Supporting Information

Edge-functionalized Graphene Nanoribbon Frameworks for the Capture and Separation of Greenhouse Gases

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A. Materials and Methods

Deuterated solvents were obtained from Cambridge Isotope Laboratories. All the gases used for the adsorption/desorption experiments as well as breakthrough experiments were ultra-high purity, grade 5. High-resolution mass spectra (HR-MS) were obtained through Bruker autoflex III Matrix Assisted Laser Desorption Ionization Mass Spectrometer. Single crystal X-ray diffraction was performed using Bruker APEX II single crystal X-ray diffractometer. Thermogravimetric analysis (TGA) were performed with a NETZSCH-TG 209 F3 by heating at rate of $10^{o}C\ min^{-1}$, up to $800^{o}C$ under air. Prior to the gas sorption experiments, polymers were kept under vacuum at $150^{o}C$ for 5 h for degassing. Ar adsorption and desorption isotherms were performed at 87 K and the specific surface areas were calculated using the Brunauer-Emmet-Teller (BET) model in the range of $0.01 < P/P_0 < 0.10$. H_2 adsorption isotherms were measured at 77 and 87 K. CO_2 and CH_4 uptake measurements were performed at 273 and 298 K. The collected isotherms data for each gas was fitted in Clausius-Clapeyron equation in order to calculate isosteric heats of adsorption (Q_{st}):

$$\Delta H = R\left[\frac{\partial lnP}{\partial\left(\frac{1}{T}\right)}\right]_{\theta} \qquad \text{Eq. 1}$$

where R is the universal gas constant ($8.314\ J\ mol^{-1}\ K^{-1}$), θ is the fraction of the adsorbed sites at a pressure P and temperature T.

The H_2 adsorption isotherms at 77 and 87 K were fit with a dual-site Langmuir-Freundlich model. The isotherms of CO_2 measured at 273 and 298 K were also fitted with the dual-site Freundlich-Langmuir (DSL) model:

$$q = \frac{q_{m,1}b_1p^{1/n_1}}{1+b_1p^{1/n_1}} + \frac{q_{m,2}b_2p^{1/n_2}}{1+b_2p^{1/n_2}} \qquad \text{Eq. 2}$$

where q is the molar loading of adsorbent ($mmol\ g^{-1}$), $q_{m,1}$ and $q_{m,2}$ are the saturation loading of site 1 and 2 ($mmol\ g^{-1}$), p is the pressure of the bulk gas (bar), b_1 and b_2 are the affinity coefficients of site 1 and 2 (bar^{-1}), and n_1 and n_2 are the deviations from an ideal homogeneous surface.

The methane adsorption data at 273 and 298 K were fitted using the single-site Langmuir (SSL) model:

$$q = \frac{q_{m,1}b_1p^{1/n_1}}{1+b_1p^{1/n_1}} \qquad \text{Eq. 3}$$

These models were fitted purely on the basis of giving the best fit with adjusted R^2 values exceeding 0.99. The calculations of all the equations were done using of Wolfram Mathematica 10.2.

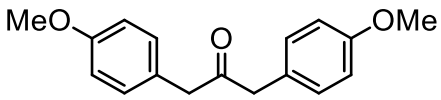
Breakthrough test was conducted by the apparatus illustrated in the Figure S13. Adsorbents were packed in the testing column for CO_2/CH_4 separation. Before the measurement, the column containing adsorbent was evacuated for 30 min and flushed with He gas for 10 min at $80^{o}C$, by

which adsorbents were activated. After stabilizing the temperature of testing apparatus at 298 K, gas mixtures were injected at the target pressure and flow rate. Effluent from the column was collected by automatic sampling valve and then injected into GC and its composition was analyzed *in-situ*. Breakthrough time was determined to be when CH_4 was firstly detected. The CO_2 storage capacity of adsorbents was calculated by using the following equation:

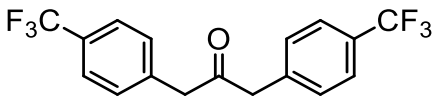
$$N_{CO2,ads} = F_{in}\, C_{in}\, T_{BT} - \int_0^{T_{BT}} F_{out}\, C_{CO2,out}(t)dt\text{-}V_{reactor} C_{CO2,in} \qquad \text{Eq. 4}$$

B. Synthesis

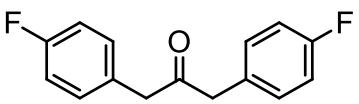
1,3-bis(4-methoxyphenyl)propan-3-one, 2a: The synthesis was performed using previously reported literature procedure. [S1] ^{1}H NMR (300 MHz. $CDCl_3$. 298 K): δ 7.04 (d, 4H, Ar-H), 6.83 (d, 4H, Ar-H), 3.78 (s, 6H, OCH_3), 3.63 (s, 4H, CH_2).



1,3-bis(4-(trifluoromethyl)phenyl)propan-3-one, 2c: The synthesis was performed using previously reported literature procedure. [S1] ^{1}H NMR (300 MHz. $CDCl_3$. 298 K): δ 7.58 (d, 4H, Ar-H), 7.27 (d, 4H, Ar-H), 3.82 (s, 4H, CH_2).



1,3-bis(4-fluorophenyl)propan-3-one, 2d: The synthesis was performed using previously reported literature procedure. [S1] ^{1}H NMR (300 MHz. $CDCl_3$. 298 K): δ 7.08 (m, 4H, Ar-H), 6.99 (m, 4H, Ar-H), 3.68 (s, 4H, CH_2).



C. Computational Studies of Model Reaction

The optimizations were carried out using B3LYP/6-31G* level along with Grimme's DFT-D3 corrections. Minimum energy structures were confirmed by all positive Harmonic frequencies. Transition states (first-order saddle points) were characterized by a single imaginary frequency (negative eigenvalue for the Hessian) pertaining to the desired reaction coordinates. The energy was further refined by single point calculation at the B3LYP/6-311+G*/Grimme's DFT-D3 corrections level.

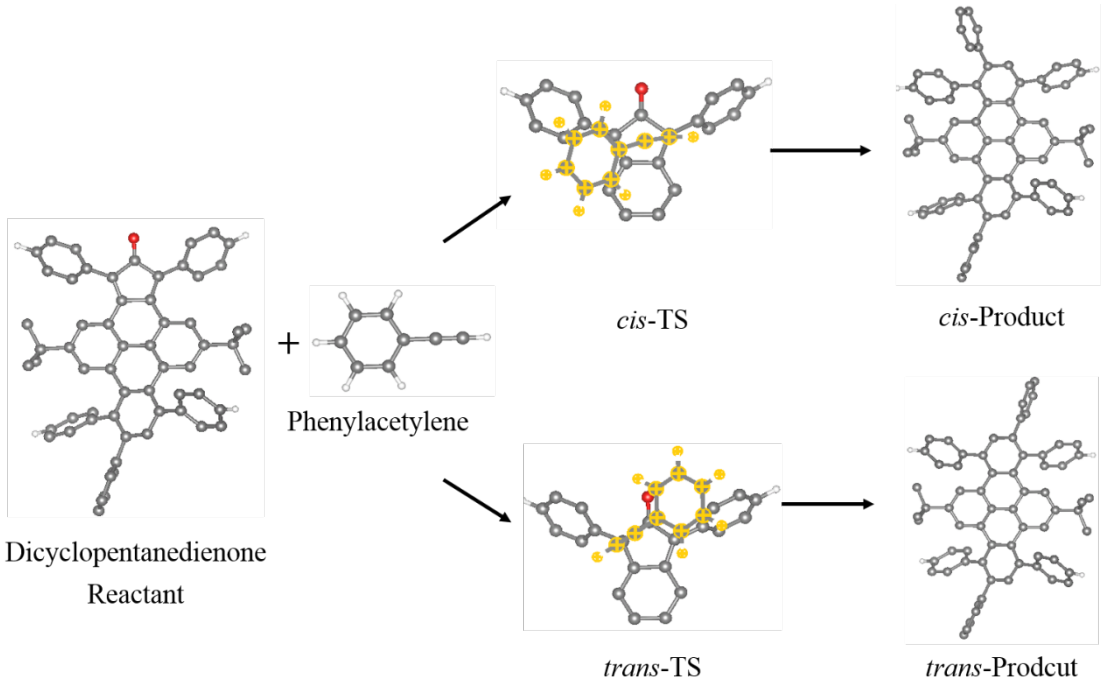


Figure S1. The model that was used to calculate transition state structures for the Diels-Alder cycloaddition reactions.

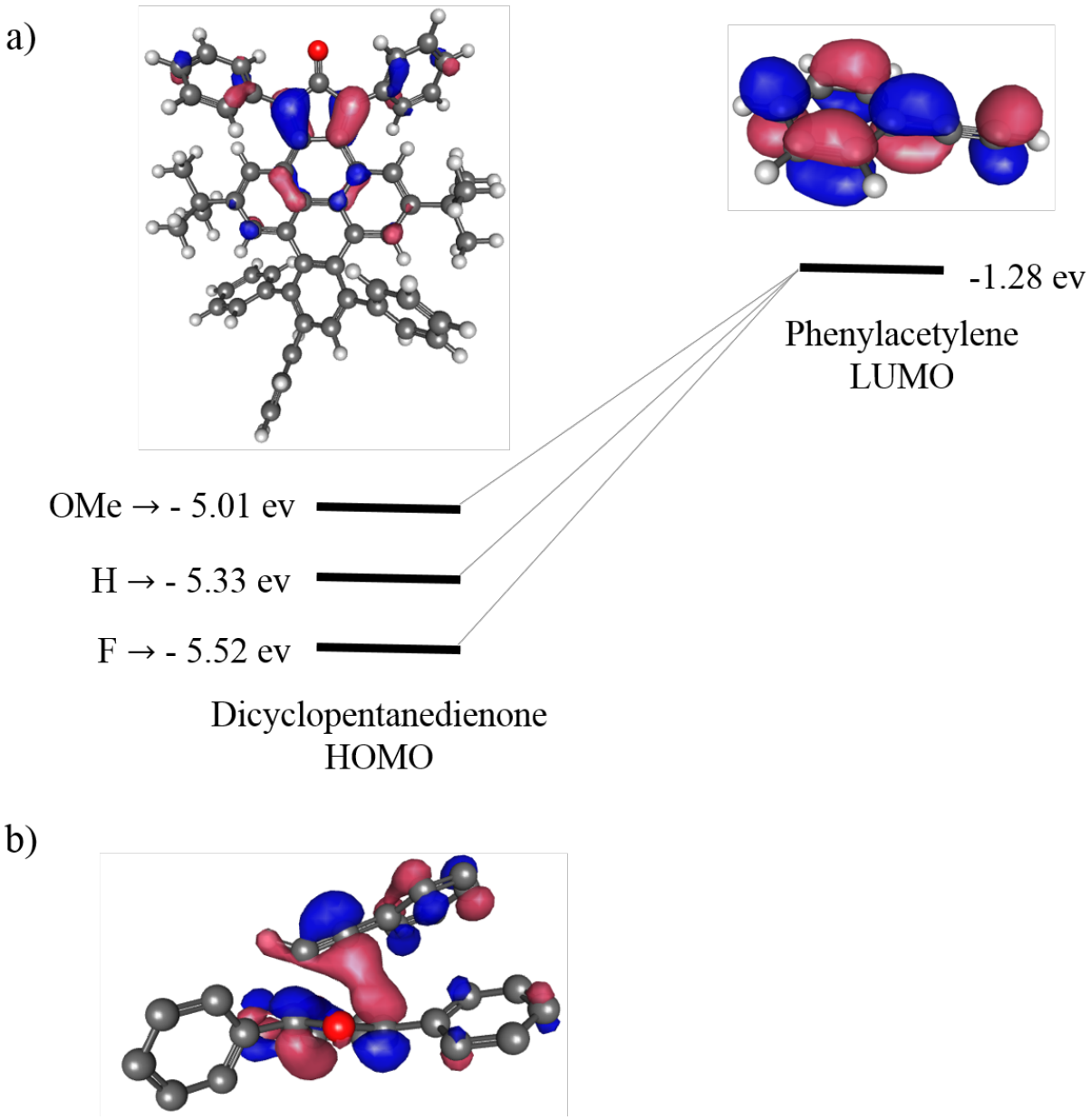


Figure S2. a) The HOMO-LUMO gap shown between substituted-dienes and phenylacetylene, along with the corresponding orbitals participating in the [4+2] symmetry allowed cycloaddition. b) The HOMO of *cis* TS geometry for –H functional group, representing the asymmetric [4+2] bond formation.

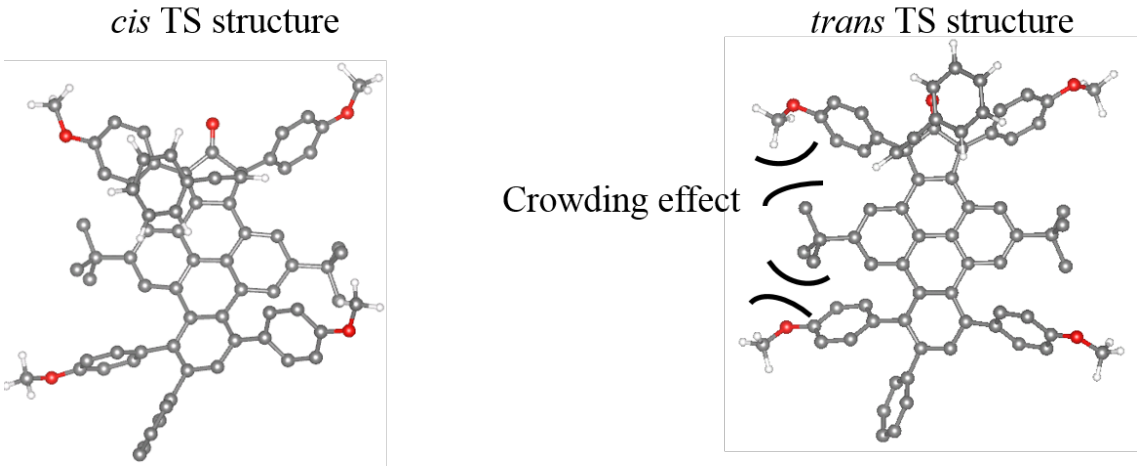


Figure S3. The front view of TS structure for compound **5**

D. Characterization of GNFs

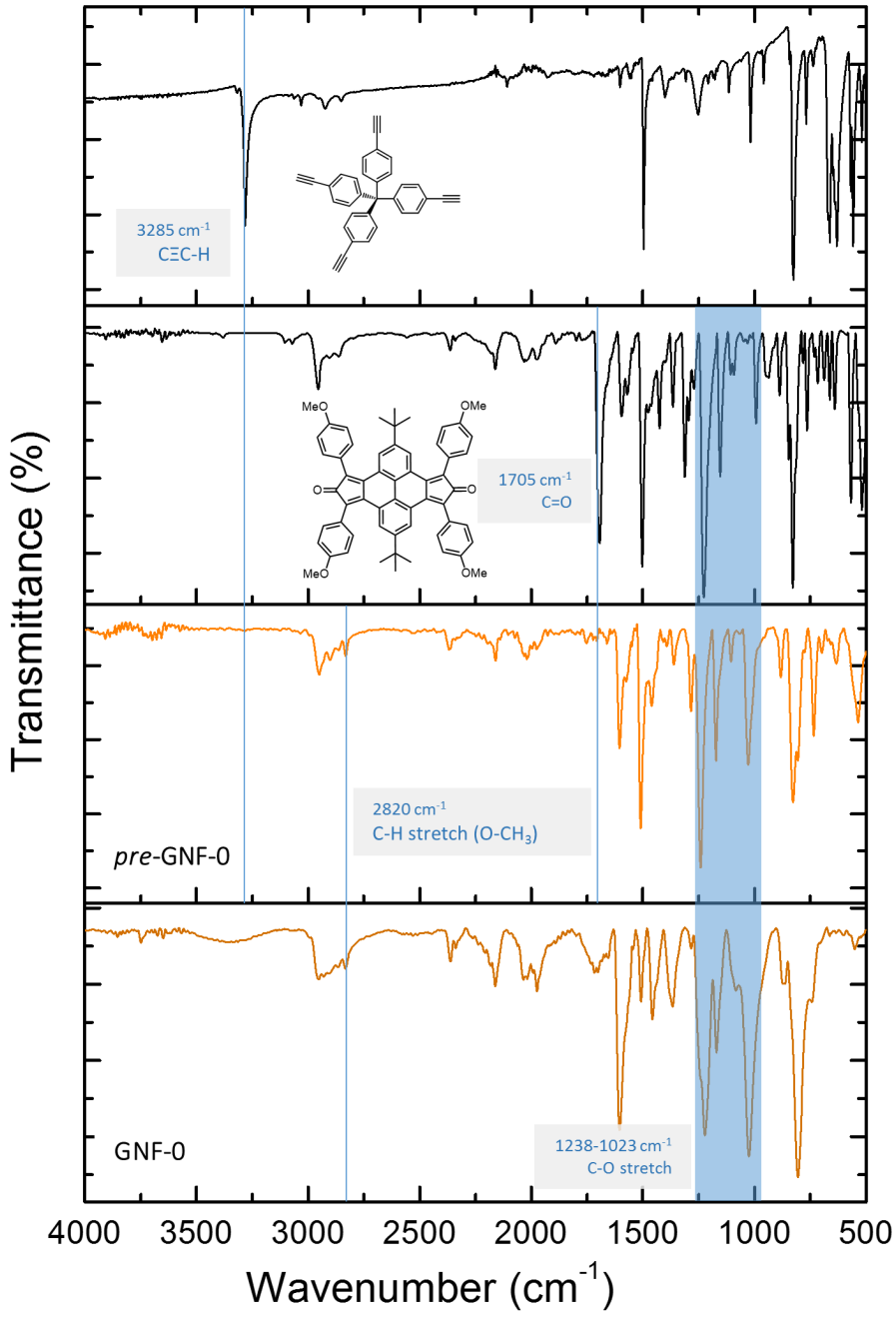


Figure S4. FT-IR spectra of tetrakis(4-ethynylphenyl)tetraphenylmethane (first), 2,8-di-tert-butyl-4,6,10,12-tetrakis(4-methoxyphenyl)dicyclopenta[e,l]pyrene-5,11-dione (second), *pre*-GNF-0 (third) and GNF-0 (last). The complete disappearance of the stretching bands at 3285 cm^{-1} (alkyne, C-H) and 1705 cm^{-1} (ketone, -C=O) indicate that both monomers were consumed to form *pre*-GNF-0 *via* the Diels-Alder cycloaddition polymerization. Maintenance of C-O stretching band at 1238-1023 cm^{-1} provides clear evidence that –OMe group is remained intact after the cyclodehydrogenation reaction.

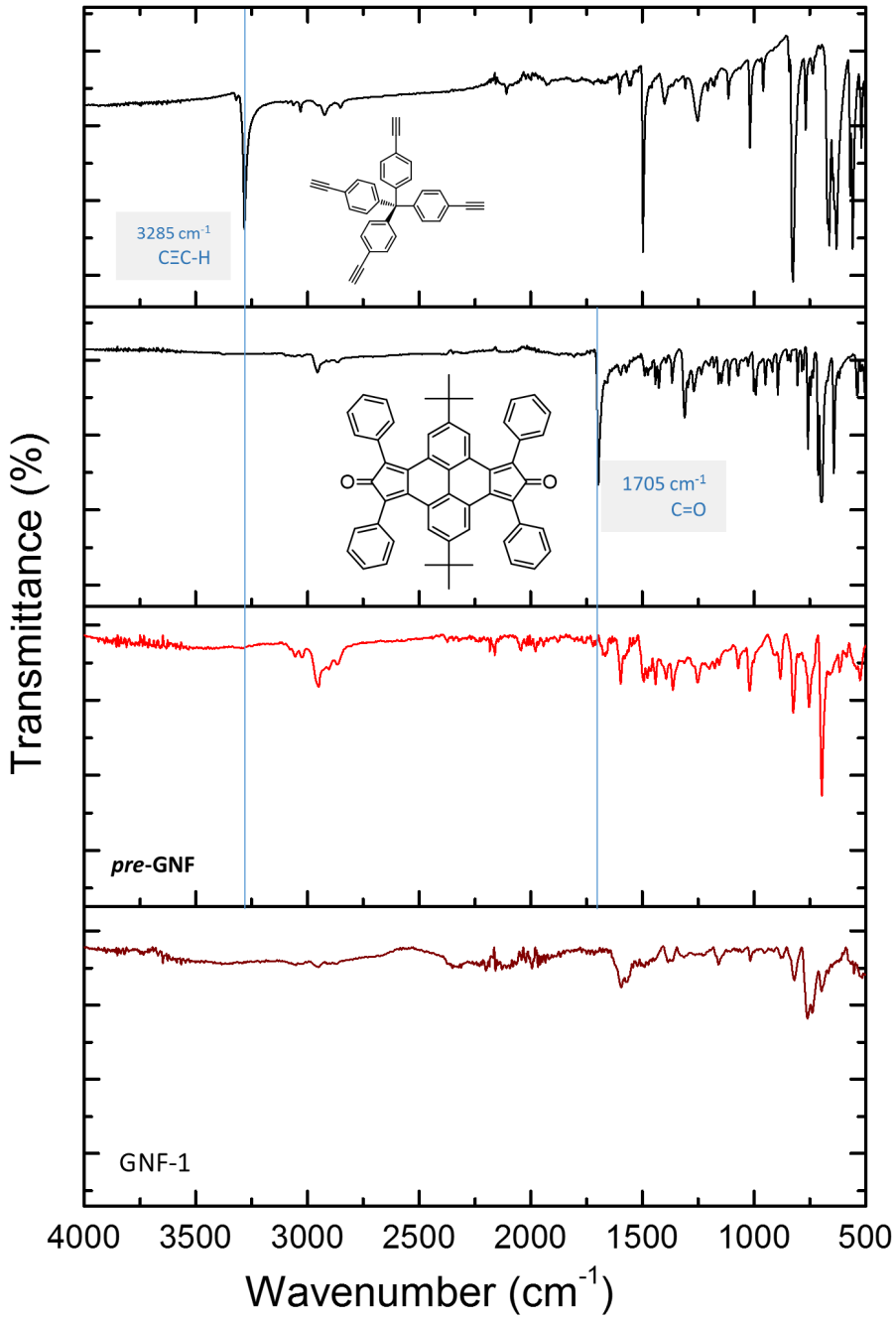


Figure S5. FT-IR spectra of tetrakis(4-ethynylphenyl)tetraphenylmethane (first), 2,8-di-tert-butyl-4,6,10,12-tetraphenyldicyclopenta[e,l]pyrene-5,11-dione (second), *pre*-GNF (third) and GNF-1 (last). The complete disappearance of the stretching bands at 3285 cm^{-1} (alkyne, C-H) and 1705 cm^{-1} (ketone, -C=O) indicate that both monomers were fully consumed to form *pre*-GNF-0 *via* the Diels-Alder polymerization.

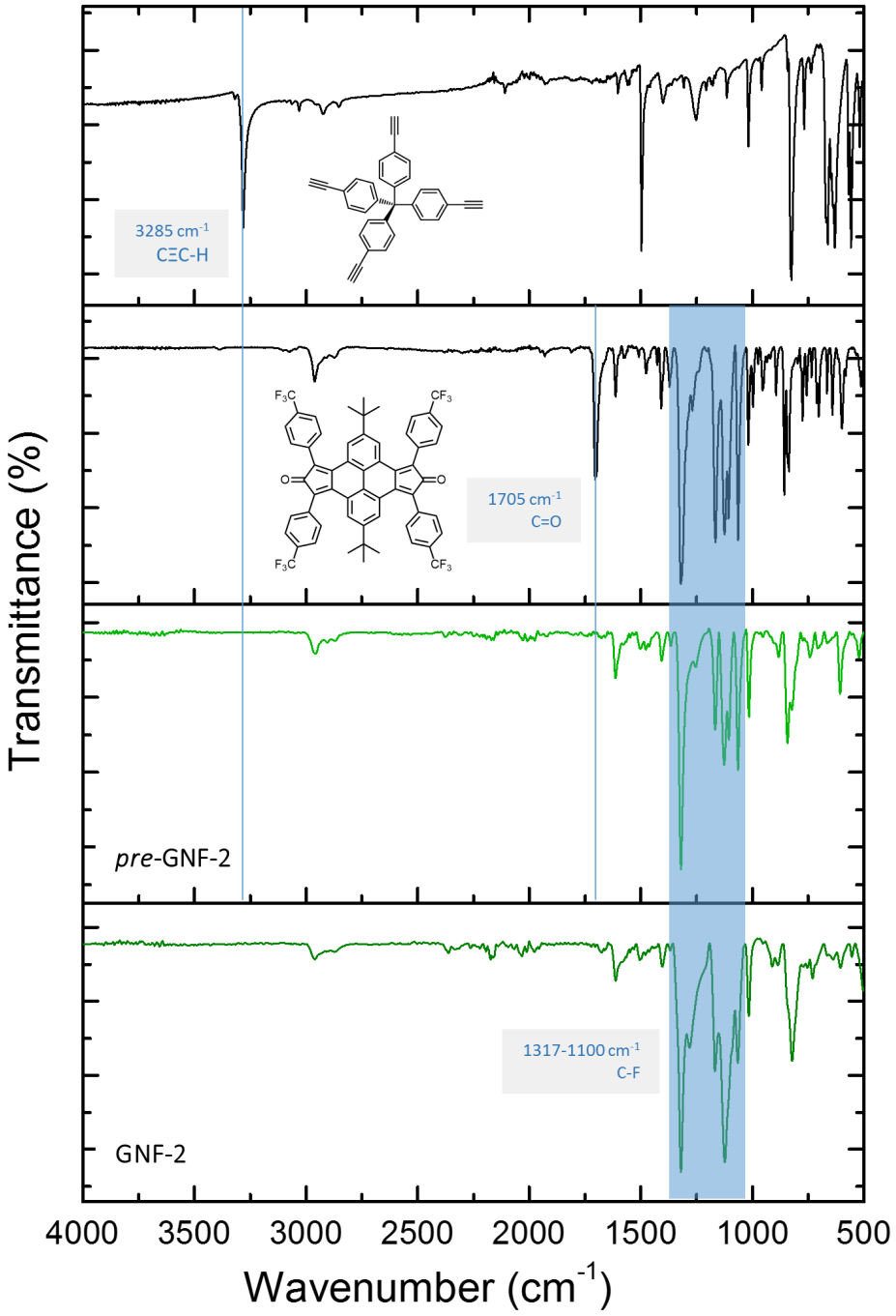


Figure S6. FT-IR spectra of tetrakis(4-ethynylphenyl)tetraphenylmethane (first), 2,8-di-tert-butyl-4,6,10,12-tetrakis(4-(trifluoromethyl)phenyl)dicyclopenta[e,l]pyrene-5,11-dione (second), *pre*-GNF-2 (third) and GNF-2 (last). The complete disappearance of the stretching bands at 3285 cm^{-1} (alkyne, C-H) and 1705 cm^{-1} (ketone, -C=O) indicate that both monomers fully reacted to form *pre*-GNF-2 *via* the Diels-Alder cycloaddition polymerization. The presence of C-F stretching bands at 1317-1100 cm^{-1} in GNF-2 provides clear evidence for the retention of -CF_3 groups following cyclodehydrogenation reaction.

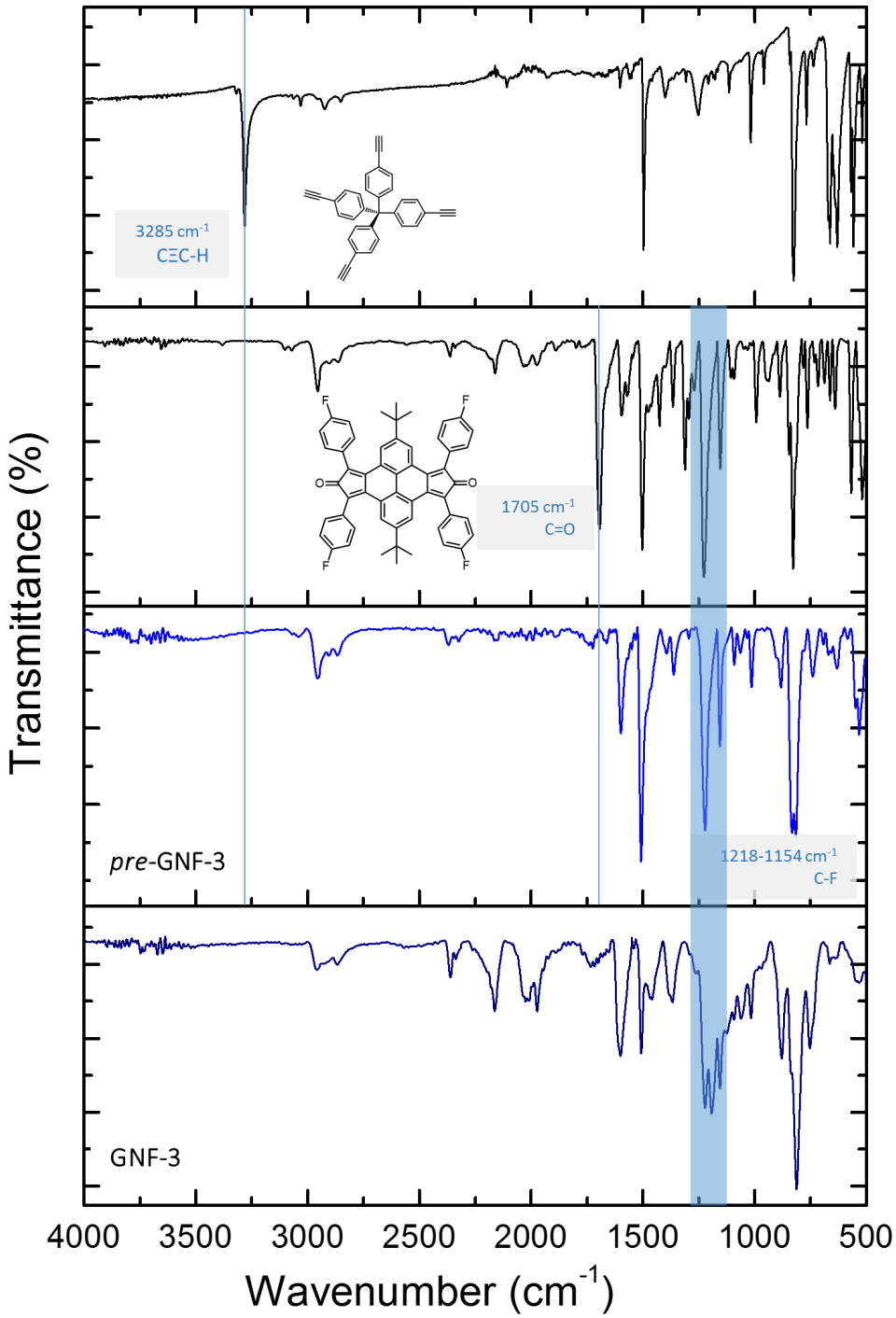


Figure S7. FT-IR spectra of tetrakis(4-ethynylphenyl)tetraphenylmethane (first), 2,8-di-tert-butyl-4,6,10,12-tetrakis(4-fluoromethylphenyl)dicyclopenta[e,l]pyrene-5,11-dione (second), *pre*-GNF-3 (third) and GNF-3 (last). The complete disappearance of the stretching bands at 3285 cm^{-1} (alkyne, C-H) and 1705 cm^{-1} (ketone, -C=O) indicate that both monomers fully reacted to form *pre*-GNF-3 *via* the Diels-Alder cycloaddition polymerization. The presence of C-F stretching bands at 1218-1154 cm^{-1} provides evidence that –F groups remained intact after the cyclodehydrogenation reaction.

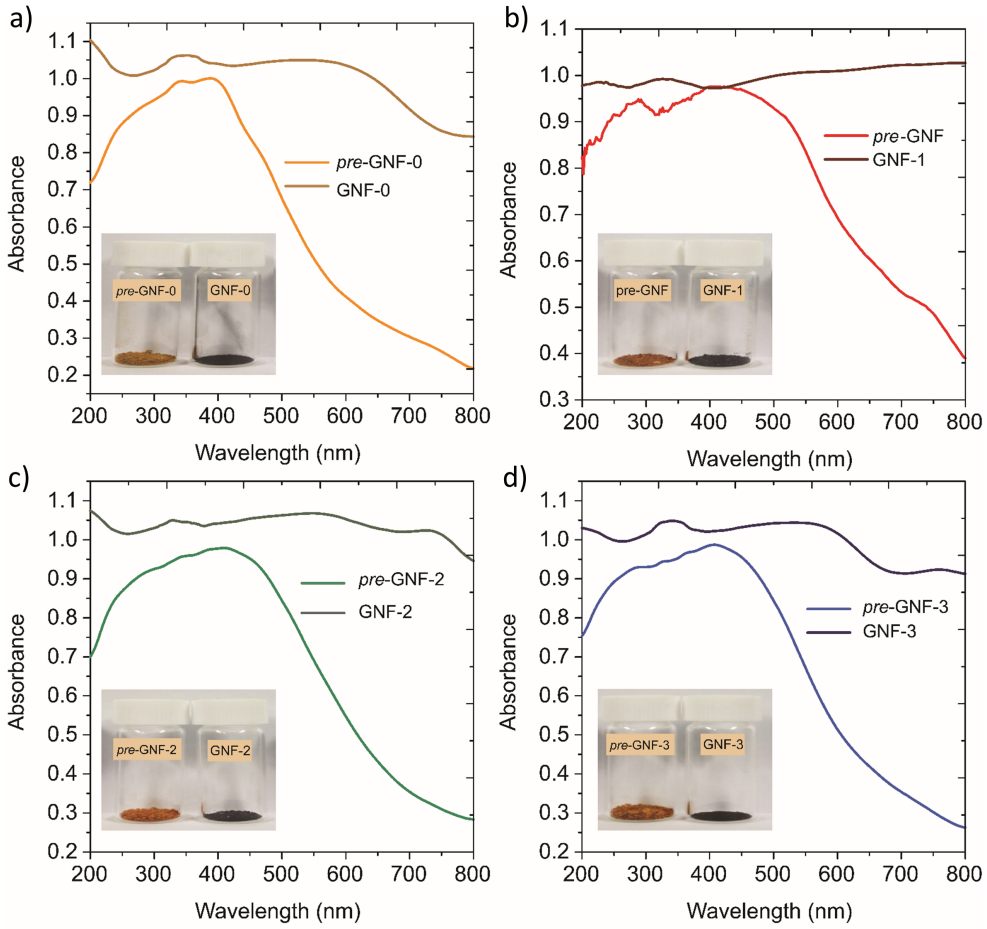


Figure S8. UV-Vis adsorption spectra of *pre*-GNFs and GNFs. Inset: Photographic images of *pre*-GNFs and GNFs powders before and after cyclodehydrogenation reaction.

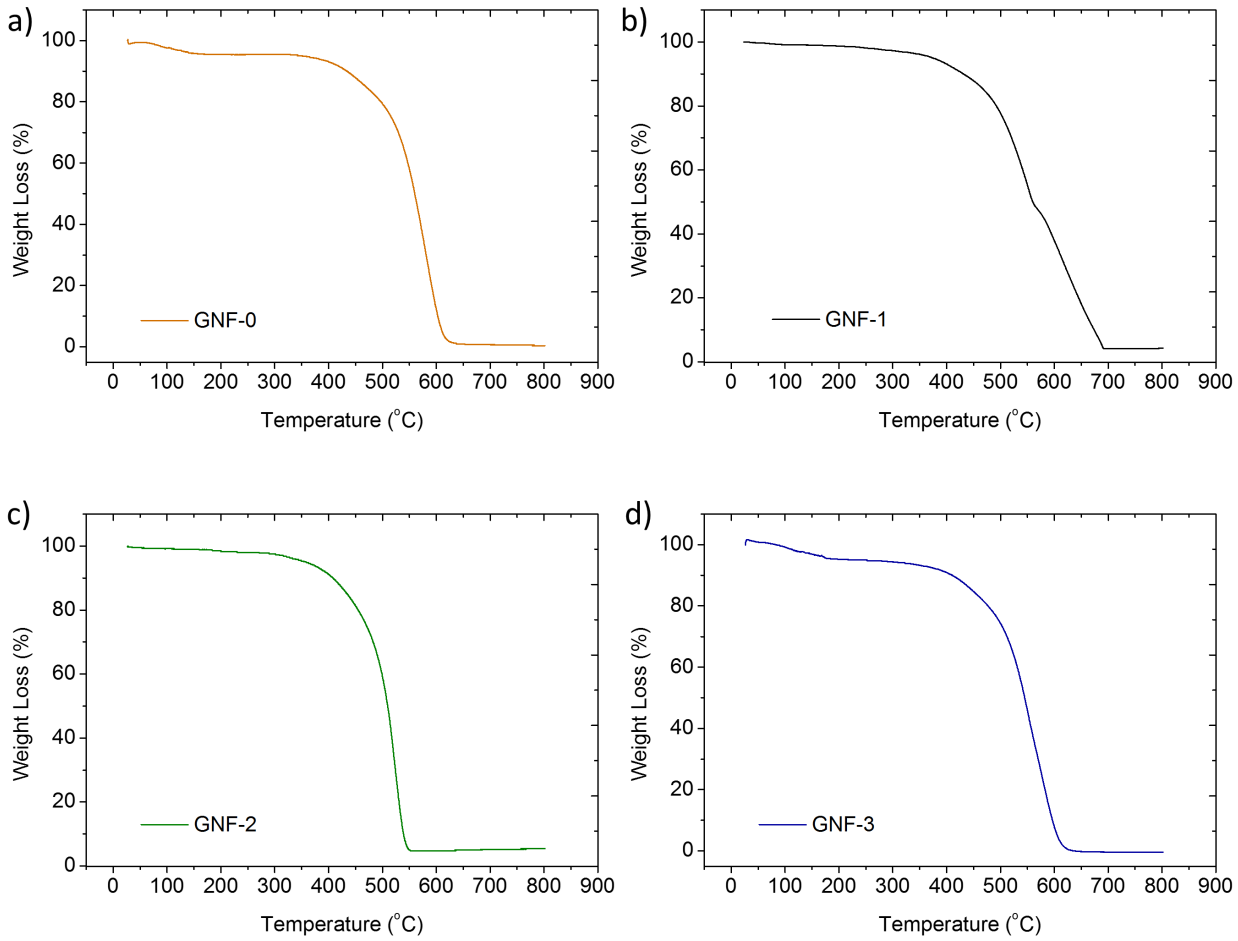


Figure S9. Thermogravimetric analysis of GNFs under air atmosphere up to 800°C at heating rate of 10°C min^{-1}.

E. Gas Sorption Studies of GNFs

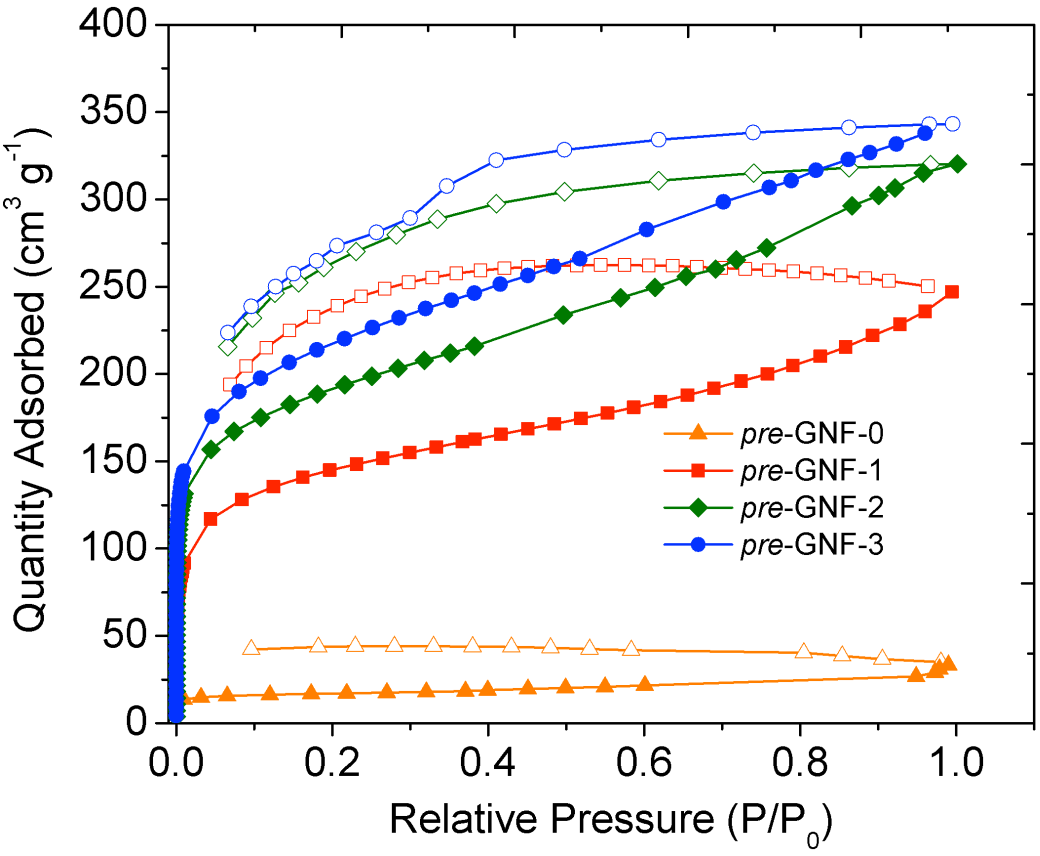


Figure S10. Argon adsorption-desorption isotherms (87 K) of *pre*-GNFs. Filled (●) and empty (○) symbols represent gas adsorption and desorption, respectively.

Table S1. BET surface areas for *pre*-GNFs.

	BET Ar (m^2 g^{-1})	Micropore area (m^2 g^{-1})
***pre*-GNF-0**	139	19
***pre*-GNF-1**	457	212
***pre*-GNF-2**	600	321
***pre*-GNF-3**	678	350

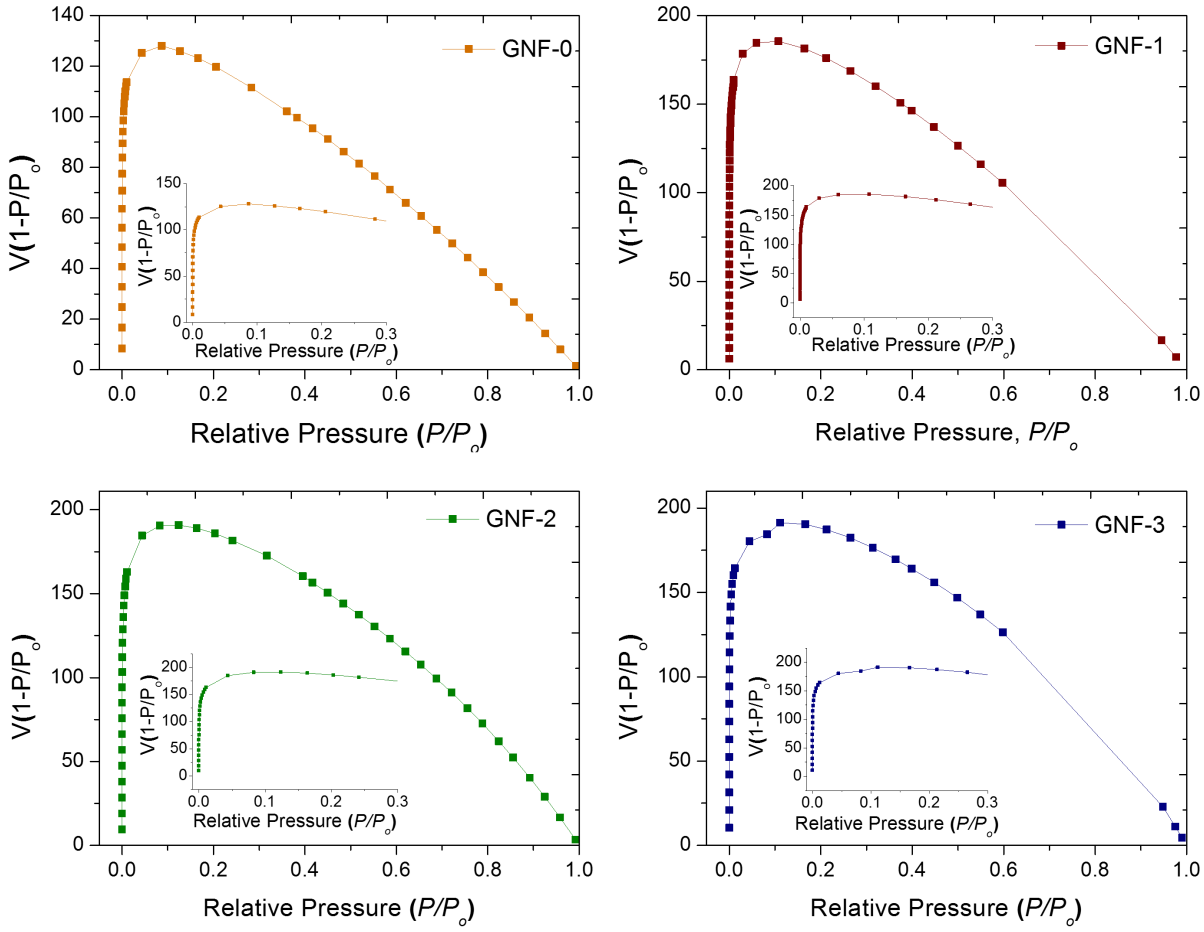


Figure S11. Rouquerol plots of GNFs (Inset: Expanded P/P_0 region). For BET surface area calculations, we utilized the relative pressure range between 0.01-0.1, where shows the continuous increase on Rouquerol plots.

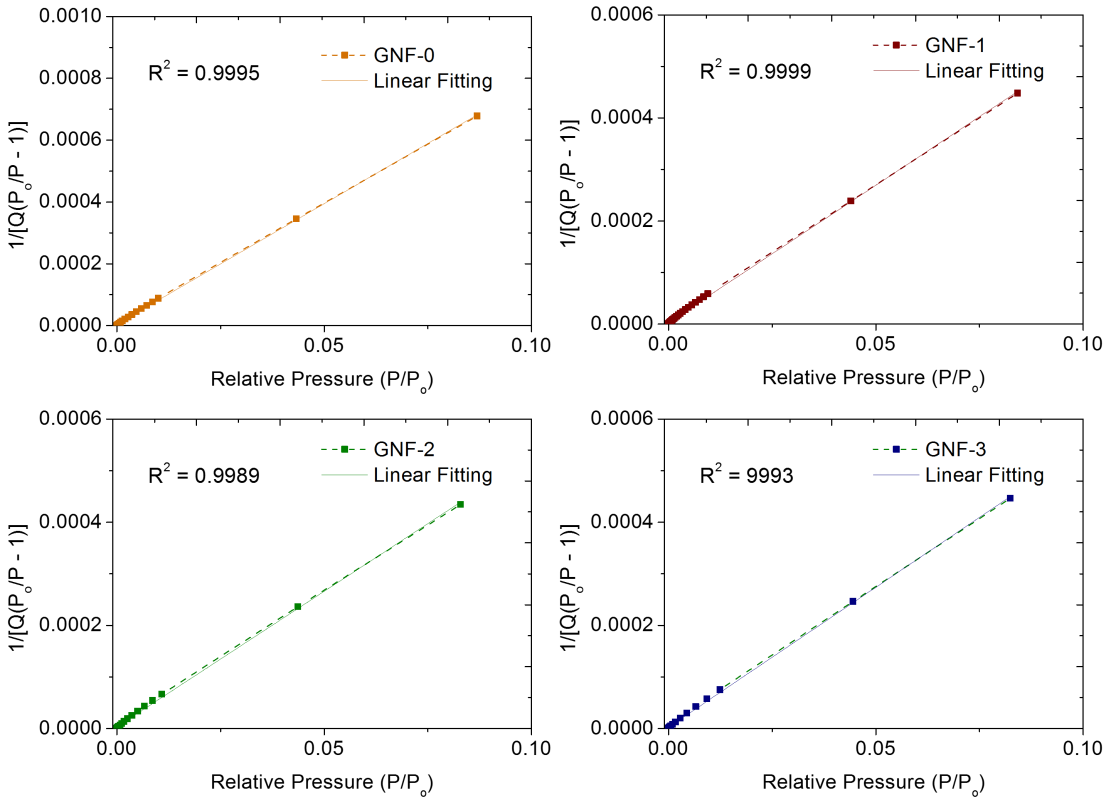


Figure S12. BET linear plots of GNFs obtained from Ar adsorption isotherms at 87 K. The relative pressure ranges were determined from the corresponding Rouquerol plots.

Table S2. Dual-site Langmuir-Freundlich fitting parameters for CO_2 adsorption for GNFs

	GNF-0		**GNF-1**		**GNF-2**		**GNF-3**	
	273 K	298 K	273 K	298 K	273 K	298 K	273 K	298 K
q_1	6.07	0.93	6.68	1.78	8.57	521.83	4.55	2.08
b_1	0.22	0.92	0.22	0.57	0.08	0.001	0.33	0.82
n_1	1	1	1	1	1	1	1	1
q_2	0.96	1.05	1.15	1.51	8.04	513.55	1.69	1.28
b_2	4.80	0.92	3.8	0.55	0.30	0.002	2.72	0.69
n_2	1	1	1	1	1	1	1	1

Table S3. Single-site Langmuir fitting parameters for CH_4 adsorption for GNFs

	GNF-0		**GNF-1**		**GNF-2**		**GNF-3**	
	273 K	298 K	273 K	298 K	273 K	298 K	273 K	298 K
q_1	2.38	1212.92	2.19	1.29	2.33	63.28	2.08	2.29
b_1	1.02	0.03	1.55	0.59	0.32	0.005	0.53	0.21
n_1	1	1	1	1	1	1	1	1

Table S4. Dual-site Langmuir-Freundlich fitting parameters for H_2 adsorption for GNFs

	GNF-0		**GNF-1**		**GNF-2**		**GNF-3**	
	273 K	298 K	273 K	298 K	273 K	298 K	273 K	298 K
q_1	1.23	0.87	3.68	8.32	2.87	1.76	3.56	4.20
b_1	34.93	14.99	3.72	0.77	14.34	8.88	18.49	0.23
n_1	1	1	0	1	1	1	1	1
q_2	1.23	0.87	9.93	4.29	3.07	5.83	2.35	2.49
b_2	34.94	14.99	2.76	11.55	0.40	0.15	0.61	10.41
n_2	1	1	1	1	1	1	1	1

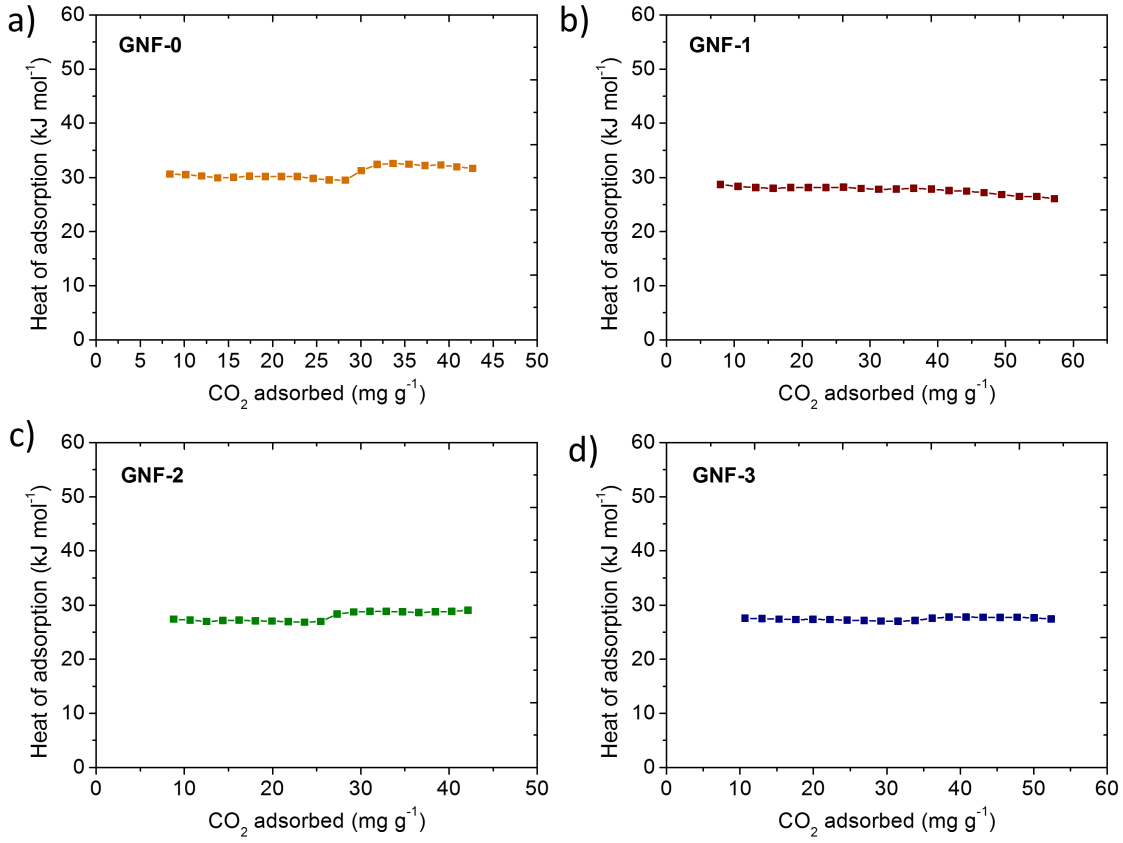


Figure S13. The isosteric heats of adsorption (Q_{st}) of CO_2 for GNFs calculated from Eq. 1 using the adsorption data at 273 and 298 K

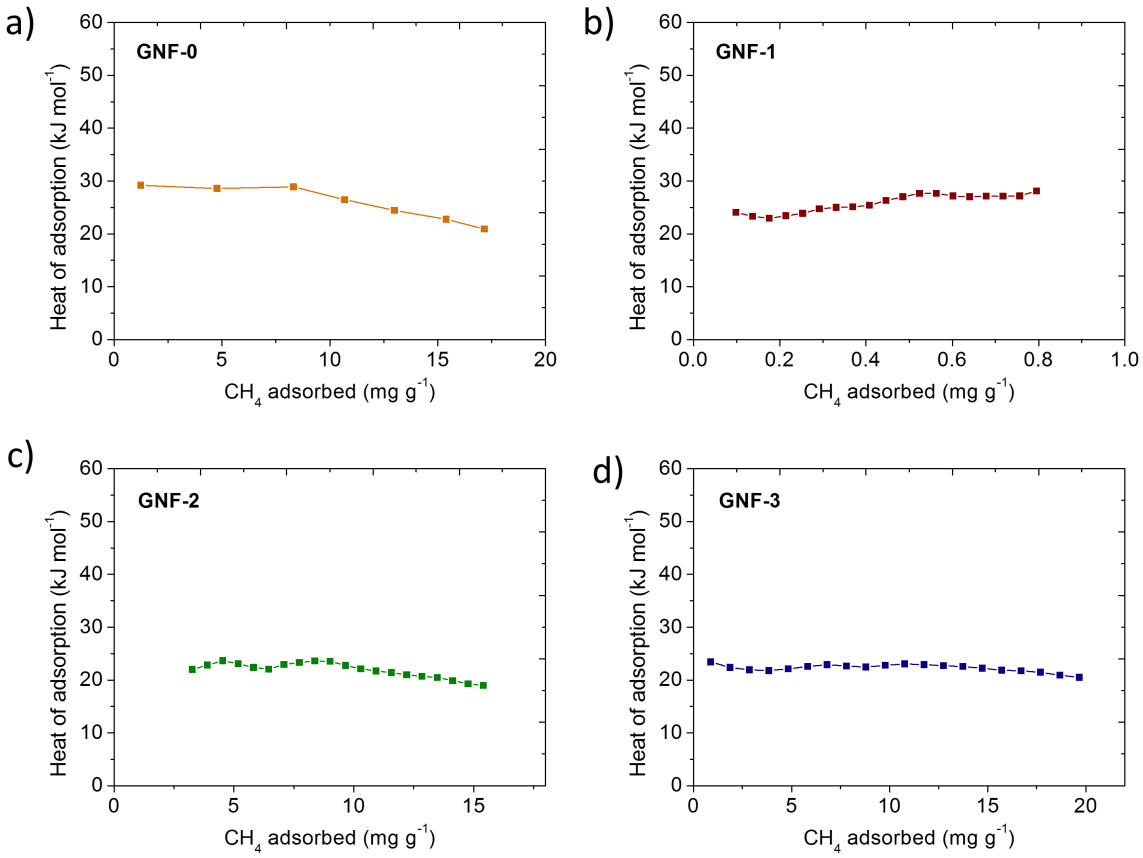


Figure S14. The isosteric heats of adsorption (Q_{st}) of CH_4 for GNFs calculated from Eq. 2 using the adsorption data at 273 and 298 K

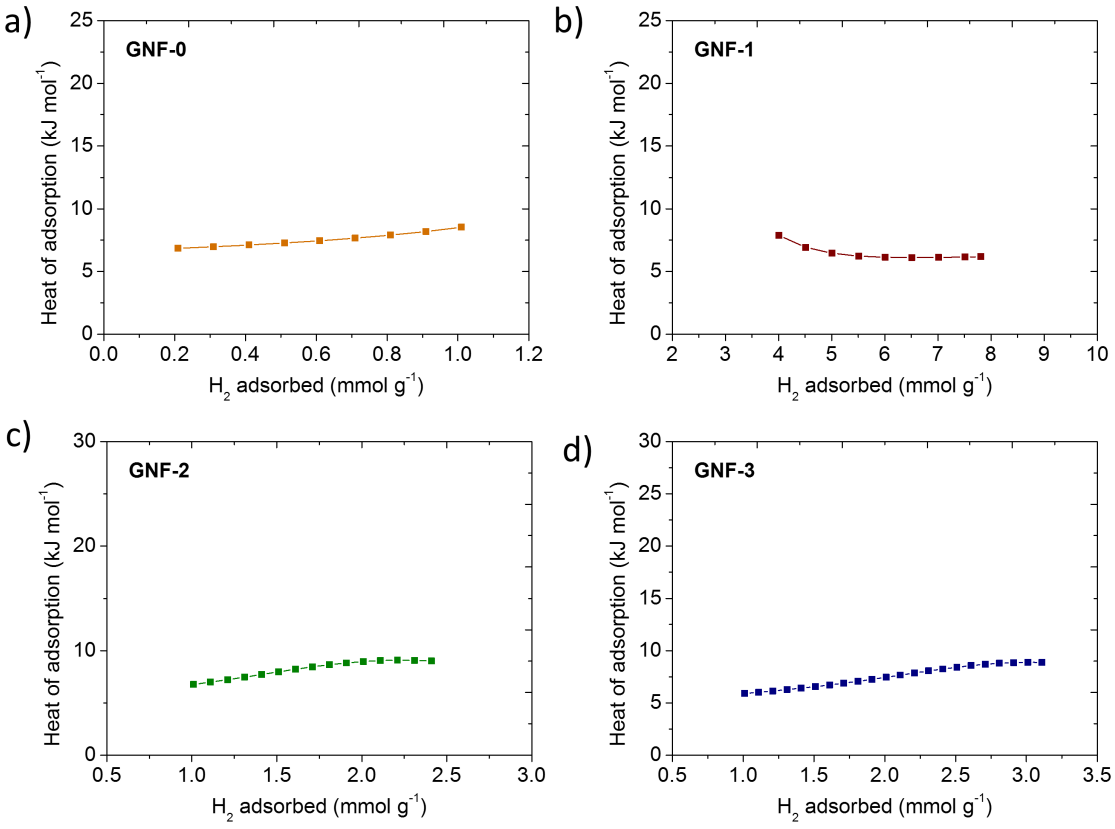


Figure S15. The isosteric heats of adsorption (Q_{st}) of H_2 of GNFs calculated from Eq. 1 using the adsorption data at 77 and 87 K

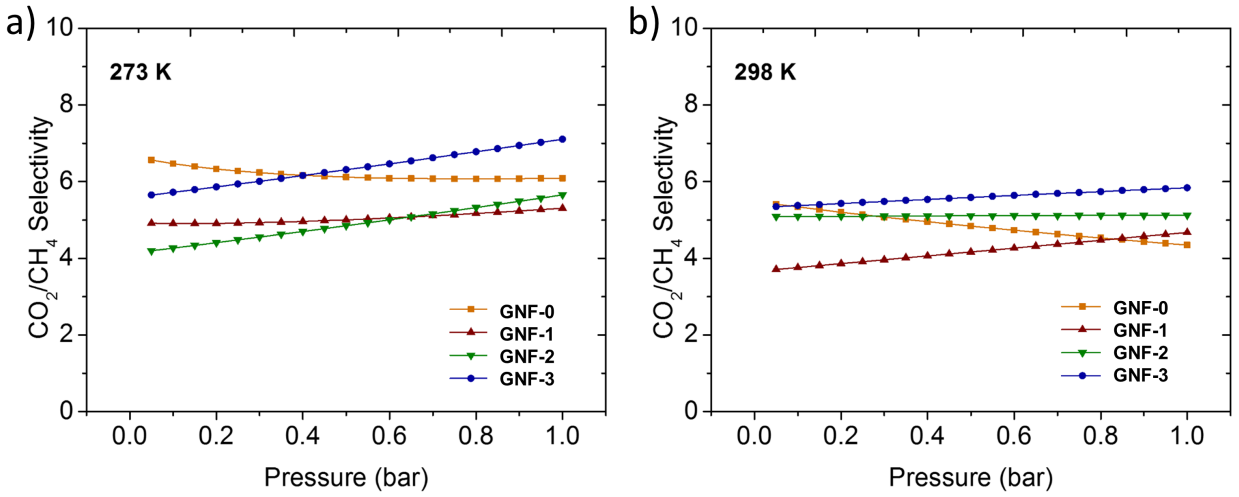


Figure S16. IAST selectivities of GNFs for a 50:50 CO_2/CH_4 mixture at (A) 273 K and (B) 298 K, respectively.

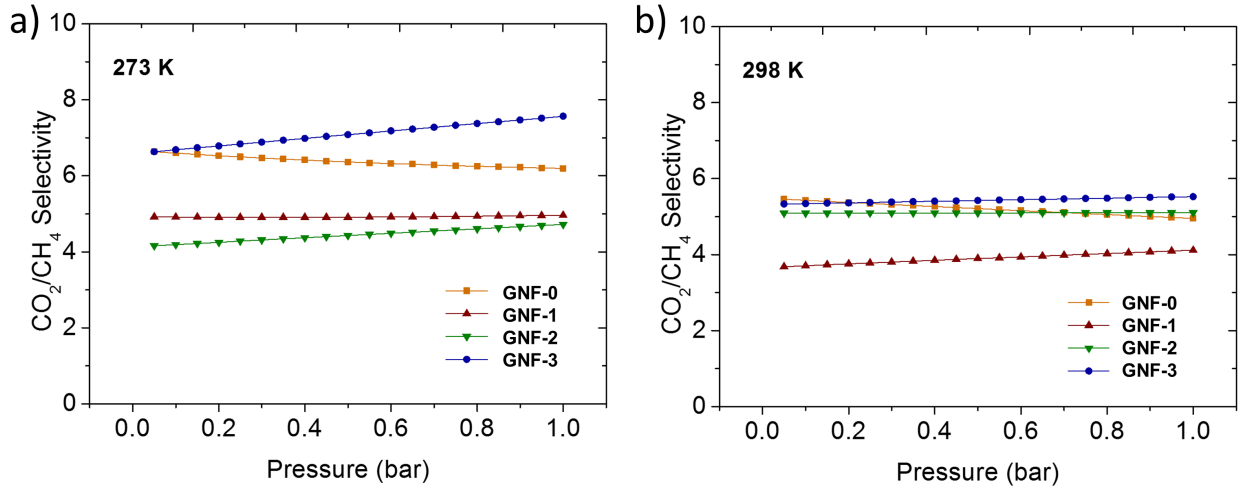


Figure S17. IAST selectivities of GNFs for a 5:95 CO_2/CH_4 mixture at (A) 273 K and (B) 298 K, respectively.

Table S5. IAST selectivities of GNFs for CO_2/CH_4 mixtures

	CO_2/CH_4 (50:50)		**CO_2/CH_4 (5:95)**	
	273 K	298 K	273 K	298 K
GNF-0	6.1	4.3	6.2	5.0
GNF-1	5.3	4.7	5.0	4.1
GNF-2	5.7	5.1	4.7	5.1
GNF-3	7.1	5.8	7.6	5.5

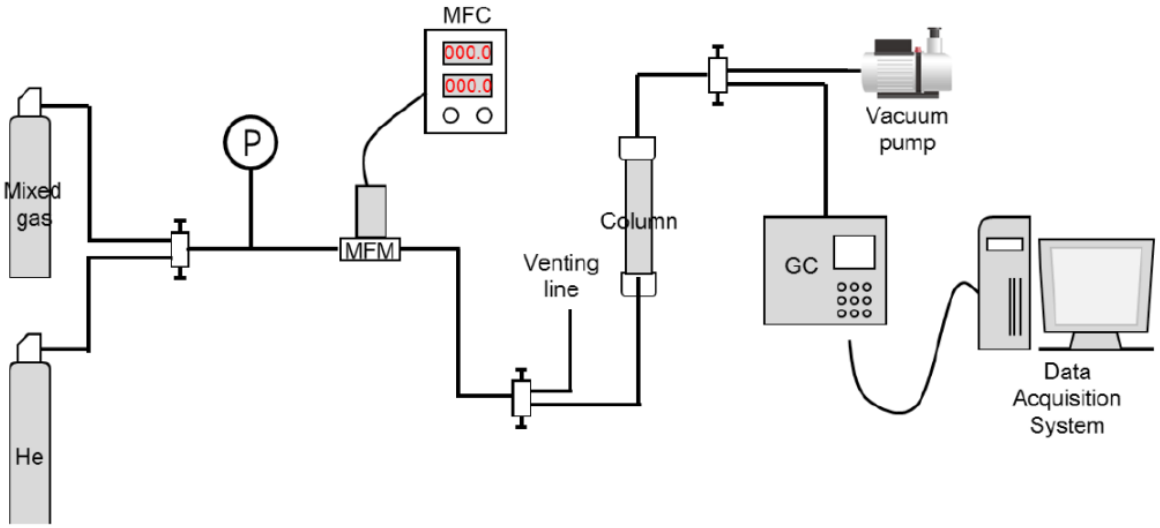


Figure S18. Schematic description of experimental set-up for the breakthrough studies.

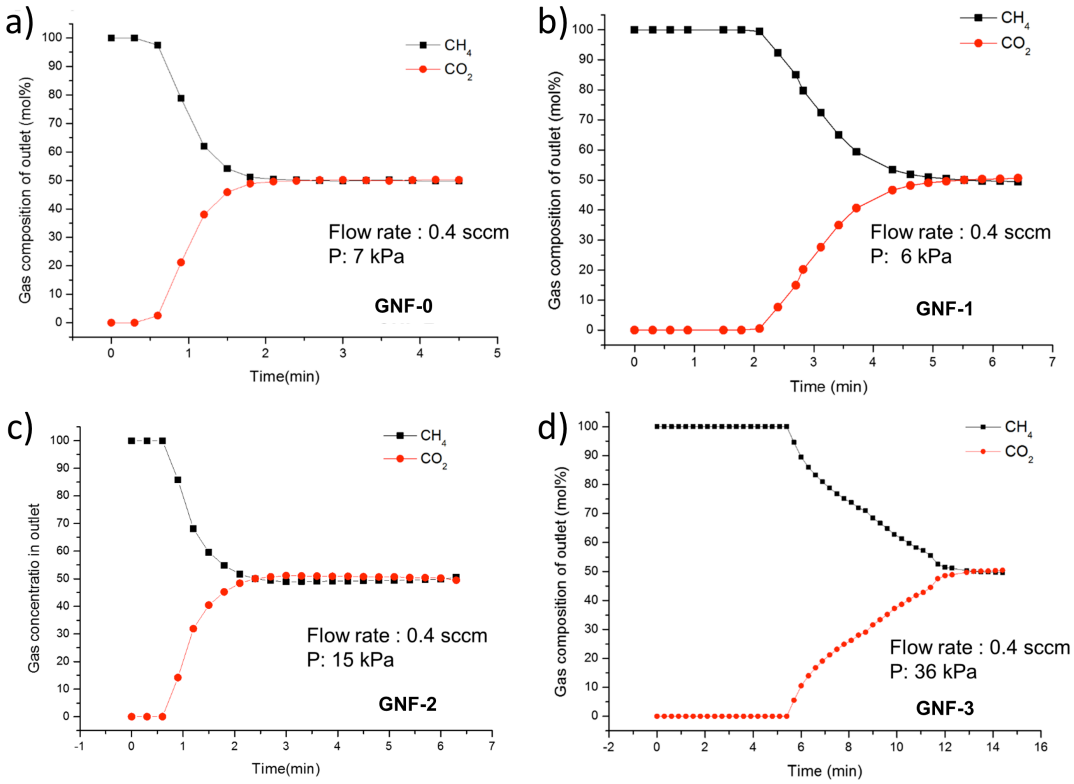


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Figure S19. Breakthrough experiments of GNFs for a binary CO_2/CH_4 (50:50) gas mixture at 298 K

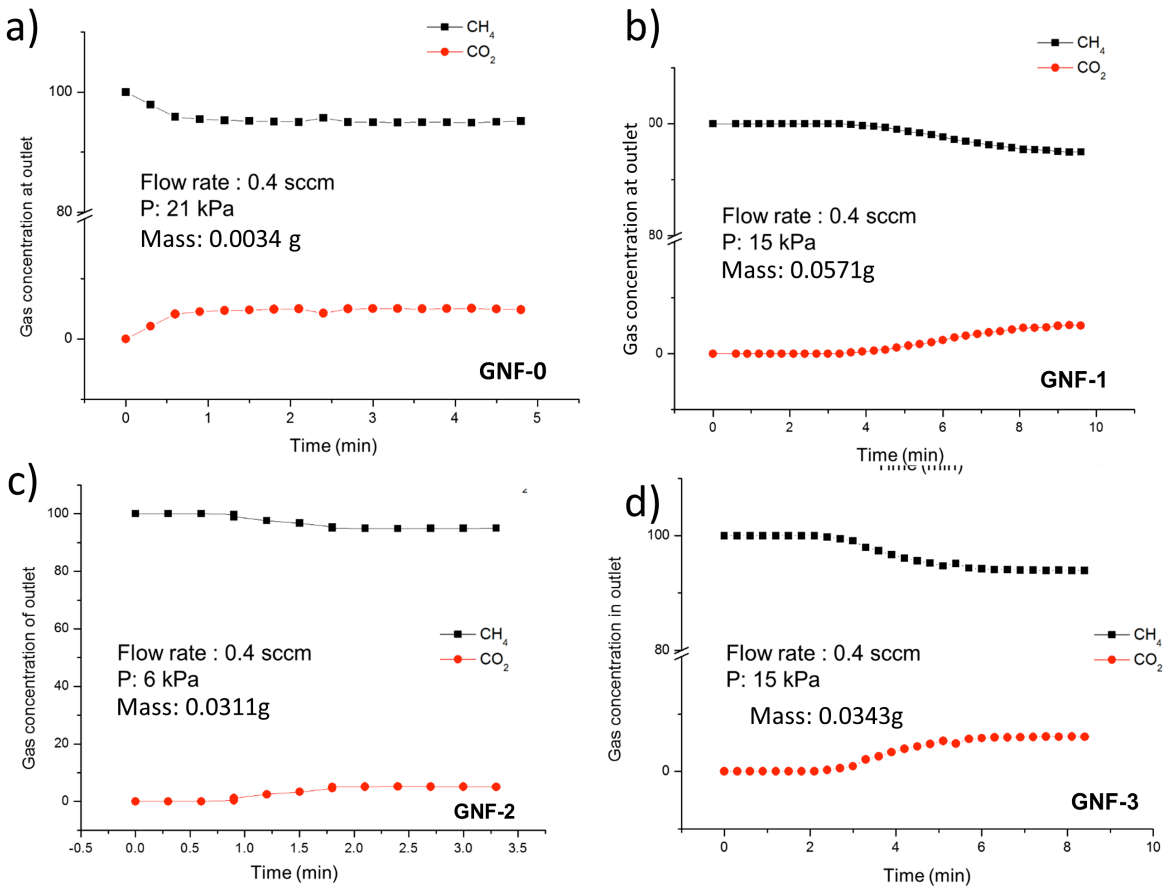

Figure S20. Breakthrough experiments of GNFs for a binary CO_2/CH_4 (5:95) gas mixture at 298 K

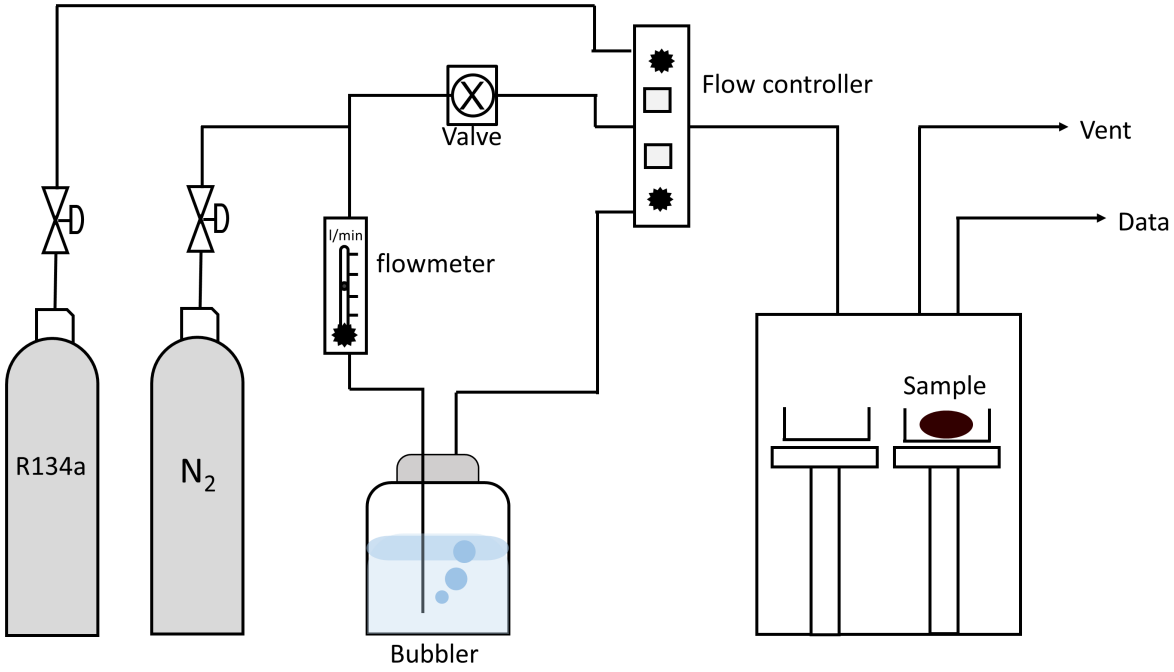

Figure S21. Schematic description of experimental set-up for the CFCs and fluorocarbon gravimetric uptake experiments using thermogravimetric analysis instrument.

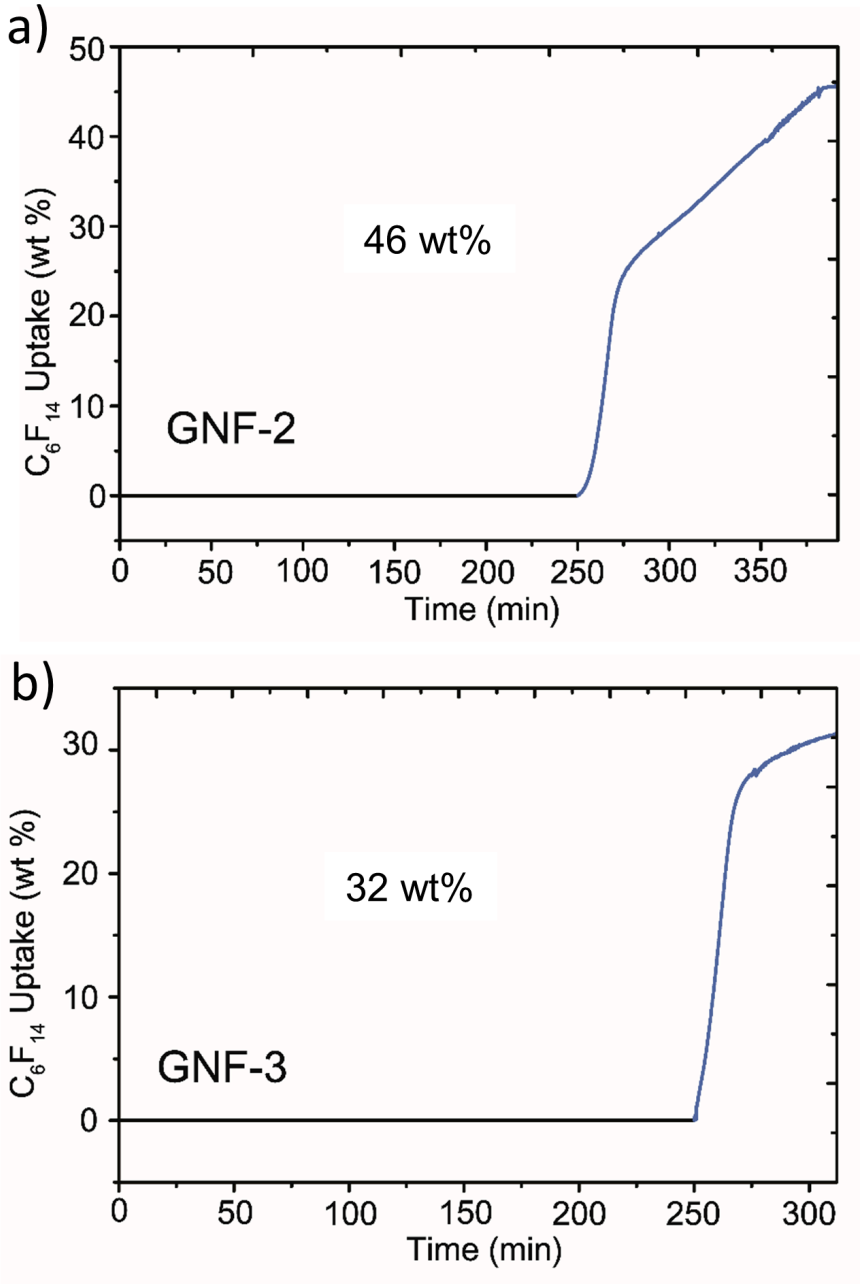

Figure S22. Perfluorohexane uptake experiments of (a) GNF-2 and (b) GNF-3. Black and blue line represent pure nitrogen atmosphere and vapor mixture of nitrogen and perfluorohexane, respectively.

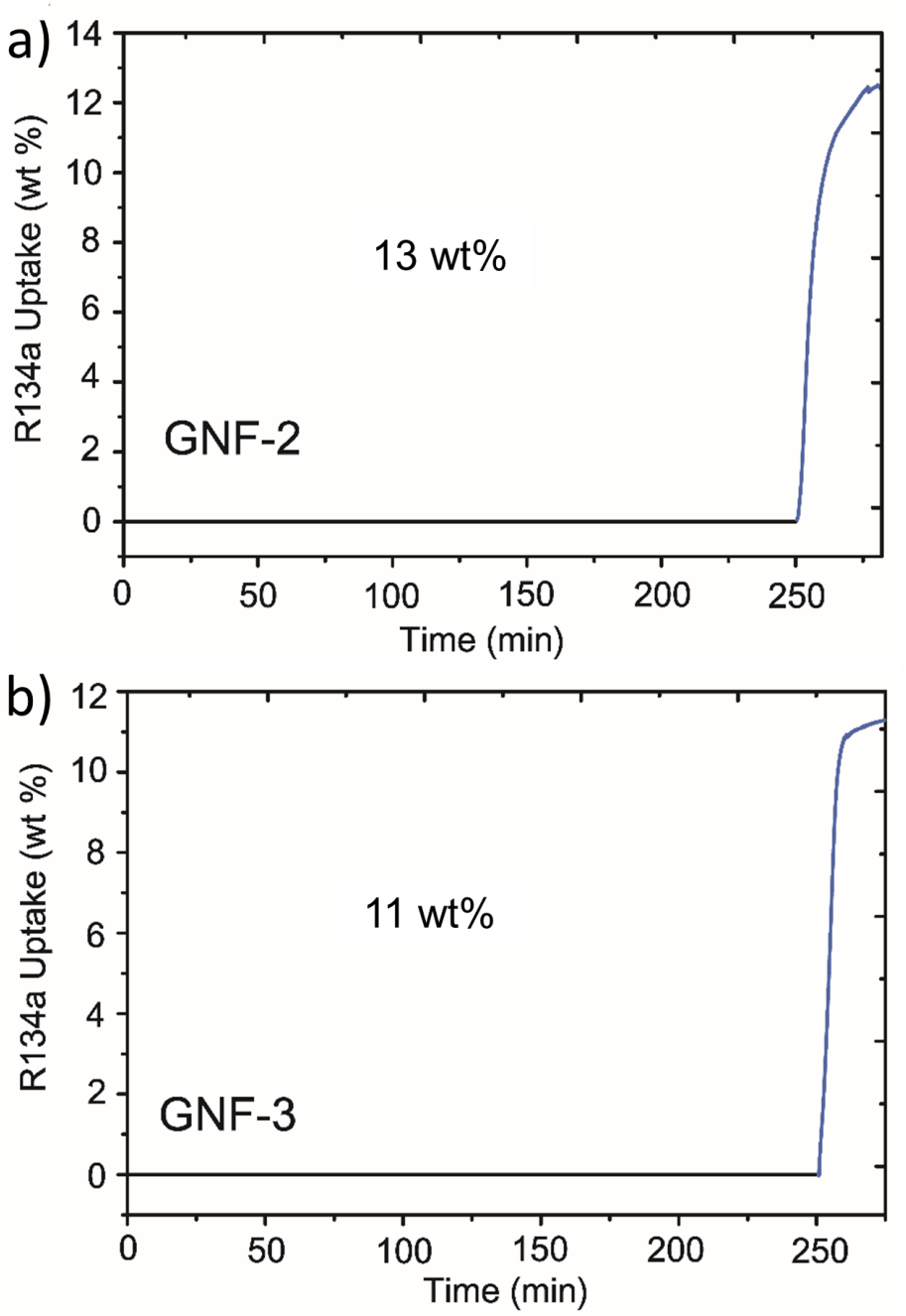

Figure S23. R134a uptake experiments of (a) GNF-2 and (b) GNF-3. Black and blue line represent pure nitrogen atmosphere and vapor mixture of nitrogen and R134a, respectively.

Table S6. ICP-MS analysis of GNFs

	Fe (wt %)
GNF-0	0.0007
GNF-1	0.0004
GNF-2	0.0003
GNF-3	0.0004

F. [1]H-NMR Spectra of Monomers

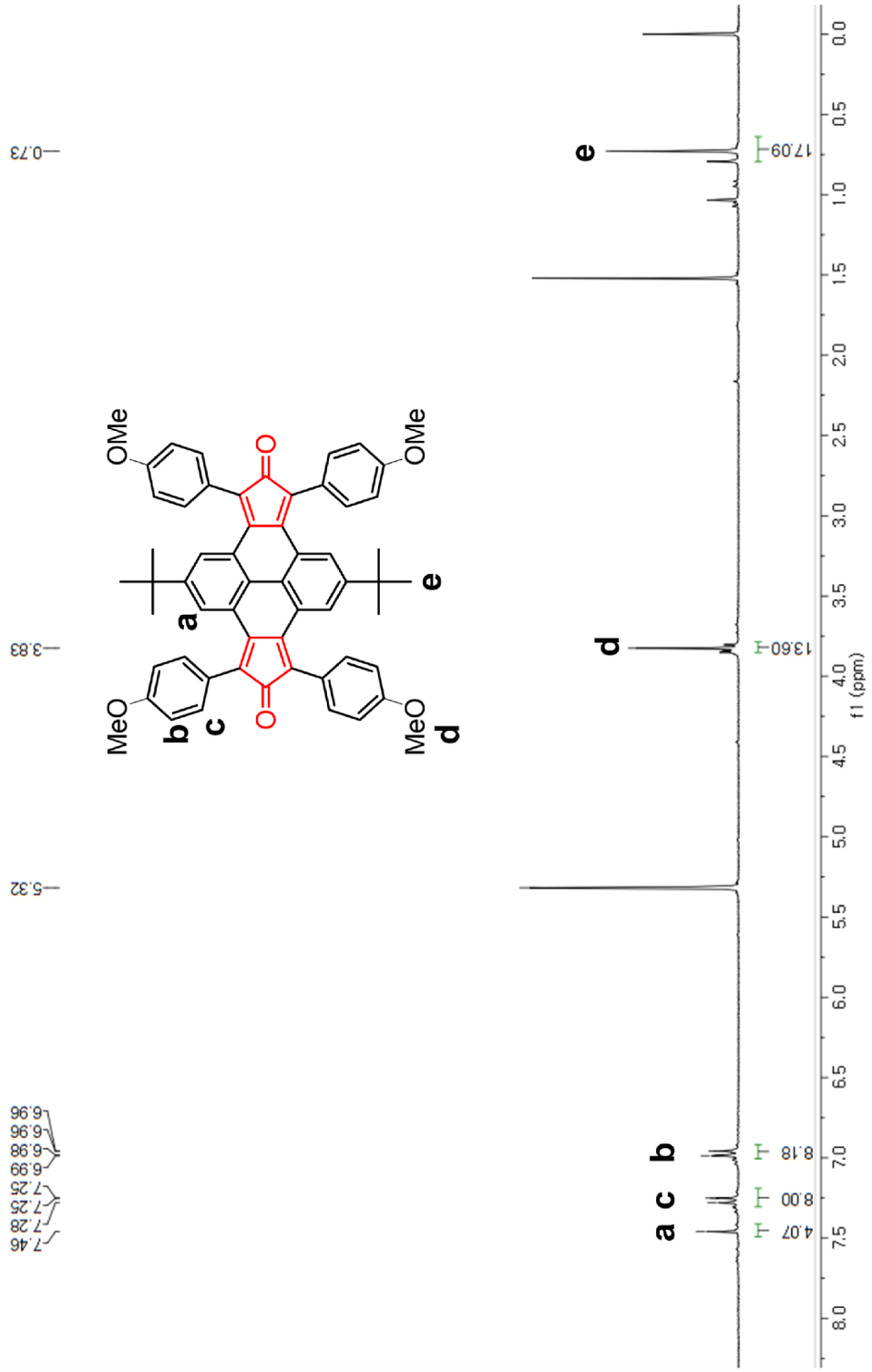

Figure S24. [1]H-NMR (300 MHz, CD_2Cl_2, 298 K) spectrum of compound **3a**.

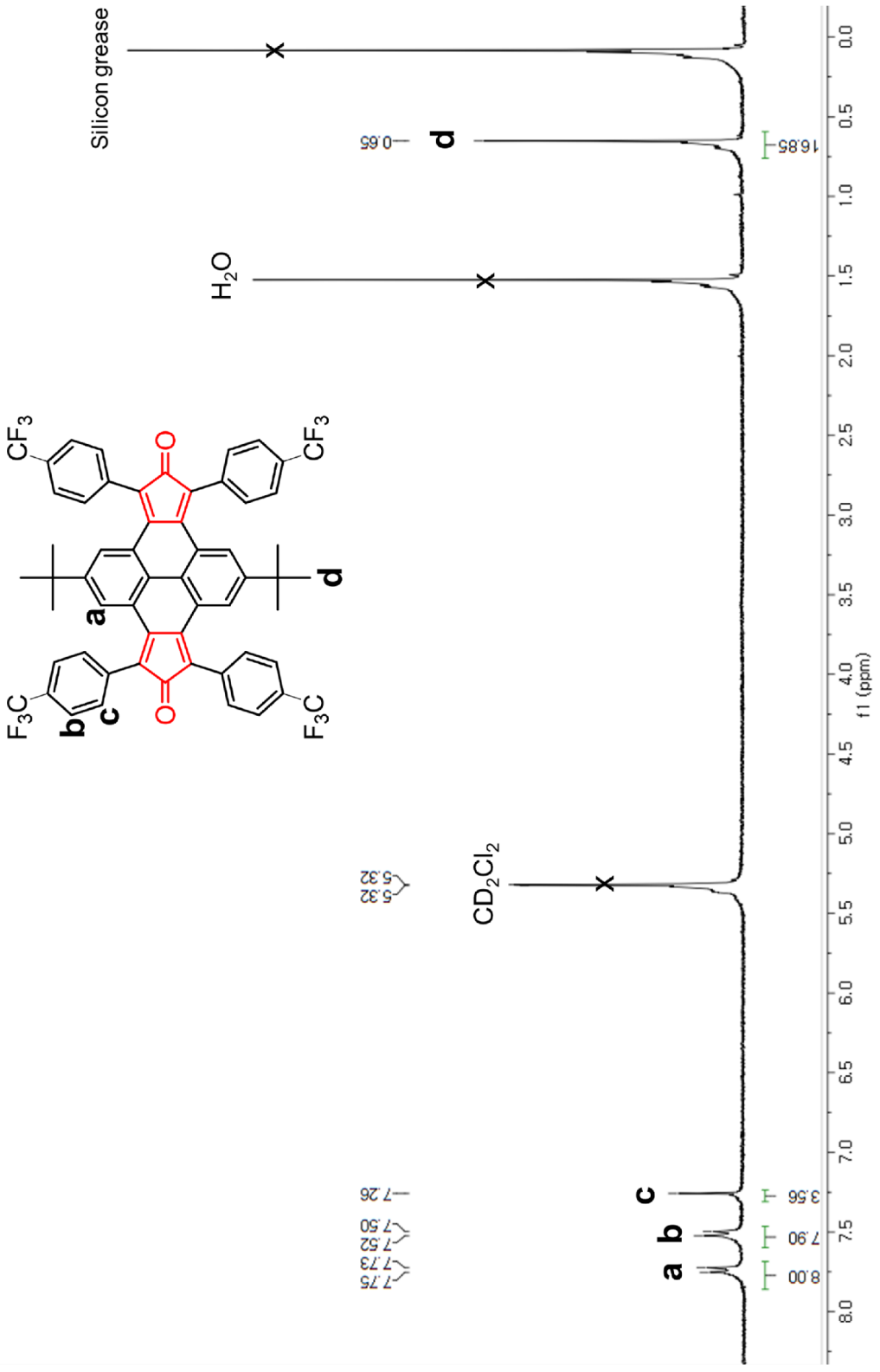

Figure S25. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298 K) of compound **3c**.

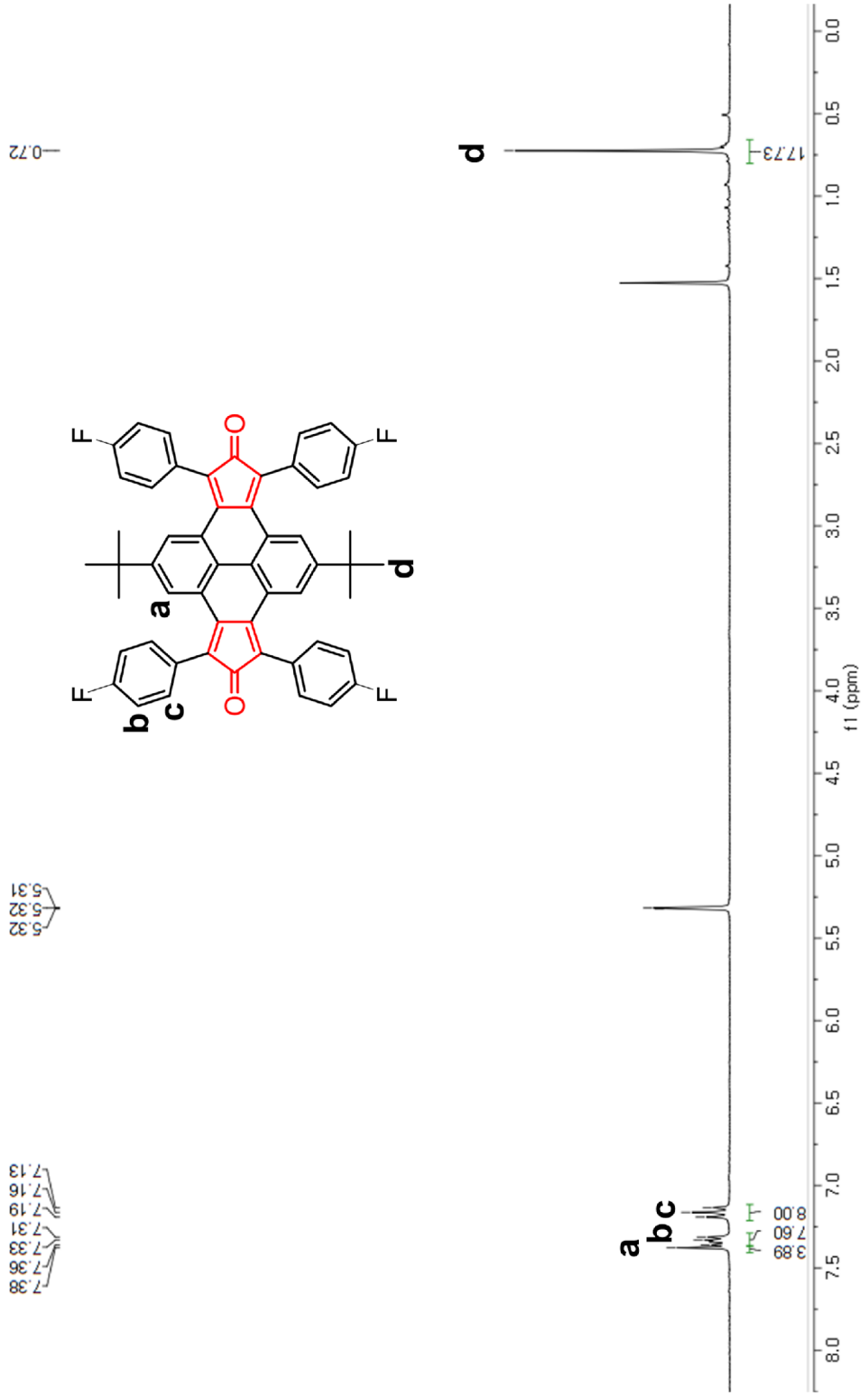

Figure S26. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298 K) of compound **3d**.

G. Crystal Data for Model Compounds *cis*-5 and *trans*-7

Table S7. Crystal data and structure refinement for ***cis*-5** and ***trans*-7**

Compound	*cis*-5	*trans*-7
Empirical formula	C84 H90 O6	C72 H50 F12
Formula weight	1195.55	1143.12
Temperature	296(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	C 2/c	C 2/c
Unit cell dimensions	a = 22.689(7) Å a= 90°. b = 15.773(5) Å b= 97.25(2)°. c = 20.036(6) Å g = 90°.	a = 21.1206(8) Å a= 90°. b = 21.8158(9) Å b= 111.402(3)°. c = 15.5581(6) Å g = 90°.
Volume	7113(4) Å3	6674.3(5) Å3
Z	4	4
Density (calculated)	1.116 Mg/m3	1.138 Mg/m3
Absorption coefficient	0.068 mm-1	0.089 mm-1
F(000)	2568	2360
Crystal size	0.23 x 0.21 x 0.19 mm3	0.27 x 0.26 x 0.05 mm3
Theta range for data collection	1.576 to 25.498°.	1.394 to 26.999°.
Index ranges	-27<=h<=27, -19<=k<=19, -24<=l<=18	-26<=h<=26, -27<=k<=27, -17<=l<=19
Reflections collected	35535	35320
Independent reflections	6619 [R(int) = 0.0653]	7278 [R(int) = 0.0672]
Completeness to theta = 25.242°	99.90%	100.00%
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Data / restraints / parameters	6619 / 6 / 413	7278 / 0 / 444
Goodness-of-fit on F2	1.049	1.007
Final R indices [I>2sigma(I)]	R1 = 0.0984, wR2 = 0.2763	R1 = 0.0759, wR2 = 0.2065
R indices (all data)	R1 = 0.1993, wR2 = 0.3535	R1 = 0.1759, wR2 = 0.2606
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	0.500 and -0.378 e.Å-3	0.281 and -0.351 e.Å-3

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ***cis*-5** and ***trans*-7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	Crystal ***cis*-5**					Crystal ***trans*-7**				
		x	y	z	U(eq)		x	y	z	U(eq)
1	C(1)	5000	8432(3)	7500	70(2)	C(1)	5125(2)	3292(1)	306(2)	57(1)
2	C(2)	4911(2)	7971(2)	6907(2)	64(1)	C(2)	4503(2)	3362(1)	404(2)	53(1)
3	C(3)	4920(2)	7087(2)	6883(2)	53(1)	C(3)	4428(1)	3387(1)	1249(2)	44(1)
4	C(4)	5000	6644(3)	7500	53(1)	C(4)	5021(1)	3308(1)	2052(2)	42(1)
5	C(5)	5000	5731(3)	7500	51(1)	C(5)	5662(1)	3218(1)	1974(2)	46(1)
6	C(6)	4746(2)	5293(2)	6923(2)	52(1)	C(6)	5696(2)	3233(1)	1098(2)	55(1)
7	C(7)	4754(2)	4408(2)	6942(2)	59(1)	C(7)	5164(2)	3274(2)	-662(2)	78(1)
8	C(8)	5000	3950(3)	7500	65(2)	C(8)	5642(5)	2701(5)	-709(6)	96(2)
9	C(9)	5000	9393(4)	7500	95(2)	C(9)	4504(5)	3233(6)	-1419(6)	93(3)
10	C(10)	4950(6)	9784(7)	6840(6)	104(4)	C(10)	5570(6)	3802(5)	-781(7)	105(2)
11	C(11)	5612(6)	9662(10)	7898(8)	159(6)	C(8A)	5869(5)	3219(5)	-632(5)	102(3)
12	C(12)	4637(7)	9723(8)	7993(6)	116(4)	C(9A)	4652(5)	2807(5)	-1255(7)	101(2)
13	C(13)	5000	2988(4)	7500	80(2)	C(10A)	4945(6)	3931(4)	-1093(5)	110(3)
14	C(14)	5352(6)	2592(7)	8071(6)	99(3)	C(11)	3759(1)	3393(1)	1350(2)	44(1)
15	C(15)	4361(7)	2743(12)	7575(11)	193(7)	C(12)	3142(1)	3563(1)	625(2)	47(1)
16	C(16)	5059(7)	2600(7)	6859(6)	113(4)	C(13)	2520(1)	3387(1)	683(2)	51(1)
17	C(17)	4546(2)	5776(2)	6304(2)	53(1)	C(14)	2523(1)	3022(1)	1420(2)	55(1)
18	C(18)	4175(2)	5425(2)	5743(2)	56(1)	C(15)	3114(1)	2908(1)	2174(2)	50(1)
19	C(19)	4157(2)	5824(2)	5124(2)	59(1)	C(16)	3731(1)	3161(1)	2180(2)	45(1)
20	C(20)	4513(2)	6535(3)	5064(2)	63(1)	C(17)	3148(1)	3949(1)	-162(2)	53(1)
21	C(21)	4816(2)	6948(2)	5606(2)	57(1)	C(18)	3472(2)	4513(2)	2(2)	74(1)
22	C(22)	4779(2)	6600(2)	6257(2)	55(1)	C(19)	3485(2)	4871(2)	-716(3)	101(1)
23	C(23)	3782(2)	4676(2)	5828(2)	58(1)	C(20)	3174(2)	4679(2)	-1607(3)	103(1)
24	C(24)	3370(2)	4713(3)	6286(2)	71(1)	C(21)	2846(2)	4123(2)	-1788(2)	89(1)
25	C(25)	3016(2)	4029(3)	6390(3)	87(1)	C(22)	2829(2)	3761(2)	-1069(2)	62(1)
26	C(26)	3061(2)	3295(3)	6028(3)	87(2)	C(23)	3210(5)	5022(4)	-2483(7)	160(3)
27	C(27)	3465(2)	3239(3)	5572(2)	81(1)	F(24)	3829(6)	5102(9)	-2344(12)	206(5)
28	C(28)	3817(2)	3934(3)	5470(2)	70(1)	F(25)	2970(10)	5709(4)	-2261(11)	245(7)
29	O(29)	2684(2)	2647(2)	6166(2)	124(1)	F(26)	2681(5)	4969(5)	-3180(5)	194(5)
30	C(30)	2773(4)	1842(4)	5889(4)	156(3)	F(24A)	3464(13)	4607(7)	-3000(10)	235(11)
31	C(31)	3771(2)	5524(3)	4510(2)	64(1)	F(25A)	2891(13)	5322(13)	-2680(20)	317(14)
32	C(32)	3160(2)	5545(3)	4456(3)	89(2)	F(26A)	3591(13)	5435(6)	-2287(11)	176(6)
33	C(33)	2820(3)	5318(4)	3859(3)	107(2)	C(27)	1845(2)	3560(1)	-17(2)	56(1)

34	C(34)	3084(4)	5056(4)	3323(3)	116(2)	C(28)	1672(2)	4171(2)	-232(2)	79(1)
35	C(35)	3686(4)	5014(5)	3378(3)	133(3)	C(29)	1027(2)	4321(2)	-839(3)	94(1)
36	C(36)	4027(2)	5244(4)	3963(2)	102(2)	C(30)	556(2)	3876(2)	-1234(3)	99(1)
37	C(37)	5204(2)	7677(2)	5483(2)	62(1)	C(31)	715(2)	3274(2)	-1028(3)	89(1)
38	C(38)	5006(2)	8307(3)	5018(2)	80(1)	C(32)	1364(2)	3121(2)	-422(2)	71(1)
39	C(39)	5391(3)	8967(3)	4885(3)	98(2)	C(33)	3076(2)	2474(1)	2890(2)	54(1)
40	C(40)	5949(3)	9011(4)	5202(3)	100(2)	C(34)	2574(2)	2527(2)	3264(2)	67(1)
41	C(41)	6155(2)	8397(3)	5659(3)	90(2)	C(35)	2542(2)	2108(2)	3916(2)	77(1)
42	C(42)	5786(2)	7738(3)	5791(2)	74(1)	C(36)	3000(2)	1643(2)	4212(3)	75(1)
43	O(43)	6292(4)	9677(4)	5039(4)	174(2)	C(37)	3498(2)	1581(2)	3840(2)	77(1)
44	C(44)	6371(10)	10188(9)	4684(12)	206(12)	C(38)	3534(2)	1988(2)	3188(2)	65(1)
45	C(44A)	6728(7)	9829(12)	5309(8)	135(5)	C(39)	2992(4)	1216(3)	4954(4)	112(2)
46	O(45)	2586(4)	3271(5)	1700(5)	237(4)	F(40)	3357(9)	1466(4)	5806(4)	158(4)
47	C(46)	2957(6)	2554(7)	1773(8)	191(4)	F(41)	3238(8)	694(3)	4947(10)	169(6)
48	C(47)	3218(5)	2483(8)	1141(6)	217(5)	F(42)	2415(5)	1134(6)	4981(9)	178(6)
49	C(48)	3332(6)	2629(9)	2373(7)	257(6)	F(40A)	2351(12)	808(9)	4382(17)	201(7)
50	C(49)	2020(6)	3152(8)	1756(8)	228(6)	F(41A)	3493(18)	892(17)	5290(30)	220(11)
51	C(50)	1674(7)	2885(10)	1136(9)	310(9)	F(42A)	2709(15)	1424(7)	5498(11)	124(10)
52	C(51)	1792(7)	3983(12)	1969(8)	360(9)					

Table S9. Bond lengths [Å] and angles [°] for cis-5 and trans-7.

Crystal ***cis*-5**		Crystal ***trans*-7**	
C(1)-C(2)#1	1.386(5)	C(1)-C(6)	1.380(4)
C(1)-C(2)	1.386(5)	C(1)-C(2)	1.385(4)
C(1)-C(9)	1.516(8)	C(1)-C(7)	1.538(4)
C(2)-C(3)	1.396(5)	C(2)-C(3)	1.382(4)
C(2)-H(2)	0.93	C(2)-H(2)	0.93
C(3)-C(4)	1.412(4)	C(3)-C(4)	1.420(3)
C(3)-C(22)	1.471(5)	C(3)-C(11)	1.478(4)
C(4)-C(3)#1	1.412(4)	C(4)-C(5)	1.415(4)
C(4)-C(5)	1.440(7)	C(4)-C(4)#1	1.431(5)
C(5)-C(6)	1.406(4)	C(5)-C(6)	1.391(4)
C(5)-C(6)#1	1.406(4)	C(5)-C(16)#1	1.471(4)
C(6)-C(7)	1.397(5)	C(6)-H(6)	0.93
C(6)-C(17)	1.476(5)	C(7)-C(9)	1.462(10)
C(7)-C(8)	1.387(4)	C(7)-C(8A)	1.479(9)
C(7)-H(7)	0.93	C(7)-C(10)	1.488(10)
C(8)-C(7)#1	1.388(4)	C(7)-C(9A)	1.526(9)
C(8)-C(13)	1.517(8)	C(7)-C(10A)	1.578(8)
C(9)-C(10)#1	1.451(11)	C(7)-C(8)	1.625(9)
C(9)-C(10)	1.451(11)	C(8)-H(8A)	0.96
C(9)-C(12)	1.460(11)	C(8)-H(8B)	0.96
C(9)-C(12)#1	1.460(11)	C(8)-H(8C)	0.96
C(9)-C(11)	1.570(13)	C(9)-H(9A)	0.96
C(9)-C(11)#1	1.570(13)	C(9)-H(9B)	0.96
C(10)-H(10A)	0.96	C(9)-H(9C)	0.96
C(10)-H(10B)	0.96	C(10)-H(10A)	0.96
C(10)-H(10C)	0.96	C(10)-H(10B)	0.96
C(11)-H(11A)	0.96	C(10)-H(10C)	0.96
C(11)-H(11B)	0.96	C(8A)-H(8A1)	0.96
C(11)-H(11C)	0.96	C(8A)-H(8A2)	0.96
C(12)-H(12A)	0.96	C(8A)-H(8A3)	0.96
C(12)-H(12B)	0.96	C(9A)-H(9A1)	0.96
C(12)-H(12C)	0.96	C(9A)-H(9A2)	0.96
C(13)-C(16)	1.445(11)	C(9A)-H(9A3)	0.96
C(13)-C(16)#1	1.445(11)	C(10A)-H(10D)	0.96
C(13)-C(14)#1	1.451(11)	C(10A)-H(10E)	0.96
C(13)-C(14)	1.451(11)	C(10A)-H(10F)	0.96
C(13)-C(15)	1.526(15)	C(11)-C(16)	1.408(4)

C(13)-C(15)#1	1.526(15)	C(11)-C(12)	1.427(4)
C(14)-H(14A)	0.96	C(12)-C(13)	1.403(4)
C(14)-H(14B)	0.96	C(12)-C(17)	1.489(4)
C(14)-H(14C)	0.96	C(13)-C(14)	1.394(4)
C(15)-H(15A)	0.96	C(13)-C(27)	1.492(4)
C(15)-H(15B)	0.96	C(14)-C(15)	1.389(4)
C(15)-H(15C)	0.96	C(14)-H(14)	0.93
C(16)-H(16A)	0.96	C(15)-C(16)	1.413(4)
C(16)-H(16B)	0.96	C(15)-C(33)	1.485(4)
C(16)-H(16C)	0.96	C(16)-C(5)#1	1.471(4)
C(17)-C(22)	1.411(5)	C(17)-C(22)	1.385(4)
C(17)-C(18)	1.428(5)	C(17)-C(18)	1.386(4)
C(18)-C(19)	1.388(5)	C(18)-C(19)	1.372(5)
C(18)-C(23)	1.502(5)	C(18)-H(18)	0.93
C(19)-C(20)	1.397(5)	C(19)-C(20)	1.365(5)
C(19)-C(31)	1.494(6)	C(19)-H(19)	0.93
C(20)-C(21)	1.375(5)	C(20)-C(21)	1.373(5)
C(20)-H(20)	0.93	C(20)-C(23)	1.581(9)
C(21)-C(22)	1.426(5)	C(21)-C(22)	1.381(4)
C(21)-C(37)	1.487(5)	C(21)-H(21)	0.93
C(23)-C(28)	1.380(5)	C(22)-H(22)	0.93
C(23)-C(24)	1.391(6)	C(23)-F(25A)	0.909(19)
C(24)-C(25)	1.376(6)	C(23)-F(26A)	1.172(14)
C(24)-H(24)	0.93	C(23)-F(26)	1.246(10)
C(25)-C(26)	1.376(6)	C(23)-F(24)	1.257(13)
C(25)-H(25)	0.93	C(23)-F(24A)	1.438(17)
C(26)-C(27)	1.375(7)	C(23)-F(25)	1.658(18)
C(26)-O(29)	1.384(5)	F(25A)-F(26A)	1.40(3)
C(27)-C(28)	1.386(6)	C(27)-C(32)	1.370(4)
C(27)-H(27)	0.93	C(27)-C(28)	1.392(4)
C(28)-H(28)	0.93	C(28)-C(29)	1.383(4)
O(29)-C(30)	1.410(7)	C(28)-H(28)	0.93
C(30)-H(30A)	0.96	C(29)-C(30)	1.365(5)
C(30)-H(30B)	0.96	C(29)-H(29)	0.93
C(30)-H(30C)	0.96	C(30)-C(31)	1.366(5)
C(31)-C(36)	1.376(6)	C(30)-H(30)	0.93
C(31)-C(32)	1.378(6)	C(31)-C(32)	1.391(4)
C(32)-C(33)	1.387(7)	C(31)-H(31)	0.93
C(32)-H(32)	0.93	C(32)-H(32)	0.93

C(33)-C(34)	1.358(8)	C(33)-C(34)	1.386(4)
C(33)-H(33)	0.93	C(33)-C(38)	1.396(4)
C(34)-C(35)	1.359(9)	C(34)-C(35)	1.386(4)
C(34)-H(34)	0.93	C(34)-H(34)	0.93
C(35)-C(36)	1.369(7)	C(35)-C(36)	1.360(5)
C(35)-H(35)	0.93	C(35)-H(35)	0.93
C(36)-H(36)	0.93	C(36)-C(37)	1.382(5)
C(37)-C(42)	1.389(6)	C(36)-C(39)	1.489(6)
C(37)-C(38)	1.396(6)	C(37)-C(38)	1.371(4)
C(38)-C(39)	1.405(7)	C(37)-H(37)	0.93
C(38)-H(38)	0.93	C(38)-H(38)	0.93
C(39)-C(40)	1.345(8)	C(39)-F(41A)	1.22(2)
C(39)-H(39)	0.93	C(39)-F(42)	1.247(9)
C(40)-O(43)	1.370(7)	C(39)-F(41)	1.253(11)
C(40)-C(41)	1.373(8)	C(39)-F(42A)	1.283(15)
C(41)-C(42)	1.381(6)	C(39)-F(40)	1.378(9)
C(41)-H(41)	0.93	C(39)-F(40A)	1.59(2)
C(42)-H(42)	0.93		
O(43)-C(44A)	1.094(15)	C(6)-C(1)-C(2)	117.9(3)
O(43)-C(44)	1.105(15)	C(6)-C(1)-C(7)	122.0(3)
C(44)-H(44A)	0.96	C(2)-C(1)-C(7)	120.1(3)
C(44)-H(44B)	0.96	C(3)-C(2)-C(1)	123.4(3)
C(44)-H(44C)	0.96	C(3)-C(2)-H(2)	118.3
C(44A)-H(44D)	0.96	C(1)-C(2)-H(2)	118.3
C(44A)-H(44E)	0.96	C(2)-C(3)-C(4)	117.5(2)
C(44A)-H(44F)	0.96	C(2)-C(3)-C(11)	123.2(2)
O(45)-C(49)	1.317(12)	C(4)-C(3)-C(11)	118.6(2)
O(45)-C(46)	1.407(11)	C(5)-C(4)-C(3)	120.4(2)
C(46)-C(48)	1.386(11)	C(5)-C(4)-C(4)#1	119.0(3)
C(46)-C(47)	1.467(14)	C(3)-C(4)-C(4)#1	120.6(3)
C(46)-H(46)	0.98	C(6)-C(5)-C(4)	118.3(2)
C(47)-H(47A)	0.96	C(6)-C(5)-C(16)#1	122.6(3)
C(47)-H(47B)	0.96	C(4)-C(5)-C(16)#1	118.9(2)
C(47)-H(47C)	0.96	C(1)-C(6)-C(5)	122.4(3)
C(48)-H(48A)	0.96	C(1)-C(6)-H(6)	118.8
C(48)-H(48B)	0.96	C(5)-C(6)-H(6)	118.8
C(48)-H(48C)	0.96	C(9)-C(7)-C(10)	111.7(7)
C(49)-C(50)	1.446(15)	C(8A)-C(7)-C(9A)	116.6(6)
C(49)-C(51)	1.490(13)	C(9)-C(7)-C(1)	114.6(5)

C(49)-H(49)	0.98
C(50)-H(50A)	0.96
C(50)-H(50B)	0.96
C(50)-H(50C)	0.96
C(51)-H(51A)	0.96
C(51)-H(51B)	0.96
C(51)-H(51C)	0.96

C(2)#1-C(1)-C(2)	116.8(5)
C(2)#1-C(1)-C(9)	121.6(2)
C(2)-C(1)-C(9)	121.6(2)
C(1)-C(2)-C(3)	123.5(4)
C(1)-C(2)-H(2)	118.2
C(3)-C(2)-H(2)	118.2
C(2)-C(3)-C(4)	117.7(3)
C(2)-C(3)-C(22)	123.3(3)
C(4)-C(3)-C(22)	118.6(3)
C(3)#1-C(4)-C(3)	120.7(4)
C(3)#1-C(4)-C(5)	119.6(2)
C(3)-C(4)-C(5)	119.6(2)
C(6)-C(5)-C(6)#1	121.2(4)
C(6)-C(5)-C(4)	119.4(2)
C(6)#1-C(5)-C(4)	119.4(2)
C(7)-C(6)-C(5)	117.7(3)
C(7)-C(6)-C(17)	122.6(3)
C(5)-C(6)-C(17)	119.2(3)
C(8)-C(7)-C(6)	123.0(4)
C(8)-C(7)-H(7)	118.5
C(6)-C(7)-H(7)	118.5
C(7)-C(8)-C(7)#1	117.2(5)
C(7)-C(8)-C(13)	121.4(2)
C(7)#1-C(8)-C(13)	121.4(2)
C(10)#1-C(9)-C(10)	129.7(10)
C(10)-C(9)-C(12)	118.7(7)
C(10)#1-C(9)-C(12)#1	118.7(7)
C(12)-C(9)-C(12)#1	138.2(11)
C(10)#1-C(9)-C(1)	115.1(5)
C(10)-C(9)-C(1)	115.1(5)
C(12)-C(9)-C(1)	110.9(6)
C(8A)-C(7)-C(1)	112.6(4)
C(10)-C(7)-C(1)	109.9(5)
C(9A)-C(7)-C(1)	109.3(5)
C(8A)-C(7)-C(10A)	102.9(6)
C(9A)-C(7)-C(10A)	108.4(6)
C(1)-C(7)-C(10A)	106.3(4)
C(9)-C(7)-C(8)	110.0(6)
C(10)-C(7)-C(8)	101.1(6)
C(1)-C(7)-C(8)	108.7(4)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(8A)-H(8A1)	109.5
C(7)-C(8A)-H(8A2)	109.5
H(8A1)-C(8A)-H(8A2)	109.5
C(7)-C(8A)-H(8A3)	109.5
H(8A1)-C(8A)-H(8A3)	109.5
H(8A2)-C(8A)-H(8A3)	109.5
C(7)-C(9A)-H(9A1)	109.5
C(7)-C(9A)-H(9A2)	109.5
H(9A1)-C(9A)-H(9A2)	109.5
C(7)-C(9A)-H(9A3)	109.5
H(9A1)-C(9A)-H(9A3)	109.5
H(9A2)-C(9A)-H(9A3)	109.5

C(12)#1-C(9)-C(1)	110.9(6)
C(10)-C(9)-C(11)	108.1(8)
C(12)-C(9)-C(11)	95.7(8)
C(1)-C(9)-C(11)	105.7(6)
C(10)#1-C(9)-C(11)#1	108.1(8)
C(12)#1-C(9)-C(11)#1	95.7(8)
C(1)-C(9)-C(11)#1	105.7(6)
C(11)-C(9)-C(11)#1	148.7(13)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(16)-C(13)-C(16)#1	129.9(10)
C(16)#1-C(13)-C(14)#1	114.5(7)
C(16)-C(13)-C(14)	114.5(7)
C(14)#1-C(13)-C(14)	129.0(10)
C(16)-C(13)-C(8)	115.1(5)
C(16)#1-C(13)-C(8)	115.1(5)
C(14)#1-C(13)-C(8)	115.5(5)
C(14)-C(13)-C(8)	115.5(5)
C(16)-C(13)-C(15)	100.2(9)
C(14)-C(13)-C(15)	104.4(9)
C(8)-C(13)-C(15)	104.7(8)
C(16)#1-C(13)-C(15)#1	100.2(9)
C(14)#1-C(13)-C(15)#1	104.4(9)
C(7)-C(10A)-H(10D)	109.5
C(7)-C(10A)-H(10E)	109.5
H(10D)-C(10A)-H(10E)	109.5
C(7)-C(10A)-H(10F)	109.5
H(10D)-C(10A)-H(10F)	109.5
H(10E)-C(10A)-H(10F)	109.5
C(16)-C(11)-C(12)	119.1(2)
C(16)-C(11)-C(3)	117.2(2)
C(12)-C(11)-C(3)	123.4(2)
C(13)-C(12)-C(11)	119.0(3)
C(13)-C(12)-C(17)	119.8(2)
C(11)-C(12)-C(17)	121.2(3)
C(14)-C(13)-C(12)	119.1(2)
C(14)-C(13)-C(27)	117.5(3)
C(12)-C(13)-C(27)	123.4(3)
C(15)-C(14)-C(13)	122.0(3)
C(15)-C(14)-H(14)	119
C(13)-C(14)-H(14)	119
C(14)-C(15)-C(16)	118.5(3)
C(14)-C(15)-C(33)	118.0(3)
C(16)-C(15)-C(33)	123.1(3)
C(11)-C(16)-C(15)	118.9(2)
C(11)-C(16)-C(5)#1	118.4(2)
C(15)-C(16)-C(5)#1	122.7(2)
C(22)-C(17)-C(18)	118.2(3)
C(22)-C(17)-C(12)	121.6(3)
C(18)-C(17)-C(12)	120.1(3)
C(19)-C(18)-C(17)	120.8(3)
C(19)-C(18)-H(18)	119.6
C(17)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	120.4(4)
C(20)-C(19)-H(19)	119.8
C(18)-C(19)-H(19)	119.8
C(19)-C(20)-C(21)	120.0(4)
C(19)-C(20)-C(23)	125.0(5)
C(21)-C(20)-C(23)	114.8(5)
C(20)-C(21)-C(22)	119.9(3)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1

C(8)-C(13)-C(15)#1	104.7(8)	C(21)-C(22)-C(17)	120.7(3)
C(15)-C(13)-C(15)#1	150.6(16)	C(21)-C(22)-H(22)	119.7
C(13)-C(14)-H(14A)	109.5	C(17)-C(22)-H(22)	119.7
C(13)-C(14)-H(14B)	109.5	F(25A)-C(23)-F(26A)	84(2)
H(14A)-C(14)-H(14B)	109.5	F(26)-C(23)-F(24)	135.1(13)
C(13)-C(14)-H(14C)	109.5	F(25A)-C(23)-F(24A)	130(3)
H(14A)-C(14)-H(14C)	109.5	F(26A)-C(23)-F(24A)	105.6(17)
H(14B)-C(14)-H(14C)	109.5	F(25A)-C(23)-C(20)	112(2)
C(13)-C(15)-H(15A)	109.5	F(26A)-C(23)-C(20)	112.6(11)
C(13)-C(15)-H(15B)	109.5	F(26)-C(23)-C(20)	113.4(7)
H(15A)-C(15)-H(15B)	109.5	F(24)-C(23)-C(20)	106.9(8)
C(13)-C(15)-H(15C)	109.5	F(24A)-C(23)-C(20)	109.1(7)
H(15A)-C(15)-H(15C)	109.5	F(26)-C(23)-F(25)	91.1(12)
H(15B)-C(15)-H(15C)	109.5	F(24)-C(23)-F(25)	102.5(13)
C(13)-C(16)-H(16A)	109.5	C(20)-C(23)-F(25)	97.7(9)
C(13)-C(16)-H(16B)	109.5	C(32)-C(27)-C(28)	118.3(3)
H(16A)-C(16)-H(16B)	109.5	C(32)-C(27)-C(13)	120.6(3)
C(13)-C(16)-H(16C)	109.5	C(28)-C(27)-C(13)	121.0(3)
H(16A)-C(16)-H(16C)	109.5	C(29)-C(28)-C(27)	119.8(3)
H(16B)-C(16)-H(16C)	109.5	C(29)-C(28)-H(28)	120.1
C(22)-C(17)-C(18)	119.5(3)	C(27)-C(28)-H(28)	120.1
C(22)-C(17)-C(6)	117.0(3)	C(30)-C(29)-C(28)	121.0(4)
C(18)-C(17)-C(6)	123.3(3)	C(30)-C(29)-H(29)	119.5
C(19)-C(18)-C(17)	118.5(3)	C(28)-C(29)-H(29)	119.5
C(19)-C(18)-C(23)	120.4(3)	C(29)-C(30)-C(31)	120.1(3)
C(17)-C(18)-C(23)	121.0(3)	C(29)-C(30)-H(30)	120
C(18)-C(19)-C(20)	119.2(4)	C(31)-C(30)-H(30)	120
C(18)-C(19)-C(31)	122.8(4)	C(30)-C(31)-C(32)	119.1(4)
C(20)-C(19)-C(31)	118.0(3)	C(30)-C(31)-H(31)	120.4
C(21)-C(20)-C(19)	123.4(4)	C(32)-C(31)-H(31)	120.4
C(21)-C(20)-H(20)	118.3	C(27)-C(32)-C(31)	121.8(3)
C(19)-C(20)-H(20)	118.3	C(27)-C(32)-H(32)	119.1
C(20)-C(21)-C(22)	117.2(4)	C(31)-C(32)-H(32)	119.1
C(20)-C(21)-C(37)	118.8(3)	C(34)-C(33)-C(38)	117.9(3)
C(22)-C(21)-C(37)	123.7(3)	C(34)-C(33)-C(15)	121.4(3)
C(17)-C(22)-C(21)	118.9(3)	C(38)-C(33)-C(15)	120.7(3)
C(17)-C(22)-C(3)	117.8(3)	C(33)-C(34)-C(35)	120.1(3)
C(21)-C(22)-C(3)	123.1(3)	C(33)-C(34)-H(34)	119.9
C(28)-C(23)-C(24)	117.7(4)	C(35)-C(34)-H(34)	119.9

C(28)-C(23)-C(18)	122.3(4)
C(24)-C(23)-C(18)	120.0(3)
C(25)-C(24)-C(23)	121.4(4)
C(25)-C(24)-H(24)	119.3
C(23)-C(24)-H(24)	119.3
C(26)-C(25)-C(24)	119.7(4)
C(26)-C(25)-H(25)	120.1
C(24)-C(25)-H(25)	120.1
C(27)-C(26)-C(25)	120.3(4)
C(27)-C(26)-O(29)	124.5(5)
C(25)-C(26)-O(29)	115.3(5)
C(26)-C(27)-C(28)	119.4(4)
C(26)-C(27)-H(27)	120.3
C(28)-C(27)-H(27)	120.3
C(23)-C(28)-C(27)	121.5(4)
C(23)-C(28)-H(28)	119.2
C(27)-C(28)-H(28)	119.2
C(26)-O(29)-C(30)	117.6(5)
O(29)-C(30)-H(30A)	109.5
O(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
O(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(36)-C(31)-C(32)	117.9(4)
C(36)-C(31)-C(19)	119.7(4)
C(32)-C(31)-C(19)	122.4(4)
C(31)-C(32)-C(33)	120.4(5)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(34)-C(33)-C(32)	120.6(6)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7
C(33)-C(34)-C(35)	119.3(5)
C(33)-C(34)-H(34)	120.3
C(35)-C(34)-H(34)	120.3
C(34)-C(35)-C(36)	120.7(6)
C(34)-C(35)-H(35)	119.6
C(36)-C(35)-H(35)	119.6
C(36)-C(35)-C(34)	121.4(3)
C(36)-C(35)-H(35)	119.3
C(34)-C(35)-H(35)	119.3
C(35)-C(36)-C(37)	119.2(3)
C(35)-C(36)-C(39)	121.5(4)
C(37)-C(36)-C(39)	119.3(4)
C(38)-C(37)-C(36)	120.2(3)
C(38)-C(37)-H(37)	119.9
C(36)-C(37)-H(37)	119.9
C(37)-C(38)-C(33)	121.2(3)
C(37)-C(38)-H(38)	119.4
C(33)-C(38)-H(38)	119.4
F(42)-C(39)-F(41)	106.4(10)
F(41A)-C(39)-F(42A)	117.8(15)
F(42)-C(39)-F(40)	103.6(8)
F(41)-C(39)-F(40)	106.3(10)
F(41A)-C(39)-C(36)	116.0(11)
F(42)-C(39)-C(36)	113.8(6)
F(41)-C(39)-C(36)	116.1(8)
F(42A)-C(39)-C(36)	115.4(7)
F(40)-C(39)-C(36)	109.7(5)
F(41A)-C(39)-F(40A)	110(3)
F(42A)-C(39)-F(40A)	93.5(14)
C(36)-C(39)-F(40A)	99.4(9)

C(35)-C(36)-C(31)	121.1(5)
C(35)-C(36)-H(36)	119.4
C(31)-C(36)-H(36)	119.4
C(42)-C(37)-C(38)	117.1(4)
C(42)-C(37)-C(21)	121.9(4)
C(38)-C(37)-C(21)	120.9(4)
C(37)-C(38)-C(39)	119.8(5)
C(37)-C(38)-H(38)	120.1
C(39)-C(38)-H(38)	120.1
C(40)-C(39)-C(38)	121.3(5)
C(40)-C(39)-H(39)	119.3
C(38)-C(39)-H(39)	119.3
C(39)-C(40)-O(43)	117.1(7)
C(39)-C(40)-C(41)	119.9(5)
O(43)-C(40)-C(41)	123.0(8)
C(40)-C(41)-C(42)	119.7(5)
C(40)-C(41)-H(41)	120.1
C(42)-C(41)-H(41)	120.2
C(41)-C(42)-C(37)	122.2(5)
C(41)-C(42)-H(42)	118.9
C(37)-C(42)-H(42)	118.9
C(44A)-O(43)-C(44)	87.1(13)
C(44A)-O(43)-C(40)	123.7(15)
C(44)-O(43)-C(40)	148.9(18)
O(43)-C(44)-H(44A)	109.5
O(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
O(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
O(43)-C(44A)-H(44D)	109.5
O(43)-C(44A)-H(44E)	109.5
H(44D)-C(44A)-H(44E)	109.5
O(43)-C(44A)-H(44F)	109.5
H(44D)-C(44A)-H(44F)	109.5
H(44E)-C(44A)-H(44F)	109.5
C(49)-O(45)-C(46)	117.1(9)
C(48)-C(46)-O(45)	108.4(11)
C(48)-C(46)-C(47)	119.0(12)

O(45)-C(46)-C(47)	105.8(11)	
C(48)-C(46)-H(46)	107.7	
O(45)-C(46)-H(46)	107.7	
C(47)-C(46)-H(46)	107.7	
C(46)-C(47)-H(47A)	109.5	
C(46)-C(47)-H(47B)	109.5	
H(47A)-C(47)-H(47B)	109.5	
C(46)-C(47)-H(47C)	109.5	
H(47A)-C(47)-H(47C)	109.5	
H(47B)-C(47)-H(47C)	109.5	
C(46)-C(48)-H(48A)	109.5	
C(46)-C(48)-H(48B)	109.5	
H(48A)-C(48)-H(48B)	109.5	
C(46)-C(48)-H(48C)	109.5	
H(48A)-C(48)-H(48C)	109.5	
H(48B)-C(48)-H(48C)	109.5	
O(45)-C(49)-C(50)	113.4(14)	
O(45)-C(49)-C(51)	106.0(11)	
C(50)-C(49)-C(51)	109.4(13)	
O(45)-C(49)-H(49)	109.3	
C(50)-C(49)-H(49)	109.3	
C(51)-C(49)-H(49)	109.3	
C(49)-C(50)-H(50A)	109.5	
C(49)-C(50)-H(50B)	109.5	
H(50A)-C(50)-H(50B)	109.5	
C(49)-C(50)-H(50C)	109.5	
H(50A)-C(50)-H(50C)	109.5	
H(50B)-C(50)-H(50C)	109.5	
C(49)-C(51)-H(51A)	109.5	
C(49)-C(51)-H(51B)	109.5	
H(51A)-C(51)-H(51B)	109.5	
C(49)-C(51)-H(51C)	109.5	
H(51A)-C(51)-H(51C)	109.5	
H(51B)-C(51)-H(51C)	109.5	

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2 for ***cis*-5**

#1 -x+1,y,-z+1/2 for ***trans*-7**

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ***cis*-5** and ***trans*-7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	Crystal *cis*-5							**Crystal *trans*-7**					
	U11	U22	U33	U23	U13	U12		U11	U22	U33	U23	U13	U12
C(1)	105(5)	48(3)	59(4)	0	22(3)	0	C(1)	62(2)	78(2)	33(2)	3(2)	19(2)	1(2)
C(2)	94(3)	46(2)	57(3)	6(2)	21(2)	1(2)	C(2)	53(2)	73(2)	31(2)	3(1)	14(1)	-2(1)
C(3)	65(3)	45(2)	52(2)	2(2)	12(2)	1(2)	C(3)	44(2)	52(2)	34(2)	1(1)	13(1)	0(1)
C(4)	65(4)	48(3)	47(3)	0	9(3)	0	C(4)	47(2)	48(2)	30(1)	2(1)	12(1)	-1(1)
C(5)	62(3)	41(3)	49(3)	0	11(3)	0	C(5)	46(2)	58(2)	33(2)	0(1)	12(1)	-1(1)
C(6)	66(2)	46(2)	44(2)	-1(2)	12(2)	-3(2)	C(6)	50(2)	82(2)	36(2)	2(2)	20(1)	1(2)
C(7)	79(3)	46(2)	50(2)	-3(2)	7(2)	-3(2)	C(7)	63(2)	138(4)	38(2)	2(2)	26(2)	3(2)
C(8)	85(4)	46(3)	63(4)	0	14(3)	0	C(8)	105	124	68(5)	-11(6)	41(4)	45(5)
C(9)	172(8)	51(4)	66(4)	0	30(5)	0	C(9)	130(8)	121	30(4)	2(6)	29(5)	30(6)
C(13)	114(6)	59(4)	63(4)	0	-4(4)	0	C(10)	114	129	75(6)	14(6)	39(6)	-7(7)
C(17)	67(2)	46(2)	48(2)	-2(2)	14(2)	-3(2)	C(8A)	142(8)	124	58(5)	10(5)	56(5)	28(6)
C(18)	70(3)	51(2)	47(2)	-1(2)	13(2)	-2(2)	C(9A)	106	130	82(7)	-45(6)	49(5)	-28(6)
C(19)	68(3)	63(2)	47(2)	-1(2)	10(2)	-2(2)	C(10A)	180(10)	101	68(5)	46(4)	69(6)	38(6)
C(20)	74(3)	69(3)	48(2)	6(2)	14(2)	-2(2)	C(11)	45(2)	52(2)	33(2)	-6(1)	12(1)	-1(1)
C(21)	65(3)	59(2)	49(2)	5(2)	12(2)	3(2)	C(12)	52(2)	49(2)	37(2)	-3(1)	12(1)	0(1)
C(22)	65(3)	51(2)	50(2)	0(2)	8(2)	1(2)	C(13)	48(2)	59(2)	42(2)	-3(2)	8(1)	5(1)
C(23)	69(3)	55(2)	48(2)	-1(2)	7(2)	-2(2)	C(14)	45(2)	69(2)	49(2)	1(2)	15(2)	-1(1)
C(24)	85(3)	62(3)	70(3)	-10(2)	23(3)	-12(2)	C(15)	51(2)	59(2)	42(2)	0(2)	18(1)	0(1)
C(25)	85(3)	85(3)	96(4)	-6(3)	35(3)	-22(3)	C(16)	43(2)	57(2)	36(2)	-5(1)	15(1)	1(1)
C(26)	94(4)	71(3)	97(4)	0(3)	15(3)	-28(3)	C(17)	59(2)	54(2)	39(2)	3(2)	9(1)	5(1)
C(27)	104(4)	67(3)	70(3)	-17(2)	7(3)	-21(3)	C(18)	90(3)	64(2)	59(2)	-1(2)	18(2)	-10(2)
C(28)	83(3)	69(3)	57(3)	-14(2)	10(2)	-11(2)	C(19)	132(4)	74(3)	86(3)	11(2)	27(3)	-32(2)
O(29)	128(3)	90(3)	159(4)	-10(2)	43(3)	-53(2)	C(20)	133(4)	83(3)	73(3)	32(3)	15(3)	-20(3)
C(30)	208(8)	83(4)	177(7)	-4(4)	19(6)	-75(5)	C(21)	104(3)	103(3)	41(2)	17(2)	4(2)	-3(2)
C(31)	71(3)	70(3)	52(3)	2(2)	11(2)	-9(2)	C(22)	65(2)	69(2)	41(2)	1(2)	7(2)	-7(2)
C(32)	82(4)	105(4)	81(4)	-8(3)	8(3)	-7(3)	C(23)	120	104	229(9)	70(6)	34(6)	-9(5)
C(33)	84(4)	132(5)	95(5)	3(4)	-18(4)	-22(3)	F(24)	232(10)	224	210(11)	141(9)	137(9)	57(7)
C(34)	122(6)	157(6)	63(4)	0(4)	-10(4)	-54(4)	F(25)	352(16)	126(6)	249(11)	128(8)	101(10)	34(9)
C(35)	127(6)	208(7)	65(4)	-44(4)	14(4)	-37(5)	F(26)	203	238(12)	74(4)	96(5)	-29(4)	-64(7)
C(36)	81(3)	172(5)	55(3)	-29(3)	13(3)	-14(3)	F(24A)	470(30)	161(12)	145(10)	26(8)	195(16)	-24(13)
C(37)	84(3)	57(2)	48(2)	0(2)	17(2)	-5(2)	F(25A)	270	257	470(50)	240(20)	190(20)	167(10)

C(38)	106(4)	67(3)	66(3)	15(2)	8(3)	-4(3)
C(39)	147(6)	66(3)	86(4)	21(3)	28(4)	-17(3)
C(40)	124(5)	85(4)	97(4)	-7(3)	43(4)	-48(4)
C(41)	88(4)	90(4)	97(4)	-12(3)	31(3)	-24(3)
C(42)	77(3)	77(3)	71(3)	1(2)	17(3)	-4(2)
O(43)	166	172(5)	199(6)	-23(5)	77(5)	-93(4)
C(44)	240(20)	102(10)	310(30)	61(13)	160(20)	-37(12)
C(44A)	107(11)	162(14)	143(13)	62(11)	38(10)	-2(10)
O(45)	128(5)	181(7)	403(12)	40(7)	36(6)	-10(5)
C(46)	168(10)	143(8)	256(15)	23(8)	5(10)	23(7)
C(47)	220(11)	235(12)	210(11)	-30(9)	80(9)	-69(9)
C(48)	216(13)	324(17)	224(13)	-8(11)	-7(11)	71(11)
C(49)	137(9)	201(11)	341(18)	-88(11)	10(10)	-19(8)
C(50)	283(18)	295(17)	327(19)	-74(14)	-54(16)	-15(14)
C(51)	252(16)	440(30)	373	-191(18)	-28(15)	76(17)

F(26A)	259	97(9)	158(9)	73(9)	59(13)	-26(10)
C(27)	55(2)	58(2)	50(2)	1(2)	12(2)	8(2)
C(28)	73(2)	66(2)	80(3)	0(2)	6(2)	10(2)
C(29)	77(3)	78(3)	100(3)	10(2)	0(2)	21(2)
C(30)	69(3)	109(3)	89(3)	-1(3)	-7(2)	21(2)
C(31)	63(2)	90(3)	90(3)	-9(2)	0(2)	4(2)
C(32)	58(2)	63(2)	74(2)	-6(2)	2(2)	3(2)
C(33)	50(2)	71(2)	39(2)	-1(2)	15(1)	-4(2)
C(34)	61(2)	81(2)	63(2)	8(2)	29(2)	3(2)
C(35)	77(2)	94(3)	72(2)	9(2)	44(2)	-6(2)
C(36)	89(3)	73(2)	69(2)	12(2)	37(2)	0(2)
C(37)	92(3)	76(2)	67(2)	13(2)	33(2)	9(2)
C(38)	62(2)	75(2)	61(2)	3(2)	25(2)	7(2)
C(39)	140(6)	110(5)	108(5)	32(4)	72(4)	2(4)
F(40)	218(10)	173(6)	80(4)	42(4)	51(5)	-1(6)
F(41)	292(15)	79(4)	175(8)	54(4)	129(8)	23(5)
F(42)	157(7)	243(17)	157	100(9)	83(8)	-12(8)
F(40A)	230	214(15)	152(15)	4(12)	60(13)	-116(11)
F(41A)	250(20)	254	240(30)	199(19)	190(20)	170(19)
F(42A)	210(30)	116(9)	74(9)	25(7)	85(14)	39(12)

D. Reference

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