyl alcohol as the starting material, we report a simple one-step synthesis of 2,6-dimethylanthracene, 1, in high yield. Based on 2,6dimethylanthracene, two pseudo-triptycene compounds, cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo- α , β -succinic anhydride, **2**, and cis-2,6-dimethyl-9,10-dihydroanthracene-9,10-endo-α,β-succinyl amine, **3**, are firstly synthesized in high yield and they are characterized by single crystal X-ray diffraction. Both compound 2 and 3 exhibit the cis-configurations and endo-conformations. Compound 1 exhibits very intense photoluminescence property due to the delocalized electron in the whole molecule, whereas fluorescence quench happens to some extents due to the destruction of the conjugated structure in compound 2. Compound 1 may be an excellent candidate for potential photoactive material, whereas compound **2** may be a good ligand for the construction of porous metal-organic framework due to its unique 3D structure.

5. Supporting materials

Atomic coordinates, bond lengths and angles, and thermal parameters are available from the authors on request. Copies of X-ray crystallographic files in CIF format for the structure determination may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 IEZ, UK (fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/i.molstruc.2009.10.017.

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