Electronic Supplementary Information

for

Sumanene-stacked supramolecular polymers. Dynamic, solvation-directed control

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Experimental Procedures

Instruments. UV/vis spectra were measured using a JASCO V-560 or -650 spectrometer with a temperature controller. Fluorescence spectra were recorded using an FP-8500 spectrometer equipped with a temperature controller. All solutions were measured in a quartz cell (path lengths of 1, 2, 5, or 10 mm) or a high-pressure cell (path length of 2 mm). Atomic force microscopy (AFM) images were obtained using a Shimadzu SPM-9700HT microscope. Hydrostatic pressure measurements were performed using a custom-built high-pressure apparatus, the details of which have been reported previously.[1] Variable-temperature measurements were performed using a UNISOKU CoolSpek cryostat.

Materials. Spectroscopy grade MCH and CH_2Cl_2 were used. A commercially available highly oriented pyrolytic graphite (HOPG) substrate was used without further treatment. **Sumanene** was synthesized according to literature.[2]

AFM measurements. A solution of **sumanene** was dropped onto an HOPG surface, pre-dried by N_2 gas flow and then fully dried under high vacuum, prior to observation by AFM.

Spectroscopic measurements. For the spectral analysis, a smoothing process was performed using MATLAB. Specifically, a range of 340–400 nm was extracted from the raw data and then converted to applicable extinction coefficients by smoothing, using the "smoothing spline" method (a smoothing parameter of $5.614035861113226 \times 10^{-6}$).

Computational studies. The density functional theory (DFT) calculations were performed using the long-range and dispersion-corrected ωB97X-D functional[3] with 6-311G** basis sets.[4] All calculations were performed using the Gaussian 16.[5]

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[1] H. Mizuno, G. Fukuhara, *Acc. Chem. Res.* **2022**, *55*, 1748-1762.
[2] H. Sakurai, T. Daiko, T. Hirao, *Science* **2003**, *301*, 1878.
[3] J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys*. **2008**, *10*, 6615-6620.
[4] R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys*. **1980**, *72*, 650-654.
[5] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc. **2016**, Wallingford CT.

SAXS measurements. Small-angle X-ray scattering (SAXS) measurements were performed at the BL-6A beamline[6,7] at the Photon Factory of the High Energy Accelerator Research Organization (KEK) in Tsukuba, Japan. The **sumanene** solution was loaded into a custom-built aluminum cell sealed with polypropylene films. The optical path length is set to 18 mm. Because of its strong absorption of X-rays, CH_2Cl_2 was not used in the SAXS measurements. X-ray wavelength of 1.5 Å and a sample-detector distance of 523 mm (calibrated using silver behenate) gave a detectable *q* range of the order of 0.2 to 9.7 nm^{-1}. All data were analyzed using the SAngler software package.[8]

Variable temperature measurements. The measured temperature was decreased from 60 °C to -50 °C at -1 °C/min. To prevent frost, the cell chamber in the spectrometer was replaced with Ar, and a cell containing the **sumanene** solution was inserted and measured. Dry air flowed continuously during the measurements. However, accurate data could not be obtained below 0 °C due to the frost effect.

High-pressure measurements. Since the optical path length is fixed at 2 mm in the high-pressure cell, a 7:3 (v/v) MCH-CH_2Cl_2 mixture was used from the viewpoint of extinction coefficient.

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[6] N. Shimizu, T. Mori, N. Igarashi, H. Ohta, Y. Nagatani, T. Kosuge, K. Ito, *J. Phys.: Conf. Ser.* **2013**, *425*, 202008.

[7] H. Takagi, N. Igarashi, T. Mori, S. Saijo, H. Ohta, Y. Nagatani, T. Kosuge, N. Shimizu, *AIP Conf. Proc.* **2016**, *1741*, 030018.

[8] N. Shimizu, K. Yatabe, Y. Nagatani, S. Saijyo, T. Kosuge, N. Igarashi, *AIP Conf. Proc.* **2016**, *1741*, 050017.

AFM measurements

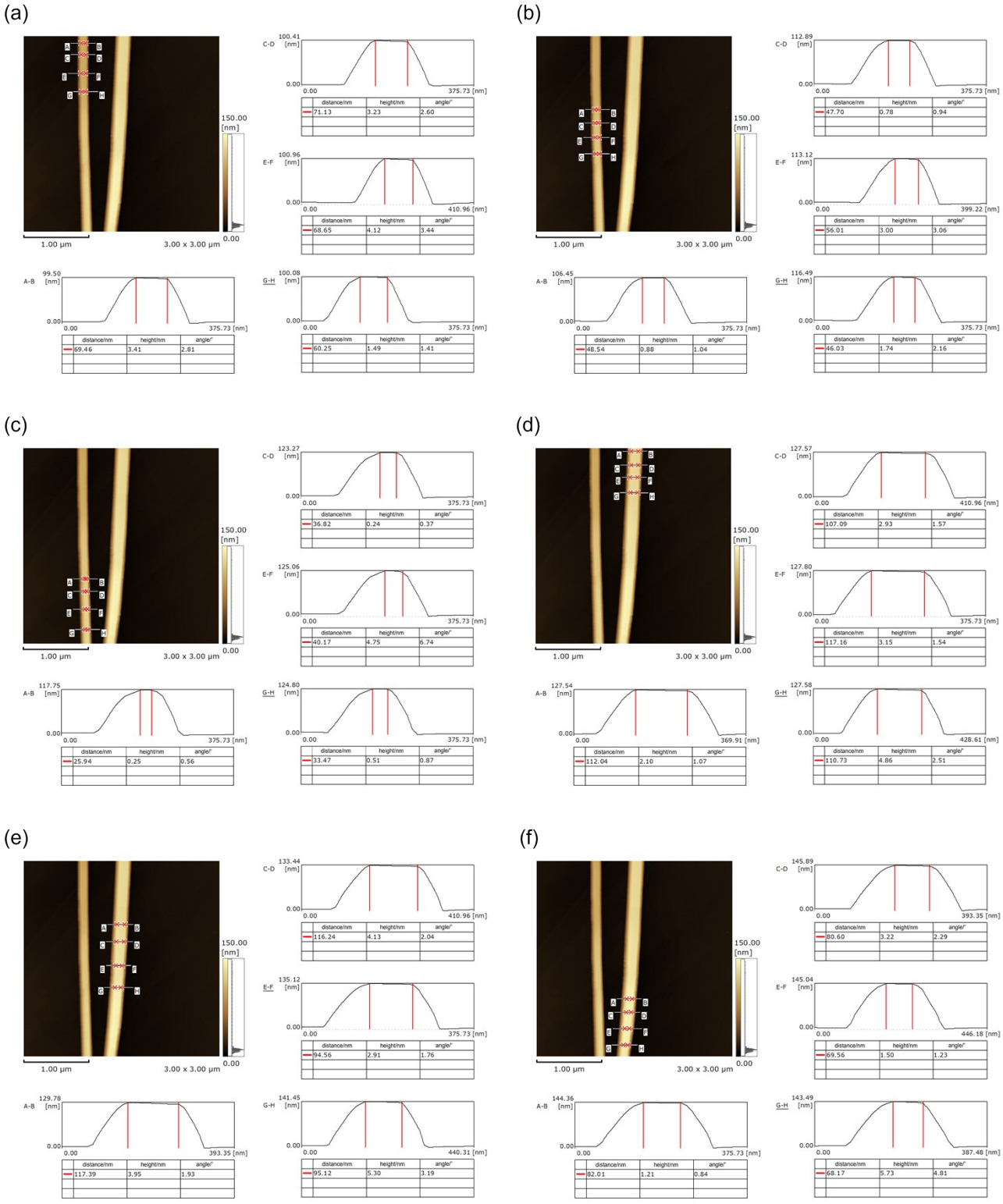

Figure S1. (a)-(f) AFM images and line profiles of **sumanene** (1.95 mM) prepared from the MCH solution on an HOPG surface.

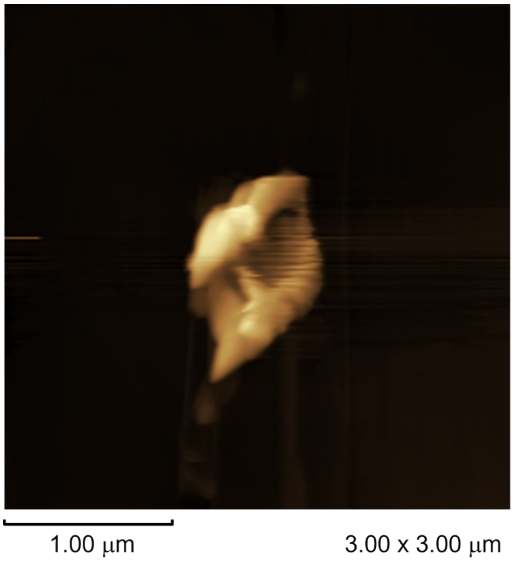

Figure S2. AFM image of **sumanene** (95.3 μM) prepared from the MCH solution on an HOPG surface.

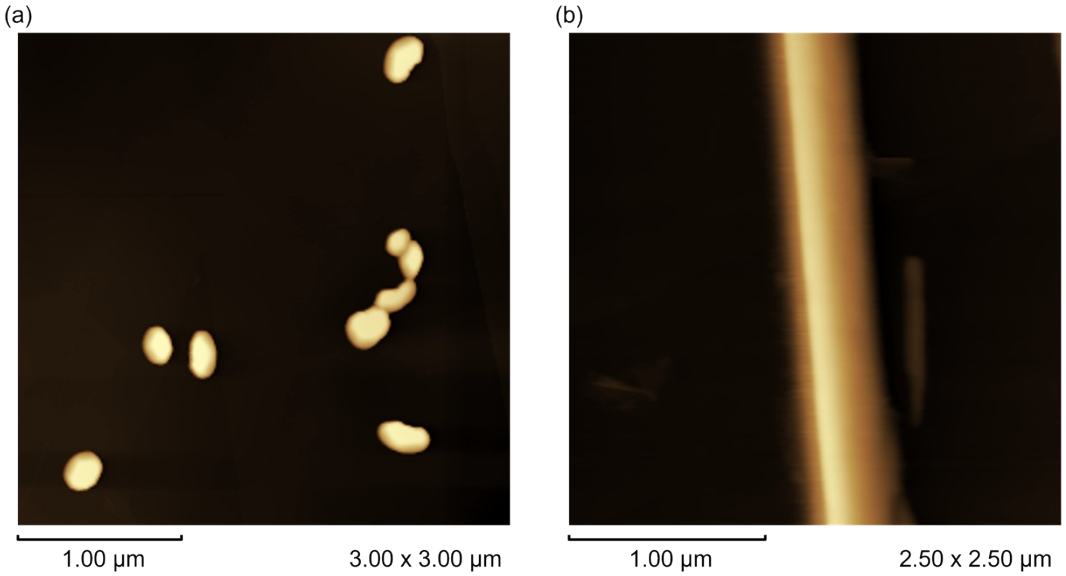

Figure S3. AFM images of **sumanene** ((a) 2.08 mM and (b) 34.3 mM) prepared from the CH_2Cl_2 solution on an HOPG surface. (b) width, 286.7 ± 68.4 nm; height, 43.7 ± 30.7 nm.

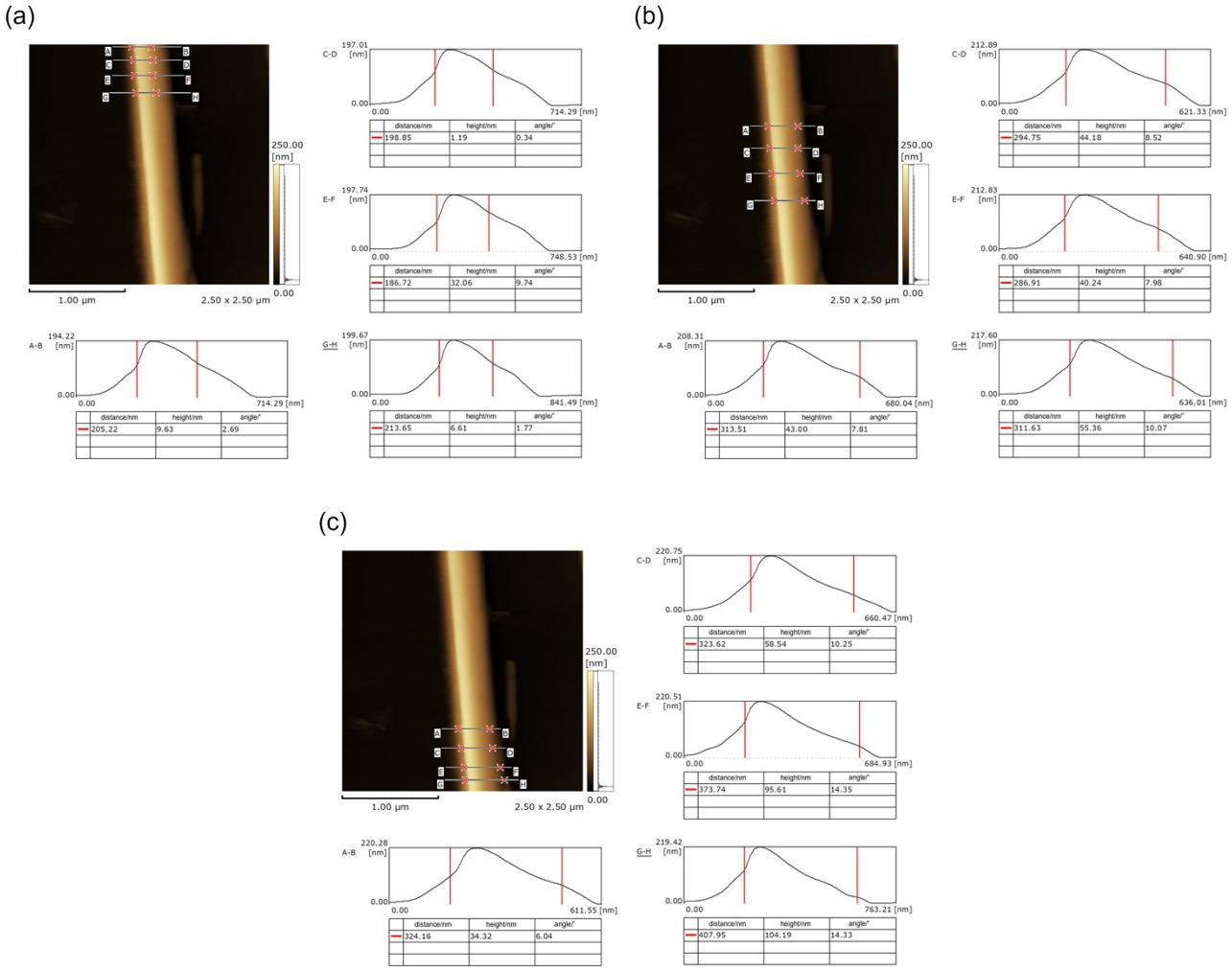

Figure S4. (a)-(c) AFM images and line profiles of **sumanene** (34.3 mM) prepared from the CH_2Cl_2 solution on an HOPG surface.

DFT calculations

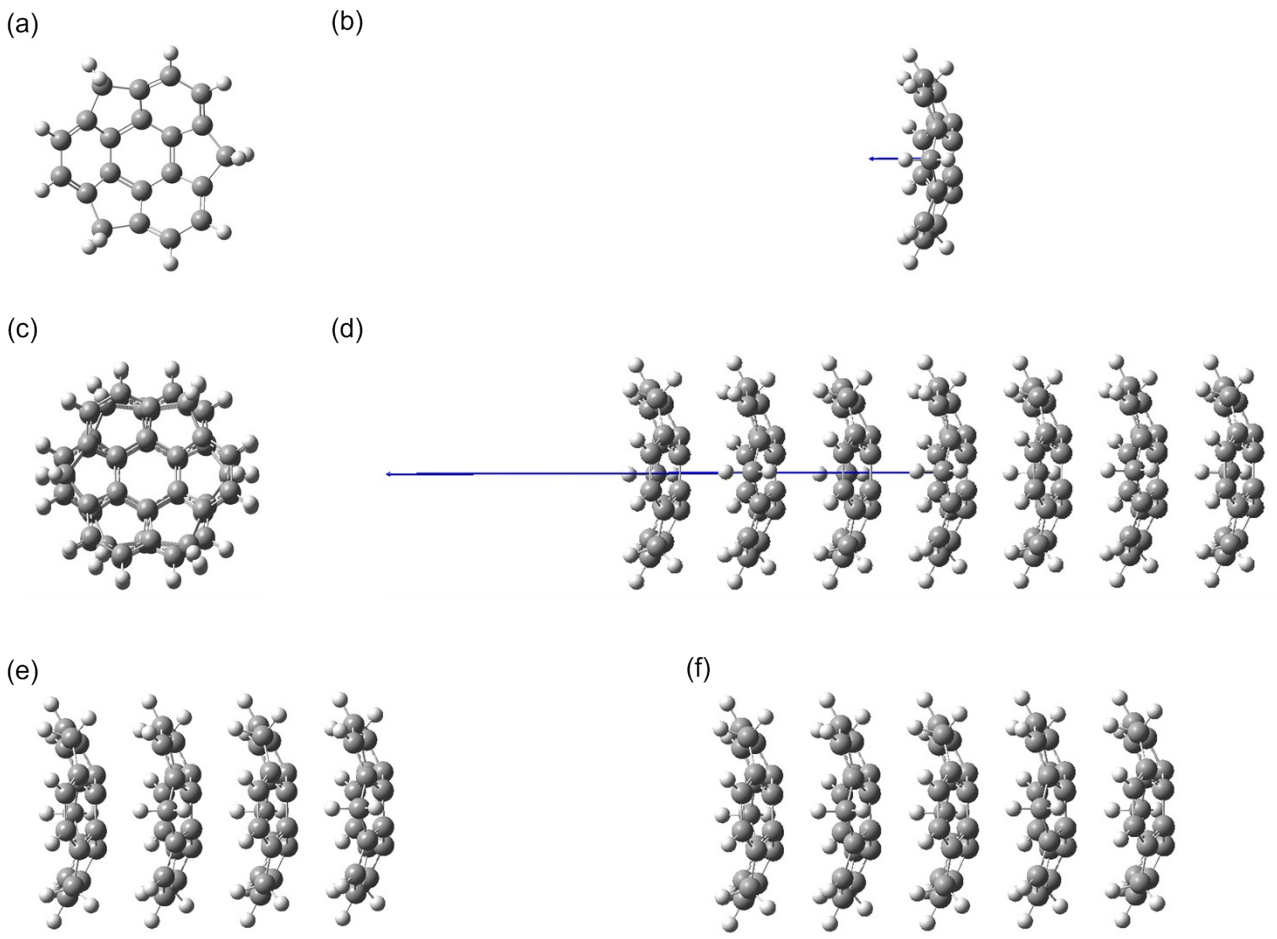

Figure S5. Optimized structures and dipole moments of **sumanene**: (a,b) monomer, (c,d) heptamer, (e) tetramer, and (f) pentamer. Dipole moment: monomer, 2.7 D; octamer, 21.7 D (3.1 D per monomer).

Supramolecular polymerization analysis[9,10]

Chemical equilibrium and sequential equations based on the (anti-)cooperative model

The (anti-)cooperative model assumes different equilibrium constants for the nucleation and elongation stages, and the chemical equilibrium and sequential equations for the formation of a supramolecular polymer of a certain chemical species "A", are given as follows.

$$A + A \rightleftarrows A_2,\ [A_2] = K_n[A]^2 \quad (1)$$

$$A_2 + A \rightleftarrows A_3,\ [A_3] = K_n K_e[A]^3 \quad (2)$$

$$A_{N-1} + A \rightleftarrows A_N,\ [A_N] = \sigma K_e^{-1}(K_e[A])^N,\ \sigma = \frac{K_n}{K_e} \quad (3)$$

where A_X represents the X-mer of A, K_n is the equilibrium constant between the two monomers, K_e is the equilibrium constant between the polymer and monomer, and σ is the cooperative factor. When σ <1, it is a cooperative model; when σ >1, it is an anti-cooperative model.

Mass balance

From the sequential equation, the material balance can be expressed as follows.

$$K_e C_t = (1-\sigma)K_e[A] + \frac{\sigma K_e[A]}{(1-K_e[A])^2} \quad (4)$$

where C_t represents the total concentration of "A". In other words,

$$C_t = [A] + \sum_{i=2}^{\infty} i[A_i] \quad (5)$$

Degree of polymerization (α_{agg})

Degree of polymerization (α_{agg}) can be expressed as follows.

$$\alpha_{agg} = 1 - \frac{K_e[A]}{K_e C_t} \quad (6)$$

On the other hand, α_{agg} is determined by the extinction coefficient as follows.

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[9] D. Zhao, J. S. Moore, *Org. Biomol. Chem.* **2003**, *1*, 3471-3491.

[10] P. P. N. Syamala, F. Würthner, *Chem.-Eur. J.* **2020**, *26*, 8426-8434.

$$\alpha_{agg} = 1 - \frac{\bar{\varepsilon}_{Ct} - \varepsilon_{agg}}{\varepsilon_{mon} - \varepsilon_{agg}} \quad (7)$$

where $\bar{\varepsilon}_{Ct}$ represents the apparent extinction coefficient at a given concentration, ε_{agg} the extinction coefficient of the aggregates and ε_{mon} the extinction coefficients of the monomers. The latter two values were determined from the concentration-dependent UV spectra.

(anti-)cooperative model

We analyzed the supramolecular polymerization based on the (anti)cooperative model by plotting and fitting α_{agg} against C_t using Equations 4 and 7.

isodesmic model

The isodesmic model assumes that the equilibrium constants for the nucleation and elongation stages are identical. In other words,

$$K_n = K_e = K, \sigma = 1 \quad (8)$$

Substituting Equation 8 into Equations (4) and (6) yields Equations 9 and 10, respectively.

$$KC_t = \frac{K[A]}{(1 - K[A])^2} \quad (9)$$

$$\alpha_{agg} = 1 - \frac{K[A]}{KC_t} \quad (10)$$

Furthermore, substituting equation 9 into equation 10 yields equation 11.

$$\alpha_{agg} = 1 - \frac{2KC_t + 1 - \sqrt{4KC_t + 1}}{2K^2C_t^2} \quad (11)$$

Finally, the supramolecular polymerization was analyzed based on the isodesmic model by plotting and fitting α_{agg} against C_t using Equation 11. The number-average degree of polymerization (DP) in the isodesmic model was calculated based on equation 12.

$$DP = \frac{C_t}{[A] + \sum_{i=2}^{\infty} [A_i]} = \frac{\sqrt{4KC_t + 1} + 1}{2} \quad (12)$$

Concentration-dependent measurements

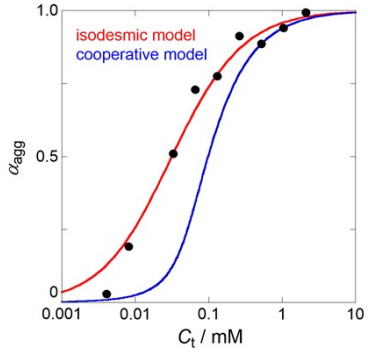

Figure S6. Plot of the degree of polymerization (α_{agg}) of **sumanene** (monitored at 356 nm in Figure 2a) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the anti-cooperative model, respectively.

Table S1. Equilibrium constants of **sumanene** supramolecular polymerization in MCH at 25 °C and 0.1 MPa based on the isodesmic and cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	18600 ± 2200	1	0.990
cooperative	15200 ± 200	0.07 ± 0.02	0.994

SAXS analysis

The equation for the cylinder model is expressed as equation 13[11]

$$I(q) = \int_0^{\frac{\pi}{2}} \frac{\sin^2\left(q\frac{L}{2}cos\theta\right)}{q^2\left(\frac{L}{2}\right)^2\cos^2\theta} \frac{4J_1^2(qR\sin\theta)}{q^2R^2\sin^2\theta} \sin\theta d\theta \quad (13)$$

$$J_1 = 3\frac{\sin qR - qR\cos qR}{(qR)^3} \quad (14)$$

where L represents the length of a cylinder, R the radius of a cylinder and J_1 the first-order Bessel function. The L and R values were obtained from the optimized structure using DFT calculations: L = 1.359 (tetramer), 1.727 (pentamer) nm and, R = 0.407 nm.

[11] A. Guinier, G. Fournet, *Small-Angle Scattering of X-rays* John Wiley & Sons, 1955.

Variable temperature measurements

To consider the effect of solvent density change with temperature, the temperature dependence data of the MCH density were obtained from the literature[12,13] and fitted with a quadratic function. Thus, equation 15 was obtained.

$$\rho(T) = -7.38 \times 10^{-7}T^2 - 4.85 \times 10^{-4}T + 0.975 \qquad (15)$$

where $\rho(T)$ represents the density of MCH at a given temperature. The absorbance was corrected by substituting $\rho(T)$ into equation 16.

$$A_{corrected} = A(T) \times \frac{\rho(T)}{\rho(298.15)} = A(T) \times \frac{\rho(T)}{0.76482} \qquad (16)$$

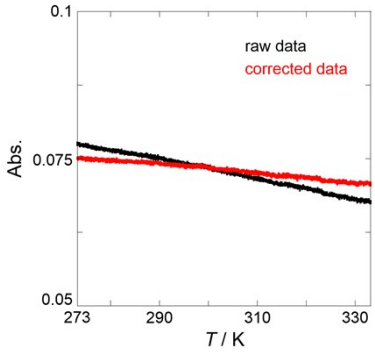

Figure S7. Temperature-dependent absorption of **sumanene** (101 μM) in MCH monitored at 356 nm (black: raw data and red: corrected data).

[12] J. Jonas, D. Hasha, S. G. Huang, *J. Chem. Phys.* **1979**, *71*, 3996-4000.

[13] M. R. Usman, Z. Shahid, M. S. Akram, R. Aslam, *Int. J. Thermophys*. **2020**, *41*, 44.

High pressure measurements

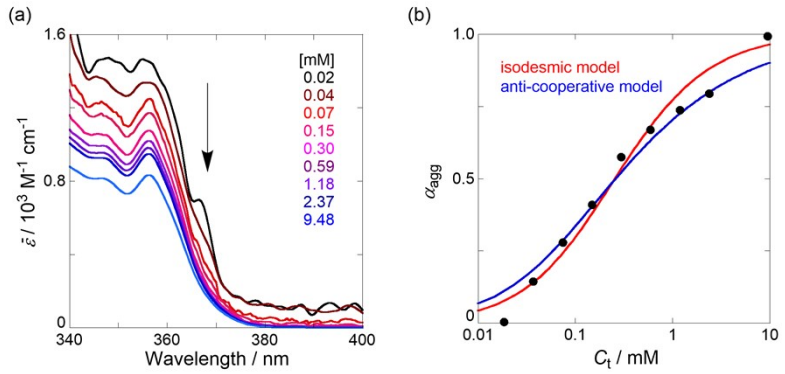

Figure S8. (a) Concentration-dependent UV spectra of **sumanene** (0.02-9.48 mM, from black to blue) in 7:3 (v/v) MCH-CH_2Cl_2 at room temperature and 100 MPa, measured in a high-pressure cell. (b) Plot of the degree of polymerization (α_{agg}) of **sumanene** (monitored at 356 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the anti-cooperative model, respectively.

Table S2. Equilibrium constants of **sumanene** supramolecular polymerization in 7:3 (v/v) MCH-CH_2Cl_2 at room temperature and 100 MPa based on the isodesmic and anti-cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	2300 ± 260	1	0.987
anti-cooperative	150 ± 90	25.4 ± 17.7	0.999

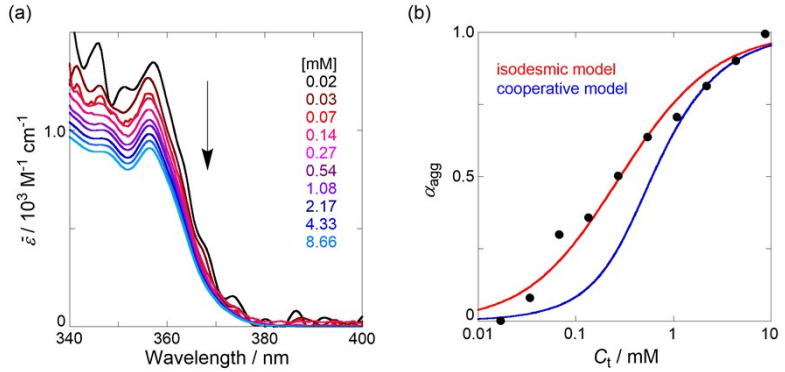

Figure S9. (a) Concentration-dependent UV spectra of **sumanene** (0.02-8.66 mM, from black to sky blue) in 7:3 (v/v) MCH-CH_2Cl_2 at room temperature and 150 MPa, measured in a high-pressure cell. (b) Plot of the degree of polymerization (α_{agg}) of **sumanene** (monitored at 356 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the cooperative model, respectively.

Table S3. Equilibrium constants of **sumanene** supramolecular polymerization in 7:3 (v/v) MCH-CH_2Cl_2 at room temperature and 150 MPa based on the isodesmic and cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	2060 ± 220	1	0.989
cooperative	2000 ± 60	0.18 ± 0.06	0.991

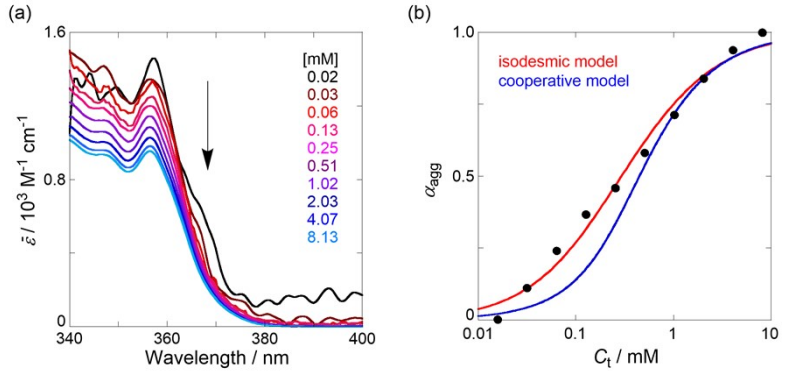

Figure S10. (a) Concentration-dependent UV spectra of **sumanene** (0.02-8.13 mM, from black to sky blue) in 7:3 (v/v) MCH-CH_2Cl_2 at room tempearture and 200 MPa, measured in a high-pressure cell. (b) Plot of the degree of polymerization (α_{agg}) of **sumanene** (monitored at 356 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the cooperative model, respectively.

Table S4. Equilibrium constants of **sumanene** supramolecular polymerization in 7:3 (v/v) MCH-CH_2Cl_2 at room temperature at 200 MPa based on isodesmic and cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	1990 ± 170	1	0.993
cooperative	2370 ± 80	0.28 ± 0.07	0.997

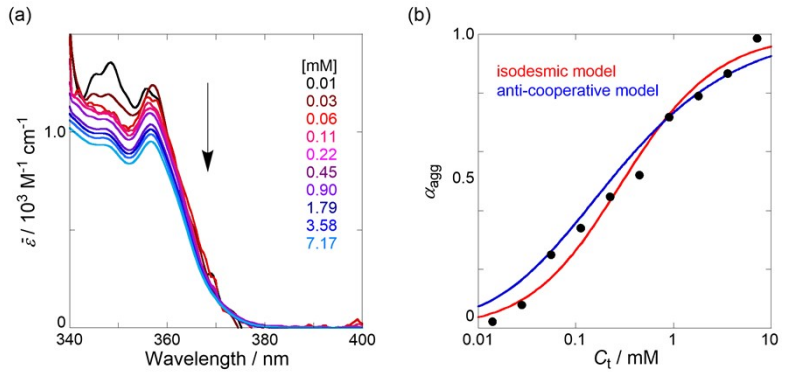

Figure S11. (a) Concentration-dependent UV spectra of **sumanene** (0.02-7.17 mM, from black to sky blue) in 7:3 (v/v) MCH-CH_2Cl_2 at room temperature and 250 MPa, measured in a high-pressure cell. (b) Plot of the degree of polymerization (α_{agg}) of **sumanene** (monitored at 356 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the anti-cooperative model, respectively.

Table S5. Equilibrium constants of **sumanene** supramolecular polymerization in 7:3 (v/v) MCH-CH_2Cl_2 at room temperature at 250 MPa based on isodesmic and anti-cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	1940 ± 190	1	0.990
anti-cooperative	490 ± 280	8.39 ± 6.82	0.993

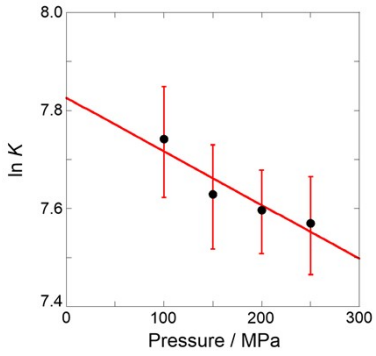

Figure S12. Natural logarithm plot of the equilibrium constants upon the **sumanene** supramolecular polymerization in 7:3 (v/v) MCH-CH_2Cl_2 as a function of pressure.

Table S6. Equilibrium constants of **sumanene** supramolecular polymerization in 7:3 (v/v) MCH-CH_2Cl_2 solution based on the isodesmic model under high pressure.

Pressure / MPa	K / M^{-1}	correlation coefficient	DP[a]
100	2300 ± 260	0.987	5.2
150	2060 ± 220	0.989	4.8
200	1990 ± 170	0.993	4.6
250	1940 ± 190	0.993	4.3

a: number-average degree of polymerization at the maximum measured concentration.

Solvent effect of sumanene supramolecular polymerization

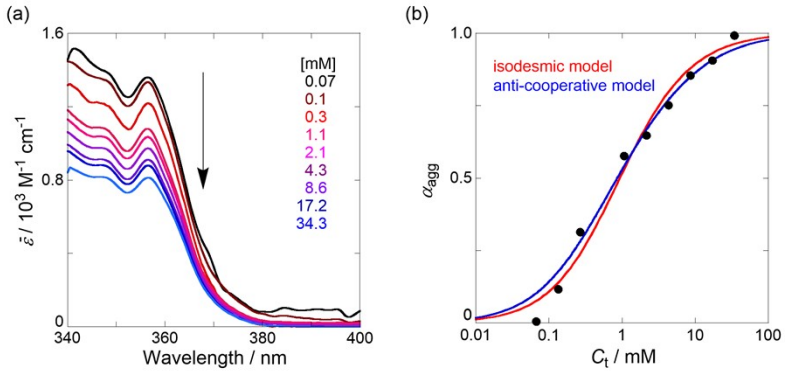

Figure S13. (a) Concentration-dependent UV spectra of **sumanene** (0.07-34.3 mM, from black to sky blue) in CH_2Cl_2 at 25 °C and 0.1 MPa, measured in a 1 mm cell. (b) Plot of the degree of polymerization (a_{agg}) of **sumanene** (monitored at 360 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the anti-cooperative model, respectively.

Table S7. Equilibrium constants of **sumanene** supramolecular polymerization in CH_2Cl_2 at room temperature at 0.1 MPa based on isodesmic and anti-cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	630 ± 70	1	0.991
anti-cooperative	320 ± 20	2.85 ± 0.59	0.997

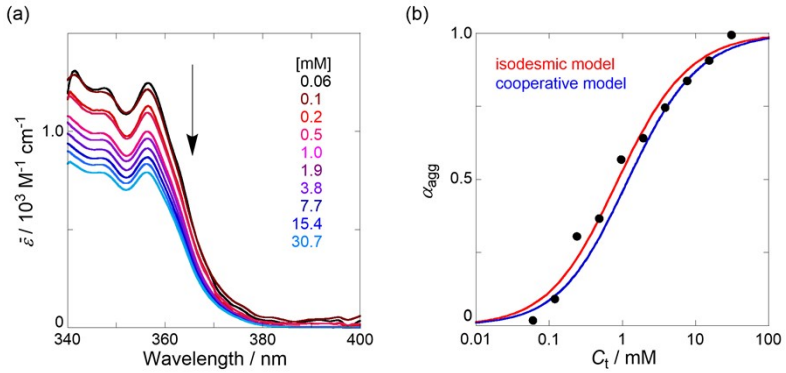

Figure S14. (a) Concentration-dependent UV spectra of **sumanene** (0.06-30.7 mM, from black to sky blue) in 1:9 (v/v) MCH-CH_2Cl_2 solution at 25 °C and 0.1 MPa, measured in a 1 mm cell. (b) Plot of the degree of polymerization (a_{agg}) of **sumanene** (monitored at 356 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the cooperative model, respectively.

Table S8. Equilibrium constants of **sumanene** supramolecular polymerization in 1:9 (v/v) MCH-CH_2Cl_2 solution at room temperature and 0.1 MPa based on isodesmic and cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	670 ± 60	1	0.991
cooperative	490 ± 10	0.99 ± 0.11	0.999

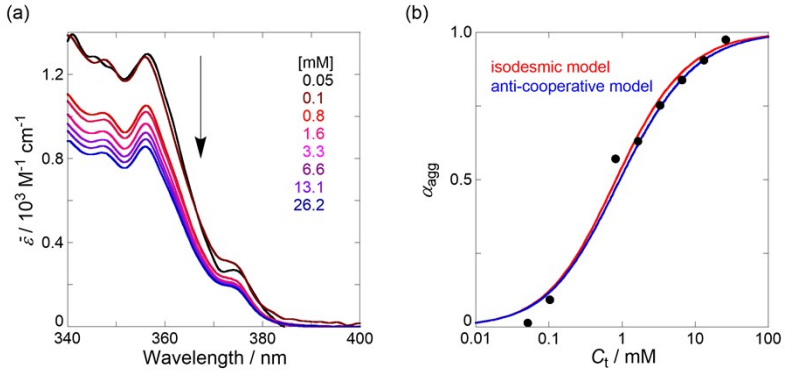

Figure S15. (a) Concentration-dependent UV spectra of **sumanene** (0.05-26.2 mM, from black to navy) in 1:3 (v/v) MCH-CH_2Cl_2 solution at 25 °C and 0.1 MPa, measured in a 1 mm cell. (b) Plot of the degree of polymerization (a_{agg}) of **sumanene** (monitored at 360 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the anti-cooperative model, respectively.

Table S9. Equilibrium constants of **sumanene** supramolecular polymerization in 1:3 (v/v) MCH-CH_2Cl_2 solution at room temperature and 0.1 MPa based on the isodesmic and anti-cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	710 ± 70	1	0.994
anti-cooperative	530 ± 10	1.30 ± 0.13	0.999

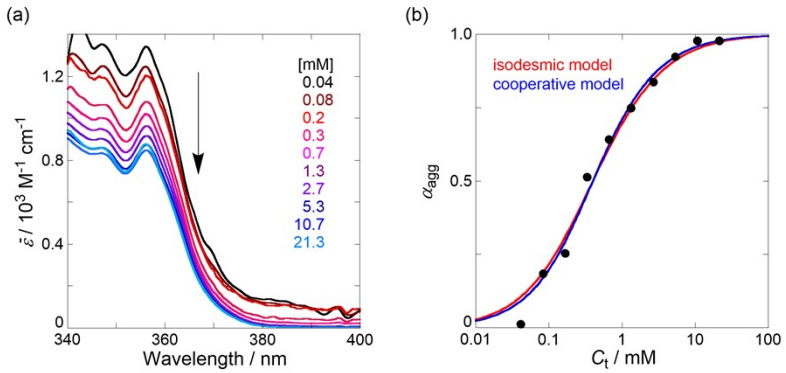

Figure S16. (a) Concentration-dependent UV spectra of **sumanene** (0.04-21.3 mM, from black to sky blue) in 2:3 (v/v) MCH-CH_2Cl_2 solution at 25 °C and 0.1 MPa, measured in a 1 mm cell. (b) Plot of the degree of polymerization (a_{agg}) of **sumanene** (monitored at 360 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the cooperative model, respectively.

Table S10. Equilibrium constants of **sumanene** supramolecular polymerization in 2:3 (v/v) MCH-CH_2Cl_2 solution at room temperature and 0.1 MPa based on the isodesmic and cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	1470 ± 140	1	0.992
cooperative	1880 ± 10	0.64 ± 0.04	0.999

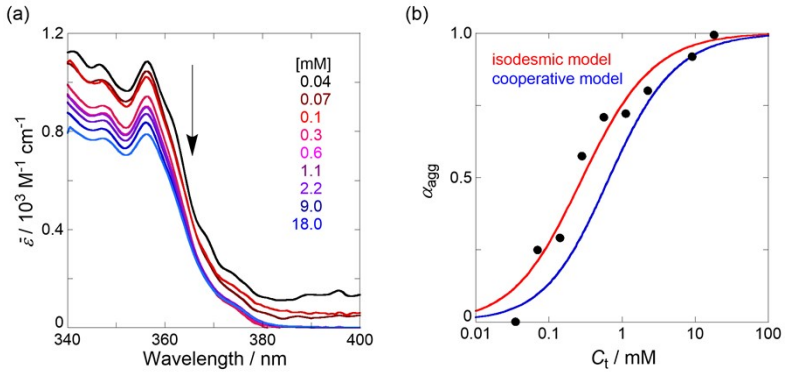

Figure S17. (a) Concentration-dependent UV spectra of **sumanene** (0.04-18.0 mM, from black to blue) in 1:1 (v/v) MCH-CH_2Cl_2 solution at 25 °C and 0.1 MPa, measured in a 2 mm cell. (b) Plot of the degree of polymerization (a_{agg}) of **sumanene** (monitored at 360 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the cooperative model, respectively.

Table S11. Equilibrium constants of **sumanene** supramolecular polymerization in 1:1 (v/v) MCH-CH_2Cl_2 solution at room temperature and 0.1 MPa based on isodesmic and cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	2030 ± 300	1	0.979
cooperative	1050 ± 40	0.73 ± 0.18	0.997

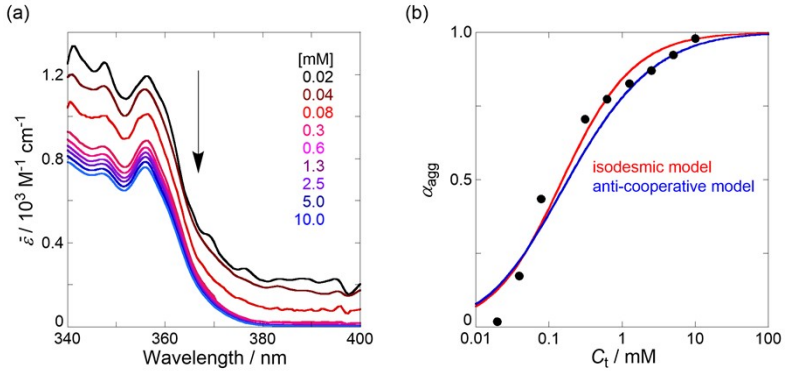

Figure S18. (a) Concentration-dependent UV spectra of **sumanene** (0.02-10.0 mM, from black to blue) in 3:1 (v/v) MCH-CH_2Cl_2 solution at 25 °C and 0.1 MPa, measured in a 5 mm cell. (b) Plot of the degree of polymerization (a_{agg}) of **sumanene** (monitored at 356 nm in (a)) as a function of C_t; the red line represents the fitting result based on the isodesmic model and the blue line represents the anti-cooperative model, respectively.

Table S12. Equilibrium constants of **sumanene** supramolecular polymerization in 3:1 (v/v) MCH-CH_2Cl_2 solution at room temperature and 0.1 MPa based on the isodesmic and anti-cooperative models.

fitting model	K or K_e / M^{-1}	σ	correlation coefficient
isodesmic	3800 ± 570	1	0.985
anti-cooperative	1420 ± 170	3.10 ± 1.04	0.994

Summary of structure optimization

Sumanene monomer

Symbol	X	Y	Z
C	1.4053125	0.0159229	-0.7013613
C	-1.4053125	0.0159229	-0.7013613
C	0.7164459	1.2090749	-0.7013613
C	0.6888666	-1.2249978	-0.7013613
C	-0.6888666	-1.2249978	-0.7013613
C	-0.7164459	1.2090749	-0.7013613
C	1.2057868	2.3481307	-0.0691930
C	2.4939784	2.2613631	0.4521217
H	2.9320307	3.0964874	0.9893603
C	2.6364343	-0.1298234	-0.0691930
C	3.2053871	1.0291671	0.4521217
H	4.1476521	0.9909694	0.9893603
C	-1.2057868	2.3481307	-0.0691930
C	-2.4939784	2.2613631	0.4521217
H	-2.9320307	3.0964874	0.9893603
C	-3.2053871	1.0291671	0.4521217
H	-4.1476521	0.9909694	0.9893603
C	-2.6364343	-0.1298234	-0.0691930
C	-1.4306475	-2.2183074	-0.0691930
C	-0.7114087	-3.2905302	0.4521217
H	-1.2156214	-4.0874568	0.9893603
C	0.7114087	-3.2905302	0.4521217
H	1.2156214	-4.0874568	0.9893603
C	1.4306475	-2.2183074	-0.0691930
C	-2.8409447	-1.6402202	0.1867129
H	-3.5886715	-2.0719205	-0.4874684
H	-3.1726400	-1.8317246	1.2096614
C	0.0000000	3.2804404	0.1867129
H	0.0000000	4.1438410	-0.4874684
H	0.0000000	3.6634492	1.2096614
C	2.8409447	-1.6402202	0.1867129
H	3.5886715	-2.0719205	-0.4874684
H	3.1726400	-1.8317246	1.2096614

Total energy: -807.330745 Hartree

Sumanene tetramer

Symbol	X	Y	Z
C	4.8421800	1.2957290	-0.5337610
C	4.8406430	-1.2855680	0.5616440
C	4.8418650	1.1280030	0.8310180
C	4.8419070	0.1545930	-1.3937490
C	4.8410800	-1.1111710	-0.8566070
C	4.8415630	-0.1874440	1.3891360
C	5.4650270	2.0269380	1.6909840
C	5.9702520	3.1860120	1.1096150
H	6.4979890	3.9228990	1.7066790
C	5.4654650	2.3761290	-1.1503090
C	5.9703340	3.3599730	-0.3054530
H	6.4982490	4.2194690	-0.7061360
C	5.4643880	-0.1940450	2.6332860
C	5.9684040	-1.4179410	3.0629970
H	6.4959960	-1.5009950	4.0078480
C	5.9673650	-2.5566420	2.2050610
H	6.4942060	-3.4425710	2.5449490
C	5.4623480	-2.4804290	0.9104690
C	5.4631780	-2.1859630	-1.4840110
C	5.9687950	-1.9466260	-2.7582540
H	6.4959070	-2.7239530	-3.3022050
C	5.9699030	-0.6341240	-3.3151710
H	6.4978040	-0.4859010	-4.2518280
C	5.4651630	0.4492980	-2.6022690
C	5.7189470	-3.2575860	-0.4003690
H	5.0429110	-4.1126390	-0.5057280
H	6.7418290	-3.6379280	-0.4468340
C	5.7231670	1.2798780	3.0188300
H	5.0501700	1.6172420	3.8140230
H	6.7472300	1.4280930	3.3687720
C	5.7233240	1.9729440	-2.6197650
H	5.0490980	2.4926380	-3.3085670
H	6.7469510	2.2022320	-2.9242550
C	1.1770420	0.1875620	-1.3876900
C	1.1772080	-0.1538370	1.3922480
C	1.1779300	1.2857470	-0.5602780

C	1.1760180	-1.1250380	-0.8305150
C	1.1762210	-1.2926660	0.5342420
C	1.1782970	1.1117690	0.8549740
C	1.7730750	2.4879710	-0.9136060
C	2.2311460	2.5732700	-2.2285740
H	2.7284940	3.4700820	-2.5845330
C	1.7716810	0.1952690	-2.6409850
C	2.2303650	1.4352740	-3.0859140
H	2.7267060	1.5296000	-4.0466960
C	1.7733650	2.1927240	1.4888180
C	2.2310060	1.9577430	2.7854820
H	2.7288030	2.7419320	3.3473840
C	2.2300750	0.6461350	3.3422230
H	2.7275700	0.5050810	4.2967360
C	1.7713910	-0.4494020	2.6104280
C	1.7698940	-2.3826480	1.1539120
C	2.2277550	-3.3880400	0.3021340
H	2.7249650	-4.2670140	0.7003250
C	2.2279910	-3.2142520	-1.1120530
H	2.7249940	-3.9708040	-1.7112670
C	1.7698550	-2.0327760	-1.6953300
C	2.0507540	-1.9712880	2.6189600
H	1.4113790	-2.5055000	3.3291320
H	3.0912650	-2.1743400	2.8873830
C	2.0540130	3.2558160	0.4001280
H	1.4150450	4.1381900	0.5088600
H	3.0948430	3.5890210	0.4409190
C	2.0515430	-1.2792430	-3.0170440
H	1.4143590	-1.6262950	-3.8367960
H	3.0926230	-1.4108640	-3.3248620
C	-2.4993900	1.2934720	-0.5336540
C	-2.5015690	-1.2860210	0.5592510
C	-2.4991320	1.1248370	0.8311060
C	-2.5007440	0.1551730	-1.3926740
C	-2.5016740	-1.1109340	-0.8561820
C	-2.4999590	-0.1883590	1.3875700
C	-1.9017720	2.0305010	1.6957140
C	-1.4402400	3.2109340	1.1131590

H	-0.9381350	3.9640920	1.7122860
C	-1.9027540	2.3823100	-1.1525680
C	-1.4406980	3.3856080	-0.3006240
H	-0.9386840	4.2617410	-0.6990300
C	-1.9028610	-0.1978920	2.6398590
C	-1.4426480	-1.4380480	3.0825330
H	-0.9411030	-1.5326120	4.0406340
C	-1.4446930	-2.5753130	2.2244740
H	-0.9443030	-3.4716740	2.5772230
C	-1.9067260	-2.4889530	0.9110900
C	-1.9068000	-2.1917520	-1.4905760
C	-1.4466490	-1.9563450	-2.7861710
H	-0.9464860	-2.7399000	-3.3466790
C	-1.4456760	-0.6446830	-3.3420000
H	-0.9453260	-0.5032440	-4.2949010
C	-1.9053080	0.4505590	-2.6103780
C	-1.6271410	-3.2558960	-0.4031050
H	-2.2672500	-4.1375240	-0.5126710
H	-0.5868430	-3.5904060	-0.4443640
C	-1.6192220	1.2756810	3.0160680
H	-2.2539830	1.6241500	3.8372620
H	-0.5772310	1.4045590	3.3218220
C	-1.6222450	1.9715220	-2.6175960
H	-2.2590830	2.5087530	-3.3279870
H	-0.5807590	2.1713870	-2.8843730
C	-6.1998550	0.1889400	-1.3905260
C	-6.1985900	-0.1539920	1.3967580
C	-6.1987030	1.2894370	-0.5609420
C	-6.2007580	-1.1277430	-0.8320010
C	-6.1998680	-1.2959780	0.5358660
C	-6.1980460	1.1147380	0.8585560
C	-5.5924370	2.4867880	-0.9123270
C	-5.1174870	2.5678490	-2.2225680
H	-4.6047730	3.4595010	-2.5694440
C	-5.5944200	0.1963960	-2.6387840
C	-5.1183260	1.4329630	-3.0779010
H	-4.6068320	1.5204570	-4.0313430
C	-5.5914210	2.1911990	1.4892810

C	-5.1160570	1.9528130	2.7799460
H	-4.6045320	2.7344110	3.3328700
C	-5.1161730	0.6444160	3.3347700
H	-4.6042070	0.4982450	4.2807400
C	-5.5922540	-0.4490200	2.6091630
C	-5.5945410	-2.3812110	1.1526860
C	-5.1206000	-3.3802120	0.3007110
H	-4.6097770	-4.2502980	0.7010600
C	-5.1212880	-3.2067310	-1.1099150
H	-4.6102110	-3.9536640	-1.7092430
C	-5.5961200	-2.0311700	-1.6939880
C	-5.3065940	-1.9696310	2.6161190
H	-5.9336060	-2.5096190	3.3334980
H	-4.2617960	-2.1651110	2.8736750
C	-5.3049780	3.2528960	0.4008880
H	-5.9316980	4.1441540	0.5108300
H	-4.2602410	3.5741400	0.4400190
C	-5.3100270	-1.2773410	-3.0144270
H	-5.9391940	-1.6268410	-3.8398310
H	-4.2661920	-1.4055150	-3.3145860

Total energy: -3229.451937 Hartree

Sumanene pentamer

Symbol	X	Y	Z
C	6.6803520	0.3129290	-1.3674630
C	6.6793670	-0.2835070	1.3723530
C	6.6811730	1.3302880	-0.4424100
C	6.6792670	-1.0482830	-0.9326590
C	6.6787490	-1.3406940	0.4109720
C	6.6805960	1.0263240	0.9538660
C	7.3050870	2.5510160	-0.6797890
C	7.8101710	2.7453420	-1.9619550
H	8.3385590	3.6579040	-2.2188390
C	7.3031330	0.4331400	-2.6058210
C	7.8091820	1.6905850	-2.9211660
H	8.3368370	1.8593600	-3.8544710
C	7.3042400	2.0377940	1.6776620
C	7.8086100	1.6815120	2.9248220

H	8.3368310	2.4046370	3.5380320
C	7.8073180	0.3234170	3.3587270
H	8.3345450	0.0889020	4.2779670
C	7.3016230	-0.6891130	2.5489140
C	7.3005330	-2.4739220	0.9256370
C	7.8050320	-3.3763530	-0.0059620
H	8.3318270	-4.2695970	0.3142890
C	7.8055840	-3.0731290	-1.3990460
H	8.3327210	-3.7525500	-2.0612220
C	7.3015550	-1.8650040	-1.8715300
C	7.5582790	-2.2081010	2.4259120
H	6.8840600	-2.7884840	3.0645190
H	8.5818480	-2.4650150	2.7077520
C	7.5635040	3.2036280	0.6969160
H	6.8905060	4.0476780	0.8806270
H	8.5875770	3.5748060	0.7780710
C	7.5600680	-0.9994740	-3.1252660
H	6.8865960	-1.2620490	-3.9478540
H	8.5839370	-1.1159510	-3.4875540
C	3.0138260	-1.0263410	-0.9525680
C	3.0140220	1.0458320	0.9322920
C	3.0138050	0.2835770	-1.3708420
C	3.0138990	-1.3298900	0.4407580
C	3.0140100	-0.3126350	1.3659530
C	3.0138100	1.3384450	-0.4113110
C	3.6087610	0.6899130	-2.5564240
C	4.0673320	-0.3337110	-3.3858410
H	4.5646850	-0.1055050	-4.3233580
C	3.6087510	-2.0445110	-1.6832810
C	4.0672300	-1.6909910	-2.9524630
H	4.5645270	-2.4202830	-3.5842870
C	3.6087230	2.4803390	-0.9276760
C	4.0675800	3.4026380	0.0129510
H	4.5652890	4.3141770	-0.3029870
C	4.0677660	3.0994380	1.4051170
H	4.5658690	3.7969950	2.0712650
C	3.6090230	1.8693780	1.8769250
C	3.6087690	-0.4363980	2.6131770

C	4.0672920	-1.7122400	2.9416250
H	4.5652720	-1.8946050	3.8888040
C	4.0672070	-2.7662330	1.9829370
H	4.5647510	-3.6921470	2.2541030
C	3.6087450	-2.5597960	0.6816970
C	3.8903320	0.9969890	3.1233910
H	3.2532190	1.2676960	3.9716420
H	4.9317900	1.0984750	3.4413800
C	3.8903820	2.2056420	-2.4239970
H	3.2539270	2.8050080	-3.0829530
H	4.9319510	2.4300180	-2.6705360
C	3.8901160	-3.2031370	-0.6970230
H	3.2529070	-4.0729140	-0.8868340
H	4.9313260	-3.5298770	-0.7681320
C	-0.6618550	0.3146090	-1.3649010
C	-0.6619840	-0.2806770	1.3723450
C	-0.6618250	1.3322380	-0.4400050
C	-0.6622580	-1.0437970	-0.9307130
C	-0.6624000	-1.3359530	0.4130870
C	-0.6619660	1.0291760	0.9535790
C	-0.0655360	2.5614510	-0.6812630
C	0.3957540	2.7666040	-1.9816170
H	0.8975440	3.6905460	-2.2514880
C	-0.0659400	0.4376680	-2.6117190
C	0.3955340	1.7124260	-2.9398750
H	0.8971590	1.8930130	-3.8854400
C	-0.0656800	2.0471840	1.6835340
C	0.3960770	1.6937510	2.9514190
H	0.8982110	2.4222130	3.5802690
C	0.3962640	0.3367650	3.3851970
H	0.8984510	0.1083480	4.3200420
C	-0.0655910	-0.6866170	2.5574530
C	-0.0666830	-2.4774190	0.9295660
C	0.3938350	-3.3993480	-0.0104790
H	0.8951020	-4.3086990	0.3058900
C	0.3938280	-3.0967200	-1.4025790
H	0.8950720	-3.7927310	-2.0678700
C	-0.0666180	-1.8675640	-1.8747930

C	0.2159690	-2.2021480	2.4253530
H	-0.4203730	-2.8014520	3.0846530
H	1.2577790	-2.4261310	2.6710030
C	0.2160560	3.2050700	0.6969820
H	-0.4204560	4.0756160	0.8864070
H	1.2575660	3.5306270	0.7678640
C	0.2156730	-0.9957350	-3.1210890
H	-0.4206650	-1.2670530	-3.9698310
H	1.2574420	-1.0973650	-3.4377520
C	-4.3377050	-1.0269180	-0.9520240
C	-4.3398960	1.0463350	0.9322020
C	-4.3384380	0.2829430	-1.3708850
C	-4.3381330	-1.3299390	0.4416990
C	-4.3392510	-0.3121830	1.3665330
C	-4.3396340	1.3384110	-0.4116580
C	-3.7415080	0.6890390	-2.5556450
C	-3.2786960	-0.3340220	-3.3832330
H	-2.7753540	-0.1050440	-4.3172840
C	-3.7398010	-2.0443200	-1.6815120
C	-3.2778400	-1.6907660	-2.9493160
H	-2.7738800	-2.4186770	-3.5773580
C	-3.7435550	2.4797750	-0.9279670
C	-3.2826560	3.4015640	0.0120630
H	-2.7802260	4.3102080	-0.3045020
C	-3.2829430	3.0990250	1.4039900
H	-2.7805740	3.7942080	2.0692910
C	-3.7441490	1.8701300	1.8762010
C	-3.7432310	-0.4348240	2.6133400
C	-3.2809020	-1.7091870	2.9418030
H	-2.7781620	-1.8888140	3.8869380
C	-3.2796500	-2.7633300	1.9837990
H	-2.7758690	-3.6862450	2.2534990
C	-3.7405180	-2.5584690	0.6832560
C	-3.4610380	0.9984900	3.1223060
H	-4.0961960	1.2699200	3.9719670
H	-2.4186440	1.0997700	3.4371760
C	-3.4594820	2.2043480	-2.4233530
H	-4.0941910	2.8040920	-3.0839390

H	-2.4169760	2.4272610	-2.6671640
C	-3.4560170	-3.2013560	-0.6946490
H	-4.0901250	-4.0735510	-0.8845720
H	-2.4134120	-3.5238260	-0.7644600
C	-8.0375220	0.3110690	-1.3710930
C	-8.0386290	-0.2852760	1.3733910
C	-8.0386920	1.3311830	-0.4442990
C	-8.0369970	-1.0513280	-0.9353400
C	-8.0376580	-1.3439000	0.4115290
C	-8.0392480	1.0274250	0.9534340
C	-7.4324520	2.5560040	-0.6840600
C	-6.9555090	2.7570040	-1.9803450
H	-6.4420030	3.6765800	-2.2430120
C	-7.4300090	0.4335050	-2.6125340
C	-6.9542570	1.7051670	-2.9359980
H	-6.4400330	1.8793180	-3.8759620
C	-7.4335510	2.0422150	1.6804350
C	-6.9577020	1.6870910	2.9436210
H	-6.4446180	2.4147020	3.5645730
C	-6.9570030	0.3334980	3.3766360
H	-6.4438080	0.1018890	4.3046680
C	-7.4321030	-0.6892480	2.5541830
C	-7.4305520	-2.4800300	0.9269910
C	-6.9531480	-3.3958480	-0.0119120
H	-6.4391200	-4.2967740	0.3080770
C	-6.9522210	-3.0940710	-1.4006240
H	-6.4373080	-3.7810040	-2.0649180
C	-7.4290240	-1.8710950	-1.8752910
C	-7.1436290	-2.2035830	2.4218820
H	-7.7698480	-2.8080360	3.0865730
H	-6.0986180	-2.4202040	2.6611050
C	-7.1461930	3.1987960	0.6937580
H	-7.7732890	4.0762170	0.8841320
H	-6.1015100	3.5150600	0.7629710
C	-7.1408780	-0.9990890	-3.1202510
H	-7.7657190	-1.2733930	-3.9767790
H	-6.0953260	-1.0966780	-3.4260910

Total energy: -4036.826565 Hartree

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Symbol	X	Y	Z
C	10.3564810	-1.0274870	-0.9518800
C	10.3559440	1.0500800	0.9311800
C	10.3539550	0.2816240	-1.3724980
C	10.3586210	-1.3292580	0.4447830
C	10.3582430	-0.3104220	1.3682280
C	10.3537260	1.3403750	-0.4128740
C	10.9744710	0.6855910	-2.5504620
C	11.4796280	-0.3279790	-3.3592890
H	12.0055330	-0.0947220	-4.2795910
C	10.9794770	-2.0399200	-1.6748470
C	11.4821240	-1.6853810	-2.9231980
H	12.0098810	-2.4091980	-3.5359750
C	10.9740040	2.4732010	-0.9302790
C	11.4790320	3.3774740	-0.0007360
H	12.0048750	4.2705370	-0.3230100
C	11.4815060	3.0764170	1.3928710
H	12.0091980	3.7571600	2.0532330
C	10.9788270	1.8687410	1.8680120
C	10.9825880	-0.4283590	2.6059580
C	11.4893310	-1.6852190	2.9227900
H	12.0181990	-1.8522550	3.8557120
C	11.4895550	-2.7415970	1.9653680
H	12.0185340	-3.6535590	2.2231660
C	10.9830910	-2.5494460	0.6834030
C	11.2399070	1.0051140	3.1226720
H	10.5684180	1.2685580	3.9465820
H	12.2645080	1.1224530	3.4826210
C	11.2291680	2.2051580	-2.4307320
H	10.5511190	2.7824470	-3.0680730
H	12.2512230	2.4640130	-2.7160520
C	11.2406700	-3.2040790	-0.6925500
H	10.5692310	-4.0499260	-0.8740690
H	12.2653170	-3.5736660	-0.7739320
C	6.6917070	-1.3385200	0.4136260
C	6.6888140	1.3289030	-0.4416330
C	6.6911850	-1.0474010	-0.9303170

C	6.6908540	-0.2824990	1.3718760
C	6.6893020	1.0269130	0.9520110
C	6.6897780	0.3105900	-1.3656760
C	7.2871810	-1.8713970	-1.8739190
C	7.7471170	-3.1005150	-1.4007200
H	8.2460480	-3.7981020	-2.0661390
C	7.2877330	-2.4792300	0.9313960
C	7.7473480	-3.4022350	-0.0082620
H	8.2462600	-4.3127560	0.3085850
C	7.2846030	0.4334740	-2.6129290
C	7.7417800	1.7095310	-2.9428110
H	8.2390220	1.8913850	-3.8905010
C	7.7404430	2.7647360	-1.9854170
H	8.2368410	3.6909730	-2.2576490
C	7.2820760	2.5593180	-0.6839750
C	7.2830710	2.0466530	1.6814710
C	7.7426010	1.6951830	2.9508020
H	8.2395840	2.4257690	3.5813940
C	7.7444040	0.3384220	3.3857820
H	8.2427090	0.1119530	4.3232150
C	7.2864860	-0.6866890	2.5578220
C	7.5629350	3.2045450	0.6939780
H	6.9255240	4.0743680	0.8831560
H	8.6039100	3.5320970	0.7645270
C	7.5681020	-1.0001220	-3.1212840
H	6.9327120	-1.2731020	-3.9700010
H	8.6099590	-1.1006700	-3.4381300
C	7.5690160	-2.2023910	2.4275230
H	6.9326390	-2.8012350	3.0871170
H	8.6105260	-2.4260780	2.6748260
C	3.0137530	-1.0290470	-0.9520070
C	3.0128130	1.0456660	0.9303080
C	3.0130180	0.2804330	-1.3719940
C	3.0142930	-1.3308960	0.4418120
C	3.0138560	-0.3124100	1.3658240
C	3.0124250	1.3366520	-0.4137380
C	3.6089580	0.6853880	-2.5576020
C	4.0708820	-0.3385150	-3.3846080

H	4.5728340	-0.1106610	-4.3196790
C	3.6102780	-2.0474720	-1.6812340
C	4.0716010	-1.6950660	-2.9495510
H	4.5743470	-2.4236020	-3.5778320
C	3.6075990	2.4778610	-0.9315770
C	4.0680160	3.4008660	0.0074930
H	4.5695470	4.3096770	-0.3099190
C	4.0684640	3.0994570	1.3998650
H	4.5701310	3.7959190	2.0643370
C	3.6086580	1.8705250	1.8733830
C	3.6105230	-0.4340640	2.6123820
C	4.0727630	-1.7083760	2.9414500
H	4.5753190	-1.8876380	3.8867250
C	4.0731300	-2.7634810	1.9842240
H	4.5760220	-3.6866720	2.2545520
C	3.6111170	-2.5596970	0.6839300
C	3.8926710	0.9997550	3.1200780
H	3.2585990	1.2718720	3.9701790
H	4.9350220	1.1015110	3.4346490
C	3.8905250	2.2009480	-2.4270910
H	3.2548510	2.7997780	-3.0875470
H	4.9323630	2.4245470	-2.6728290
C	3.8929470	-3.2043420	-0.6937850
H	3.2573410	-4.0757550	-0.8822940
H	4.9347000	-3.5291220	-0.7645080
C	-0.6621430	-1.3396950	0.4133230
C	-0.6627980	1.3277150	-0.4429900
C	-0.6622580	-1.0490460	-0.9308710
C	-0.6625620	-0.2831790	1.3713330
C	-0.6630010	1.0262320	0.9509470
C	-0.6625860	0.3089750	-1.3667740
C	-0.0651670	-1.8733540	-1.8736430
C	0.3967530	-3.1013630	-1.3998190
H	0.9008440	-3.7964730	-2.0638400
C	-0.0652100	-2.4799290	0.9313210
C	0.3967560	-3.4024330	-0.0074920
H	0.9006660	-4.3098650	0.3101100
C	-0.0659090	0.4308540	-2.6133150

C	0.3955740	1.7053330	-2.9427080
H	0.8989770	1.8841970	-3.8876020
C	0.3952340	2.7605970	-1.9858130
H	0.8985770	3.6836050	-2.2558730
C	-0.0665840	2.5567640	-0.6854770
C	-0.0669630	2.0452220	1.6797710
C	0.3947580	1.6936640	2.9481640
H	0.8978820	2.4227200	3.5754990
C	0.3953070	0.3373550	3.3835860
H	0.8985160	0.1099950	4.3181100
C	-0.0658560	-0.6871410	2.5568950
C	0.2163870	3.2014690	0.6919080
H	-0.4179910	4.0737770	0.8804870
H	1.2587870	3.5244340	0.7619760
C	0.2182580	-1.0026600	-3.1204560
H	-0.4150430	-1.2759400	-3.9708130
H	1.2610760	-1.1030020	-3.4340150
C	0.2185580	-2.2021040	2.4264590
H	-0.4145740	-2.8022970	3.0881330
H	1.2614670	-2.4227920	2.6704720
C	-4.3381440	-1.0275940	-0.9514250
C	-4.3380510	1.0477050	0.9304290
C	-4.3381430	0.2818320	-1.3718160
C	-4.3378660	-1.3290910	0.4425470
C	-4.3379800	-0.3103430	1.3663470
C	-4.3380350	1.3383640	-0.4137780
C	-3.7412270	0.6859490	-2.5572430
C	-3.2792550	-0.3382950	-3.3837360
H	-2.7749100	-0.1106540	-4.3175670
C	-3.7414550	-2.0462920	-1.6801660
C	-3.2793800	-1.6945670	-2.9483420
H	-2.7750530	-2.4232200	-3.5751860
C	-3.7412370	2.4787050	-0.9317260
C	-3.2794520	3.4013140	0.0070370
H	-2.7752690	4.3085680	-0.3106370
C	-3.2793460	3.1002510	1.3993410
H	-2.7751850	3.7952700	2.0634220
C	-3.7410050	1.8721480	1.8731230

C	-3.7409690	-0.4320200	2.6127670
C	-3.2787560	-1.7062370	2.9420770
H	-2.7744900	-1.8846950	3.8865790
C	-3.2786860	-2.7614390	1.9851790
H	-2.7742230	-3.6839240	2.2549250
C	-3.7409070	-2.5578050	0.6849980
C	-3.4567550	1.0015110	3.1197620
H	-4.0895950	1.2747860	3.9704580
H	-2.4136600	1.1019200	3.4324450
C	-3.4568480	2.2008450	-2.4267020
H	-4.0896140	2.8011200	-3.0886950
H	-2.4137420	2.4213020	-2.6701000
C	-3.4573610	-3.2022750	-0.6923130
H	-4.0910850	-4.0751030	-0.8808780
H	-2.4146270	-3.5243150	-0.7622780
C	-8.0144950	-1.3391720	0.4132380
C	-8.0145000	1.3285050	-0.4428470
C	-8.0147380	-1.0483740	-0.9309510
C	-8.0145360	-0.2826450	1.3714440
C	-8.0146220	1.0268470	0.9511840
C	-8.0147580	0.3098310	-1.3667610
C	-7.4171250	-1.8724550	-1.8736110
C	-6.9544240	-3.1002470	-1.4000060
H	-6.4493890	-3.7945140	-2.0642330
C	-7.4169060	-2.4792290	0.9309160
C	-6.9543430	-3.4014340	-0.0078630
H	-6.4492210	-4.3081500	0.3098950
C	-7.4173570	0.4315820	-2.6129950
C	-6.9546570	1.7056730	-2.9421080
H	-6.4498010	1.8839760	-3.8863230
C	-6.9545600	2.7607230	-1.9852060
H	-6.4495880	3.6830150	-2.2546660
C	-7.4171300	2.5570560	-0.6851560
C	-7.4174540	2.0453280	1.6798260
C	-6.9550210	1.6935210	2.9478730
H	-6.4504720	2.4221190	3.5746030
C	-6.9547080	0.3373130	3.3830420
H	-6.4500160	0.1094740	4.3166370

C	-7.4170150	-0.6867940	2.5565370
C	-7.1330110	3.2012700	0.6920850
H	-7.7660730	4.0744980	0.8810630
H	-6.0900150	3.5225130	0.7617880
C	-7.1331310	-1.0017840	-3.1201810
H	-7.7661270	-1.2749580	-3.9708140
H	-6.0900250	-1.1020690	-3.4329350
C	-7.1324280	-2.2015950	2.4258610
H	-7.7653360	-2.8018740	3.0877490
H	-6.0892760	-2.4219880	2.6691830
C	-11.7152970	-1.0289690	-0.9532180
C	-11.7146210	1.0514460	0.9335640
C	-11.7150980	0.2833530	-1.3744030
C	-11.7151370	-1.3315000	0.4447580
C	-11.7148310	-0.3105600	1.3706090
C	-11.7147940	1.3428890	-0.4135430
C	-11.1081520	0.6863250	-2.5551650
C	-10.6316940	-0.3369010	-3.3763540
H	-10.1176980	-0.1056550	-4.3040470
C	-11.1086970	-2.0440510	-1.6789140
C	-10.6320270	-1.6899970	-2.9421340
H	-10.1182810	-2.4180610	-3.5620340
C	-11.1076340	2.4785500	-0.9298900
C	-10.6303920	3.3952380	0.0083840
H	-10.1158490	4.2956110	-0.3122370
C	-10.6301050	3.0947270	1.3973720
H	-10.1155820	3.7822100	2.0613950
C	-11.1071100	1.8721180	1.8729700
C	-11.1076720	-0.4315800	2.6122500
C	-10.6312230	-1.7027670	2.9370010
H	-10.1171080	-1.8756180	3.8772560
C	-10.6314750	-2.7554260	1.9822780
H	-10.1173640	-3.6744240	2.2457000
C	-11.1083520	-2.5557550	0.6857340
C	-10.8195690	1.0014160	3.1189880
H	-11.4451280	1.2762070	3.9748550
H	-9.7743120	1.0995780	3.4255350
C	-10.8203400	2.2007460	-2.4244670

H	-11.4463520	2.8044840	-3.0900400
H	-9.7752590	2.4170490	-2.6635750
C	-10.8211310	-3.1996220	-0.6912880
H	-11.4476470	-4.0775950	-0.8811960
H	-9.7762340	-3.5152850	-0.7598320

Total energy: -5651.576032 Hartree