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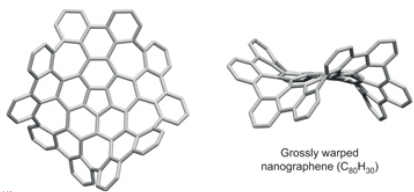
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Articles top

A grossly warped nanographene and the consequences of multiple odd-membered-ring defects pp739 - 744
Katsuaki Kawasumi, Qianyan Zhang, Yasutomo Segawa, Lawrence T. Scott & Kenichiro Itami
doi:10.1038/nchem.1704



Grossly warped nanographene (C₈₀H₃₀)

A grossly warped nanographene, C₈₀H₃₀, that incorporates five 7-membered rings and one 5-membered ring embedded in a hexagonal lattice backbone synthesized, isolated and fully

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A grossly warped nanographene and the consequences of multiple odd-membered-ring defects

Katsuaki Kawasumi, Qianyan Zhang, Yasutomo Segawa, Lawrence T. Scott & Kenichiro Itami

Affiliations | Contributions | Corresponding authors

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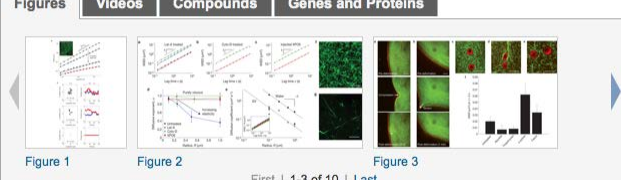



Figure 1 | Figure 2 | Figure 3

First | 1-3 of 10 | Last

solubility of this derivative permits the recording of

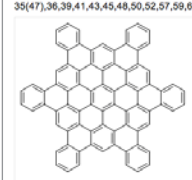
ear: NV Compound 9 Lin
ass: Pentacosacyclo[29.7.17.6^{3,8}.8^{15,22}.4^{1,19}.1^{6,18}.1^{17,21}.1^{20,24}.0^{7,16}.0^{9,14}.0^{25,30}.0^{4,18}.0^{3,7}.0^{32,56}.0^{33,66}.0^{36,87}.0^{38,89}.0^{37,62}.0^{63,65}.0^{68,70}.0^{73,78}]octaheptaconta-
ΔS 54.035.47.037.45.039.44.
tha 0^{48,53}.0^{5,72}.0^{32,56}.0^{33,66}.0^{36,67}.0^{38,89}.0⁵
(Fij) 7.62.0^{63,65}.0^{68,70}.0^{73,78}]octaheptaconta-
onl 1(38),2,4(69),5(72),6(70),7(16),8(71),9,11
D₅ 13,15(64),17,19(66),20,22,24(56),25,27,
29,31(55),32,34(54),
35(47),36,39,41,43,45,48,50,52,57,59,61,
63(65),67,73,75,77-nonatriacontaene



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that of 9 (E_{HOMO} = -5.13 and -4.95 eV, respective
9, however, remain similar (E_{LUMO} = -2.07 and -2

Compound 9
Pentacosacyclo[29.7.17.6^{3,8}.8^{15,22}.4^{1,19}.1^{6,18}.1^{17,21}.1^{20,24}.0^{7,16}.0^{9,14}.0^{25,30}.0^{4,18}.0^{3,7}.0^{32,56}.0^{33,66}.0^{36,87}.0^{38,89}.0^{37,62}.0^{63,65}.0^{68,70}.0^{73,78}]octaheptaconta-
24(56),25,27,29,31(55),32,34(54),
35(47),36,39,41,43,45,48,50,52,57,59,61,63(65),67,73,75,77-nonatriacontaene



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Chemical Formula: C₈₀H₃₀
Molecular Weight: 967.07
Elemental Analysis: C, 96.87; H, 3.13
Standard InChI=1S/C78H30/c1-2-14-32-31(13-14)-25-45-33-15-3-4-16-34(3-53-41-23-11-9-21-39(41)60-28-48-36-18-6-5-17-35(36)46-26-44(32)56-55(43-24(56),25,27,29,31(55),32,34(54),35(47),36,39,41,43,45,48,50,52,57,59,61,63(65),67,73,75,77-nonatriacontaene
Standard InChIKey: QATPKFDSJUFYEJ-UHFFFAOYSA-N
SMILES: C12=C(C3=C4C5=CC6=C3C7=C8C9=C(C%10=CC=CC=C%10%11)C15=C%16C%17=C(C%18=CC=CC=C%18%19)C=C%15C%20=CC=CC=C%14)4=CC=CC=C%245)C=C%23C%25=CC=CC=C%22%25

Previous compound | Compound 10

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Addition of synthetic procedures to the compound page

From the compound page the synthetic procedure allows the user see the procedure for making the compound and any characterization data from the Supplementary Information.

Synthetic Procedure: See article for the definitive version of this procedure and for full experiment

To a solution of pentakis(*o*-biphenyl)corannulene (**2**: 10 mg, 10 μ mol, 1.0 equiv) in dry CH_2Cl_2 (1. none (DDQ: 23 mg, 0.1 mmol, 10 equiv) at 0 °C. After stirring for 5 min, trifluoromethanesulfonic acid was further stirred for 30 min at 0 °C. The reaction mixture was neutralized with sat. NaHCO_3 aq., a organic phase was dried over MgSO_4 and the organic solvent was removed under reduced pressure and incubated at 100 °C for 30 min. The thus-obtained precipitate was collected by filtration and $\text{C}_{80}\text{H}_{30}$ (**4**: 4.9 mg, 50% yield) as a yellow powder. ^1H NMR (400 MHz, $\text{C}_2\text{D}_2\text{Cl}_4/\text{AsCl}_3 = 1:1$, 100 °C 10H), 7.40 (d, $J = 7.6$ Hz, 1H); ^{13}C NMR (100MHz, $\text{C}_2\text{D}_2\text{Cl}_4/\text{AsCl}_3 = 1:1$, 100 °C) 139.2 (4 \times), 133.8 (2 \times), 122.5 (CH). HRMS (MALDI-TOF) m/z calcd for $\text{C}_{80}\text{H}_{30}$ [M] $^+$: 990.2348, found: 990.2347. Mp: >300

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References

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