

Supporting Information

Regulating Supramolecular Interactions in Dimeric Macrocycles

Pengwei Fang,^{a,b} Muqing Chen,^{*a,b} Nan Yin,^b Guilin Zhuang,^{*c} Tianyun Chen,^b
Xinyu Zhang,^b Pingwu Du^{*b}

^a School of Environment and Civil Engineering, Dongguan University of Technology,
Dongguan, Guangdong Province, 523808, China

^b Key Laboratory of Precision and Intelligent Chemistry, Hefei National Research
Center for Physical Sciences at the Microscale, Anhui Laboratory of Advanced
Photon Science and Technology, Department of Materials Science and Engineering,
University of Science and Technology of China, 96 Jinzhai Road, Hefei, Anhui
Province, 230026, China

^c College of Chemical Engineering, Zhejiang University of Technology, 18 Chaowang
Road, Hangzhou, Zhejiang Province, 310032, China

*Corresponding authors: mqchen@ustc.edu.cn, glzhuang@zjut.edu.cn,
dupingwu@ustc.edu.cn.

Tel/Fax: 86-551-63606207

Materials and General Information.

All anhydrous solvents for syntheses and chemicals were purchased from commercial suppliers (Acros or Innochem). All the air-sensitive reactions were carried out using the standard Schlenk technique under nitrogen or argon atmosphere. The NMR spectra were recorded on a Bruker BioSpin (^1H 400 MHz, ^{13}C 100 MHz) spectrometer in CDCl_3 solution, and chemical shifts for ^1H NMR are expressed in parts per million (ppm) relative to tetramethylsilane (δ 0.00 ppm) or CHCl_3 (δ 7.26 ppm). Chemical shifts for ^{13}C NMR are expressed ppm relative to CDCl_3 (δ 77.0 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, m = multiplet, br s = broad signal), coupling constant (Hz), and integration. High-resolution mass spectrometry (HR-MS) analyses were carried out using MALDI-TOF-MS techniques and *trans*-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile as the matrix. UV-vis spectra were obtained on a UNIC-3802 spectrophotometer in standard glass cuvettes. Fluorescence spectra were obtained on a FluoroMax-4 spectrofluorometer. Preparative thin-layer chromatography (PTLC) were performed using silica gel GF254 precoated plates and flash chromatography was performed on silica gel (200~300 mesh).

Synthesis details.

Synthesis of 4a. To a mixture of **2a** (180.85 mg, 0.186 mmol), **3** (196.03 mg, 0.186 mmol), and K_2CO_3 (770 mg, 5.57 mmol) in a round-bottom flask (500 mL) was added THF (200 mL) and H_2O (40 mL), then $Pd(PPh_3)_4$ (30.06 mg, 0.026 mmol) were added under argon atmosphere. Thereafter, the solution was heated at 68 °C for 48 hours. Upon cooling to room temperature, the solvent was removed under vacuum and the residue was extracted with CH_2Cl_2 . The combined organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure to afford the crude product as a gray solid for the next step without further purification.

To a 50-mL round-bottom flask containing a magnetic stirring bar were added $SnCl_2 \cdot 2H_2O$ (274 mg, 1.21 mmol), THF (25 mL) and concentrated HCl (0.21 mL, 12 mol/L) were added, and the resultant mixture was further stirred at room temperature for 30 min. The solution of H_2SnCl_4/THF was added dropwise to a solution containing the above crude product. After stirring the mixture at room temperature for 2 h, the mixture was quenched with aqueous sodium hydroxide, extracted with CH_2Cl_2 , dried over Na_2SO_4 , and concentrated under reduced pressure. The crude product was purified by column chromatography (hexane/ CH_2Cl_2 = 4/1, v/v) to afford **4a** (50 mg, 20% yield over two steps) as a yellow solid. 1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.16 (d, J = 8 Hz, 2H), 7.69 (dd, J = 8 Hz, 2H), 7.53-7.46 (m, 18H), 7.40 (d, J = 8 Hz, 6H), 7.34-7.28 (m, 6H), 7.25 (d, J = 4 Hz, 2H), 7.16 (dd, J = 8 Hz, 2H), 7.04 (d, J = 8 Hz, 6H), 6.86 (dd, J = 8 Hz, 2H), 6.73 (dd, J = 8 Hz, 2H), 6.25 (dd, J = 8 Hz, 2H), 1.13 (s, 18H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.23, 142.62, 141.12, 138.30, 138.27, 137.99, 137.87,

137.84, 137.79, 137.01, 136.88, 134.21, 134.15, 132.56, 131.67, 131.57, 131.30, 130.58, 130.40, 130.13, 129.86, 127.43, 127.40, 127.34, 127.30, 127.19, 126.91, 123.92, 123.72, 123.43, 122.79, 120.31, 34.13, 31.15 ppm. HR-MS (MALDI-TOF) m/z calcd. for $C_{92}H_{68}Br_2 [M]^+$: 1332.3667, found: 1332.3683.

Synthesis of 1a. To a mixture of **2a** (45.21 mg, 0.046 mmol), **4a** (61.33 mg, 0.046 mmol), and Caesium carbonate (179.85 mg, 0.552 mmol) in a round-bottom flask (500 mL) was added Toluene (250 mL), MeOH (10 mL) and H₂O (10 mL), then Pd₂(dba)₃ (8.42 mg, 0.0092 mmol) and S-Phos (7.55 mg, 0.0184 mmol) were added under argon atmosphere. Thereafter, the solution was heated at 100 °C for 72 hours. Upon cooling to room temperature, the solvent was removed under vacuum and the residue was extracted with CH₂Cl₂. The combined organic layer was dried over anhydrous MgSO₄, filtered, and concentrated under reduced pressure to afford the crude product as a gray solid for the next step without further purification.

To a 50-mL round-bottom flask containing a magnetic stirring bar were added SnCl₂·2H₂O (68.5 mg, 0.303 mol), THF (8 mL) and concentrated HCl (0.05mL, 12 mol/L) were added, and the resultant mixture was further stirred at room temperature for 30 min. The solution of H₂SnCl₄/THF was added dropwise to a solution containing the above crude product. After stirring the mixture at room temperature for 2 hours, the mixture was quenched with aqueous sodium hydroxide, extracted with CH₂Cl₂, dried over Na₂SO₄, and concentrated under reduced pressure. The crude product was purified initially by silica gel column chromatography and then by preparative thin-layer chromatography (hexane/CH₂Cl₂ = 2/1) to afford **1a** (3.92 mg, 5% yield over two steps)

as a yellow solid. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 8.34 (s, 2H), 8.30 (d, $J = 8$ Hz, 2H), 7.78 (d, $J = 8$ Hz, 2H), 7.63-7.43 (m, 52H), 7.39 (d, $J = 8$ Hz, 4H), 7.34 (d, $J = 8$ Hz, 4H), 7.2 (d, $J = 8$ Hz, 4H), 7.00 (br s, 4H), 6.13 (d, $J = 8$ Hz, 2H), 5.02 (d, $J = 8$ Hz, 2H), 1.13 (s, 18H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.64, 144.27, 141.18, 140.05, 138.33, 138.31, 138.23, 138.16, 138.06, 138.00, 137.92, 137.90, 135.21, 133.19, 131.39, 130.99, 130.15, 128.82, 127.99, 127.55, 127.46, 127.37, 127.25, 127.10, 127.03, 126.78, 124.38, 123.68, 123.08, 122.22, 34.11, 31.29 ppm. HR-MS (MALDI-TOF-MS) m/z calcd. for $\text{C}_{134}\text{H}_{96}$ $[M]^+$: 1705.7501, found 1705.7546.

Synthesis of 4b. Compound **4b** was prepared by a procedure similar to that used for **4a**, starting from **2b** (194.96 mg, 0.186 mmol) and **3** (196.03 mg, 0.186 mmol). The crude product was purified by silica gel column chromatography (hexane/ $\text{CH}_2\text{Cl}_2 = 4/1$) to afford **4b** (57 mg, 22%) as a yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.22 (d, $J = 8$ Hz, 2H), 7.7 (d, $J = 8$ Hz, 2H), 7.60-7.53 (m, 20H), 7.47 (d, $J = 8$ Hz, 4H), 7.38 (m, 6H), 7.31 (m, 6H), 7.23 (d, $J = 8$ Hz, 2H), 7.14 (d, $J = 8$ Hz, 2H), 7.02 (d, $J = 8$ Hz, 4H), 6.87 (d, $J = 8$ Hz, 2H), 6.72 (d, $J = 8$ Hz, 2H), 6.25 (d, $J = 8$ Hz, 2H), 1.12 (s, 18H). ^{13}C NMR (CDCl_3 , 100 MHz): δ 148.23, 142.69, 141.35, 138.44, 138.39, 138.33, 138.19, 138.12, 138.03, 137.92, 136.85, 137.15, 136.93, 134.58, 134.19, 132.51, 131.55, 131.48, 131.33, 130.53, 130.43, 130.07, 129.91, 128.57, 127.40, 127.34, 127.21, 127.09, 126.39, 124.12, 123.71, 123.38, 122.79, 120.33, 34.13, 31.15 ppm. The analytical data is in accordance to the literature.^{S1}

Synthesis of 1b. Compound **1b** was prepared by a procedure similar to that used for **1a**, starting from **2a** (45.21 mg, 0.046 mmol) and **4b** (65.51 mg, 0.046 mmol). The

crude product was purified initially by silica gel column chromatography and then by preparative thin-layer chromatography (hexane/CH₂Cl₂ = 2/1) to afford **1b** (4.92 mg, 6%) as a yellow solid. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.42 (s, 2H), 8.36 (d, *J* = 8 Hz, 2H), 7.80 (d, *J* = 8 Hz, 2H), 7.63-7.48 (m, 56H), 7.42 (d, *J* = 8 Hz, 4H), 7.34 (d, *J* = 8 Hz, 4H), 7.21 (d, *J* = 8 Hz, 4H), 7.00 (br s, 4H), 6.14 (d, *J* = 8 Hz, 2H), 5.03 (d, *J* = 8 Hz, 2H), 1.14 (s, 18H). ¹³C NMR (100 MHz, CDCl₃) δ 147.59, 144.26, 141.70, 140.05, 138.51, 138.31, 138.17, 138.09, 137.97, 137.42, 137.32, 135.45, 133.14, 131.18, 131.13, 131.00, 128.84, 127.99, 127.55, 127.42, 127.35, 127.23, 127.08, 126.77, 124.41, 123.62, 123.06, 122.19, 34.11, 31.29 ppm. HR-MS (MALDI-TOF-MS) *m/z* calcd. for C₁₄₀H₁₀₀ [*M*]⁺: 1781.7859, found 1781.7811.

Physical characterizations.

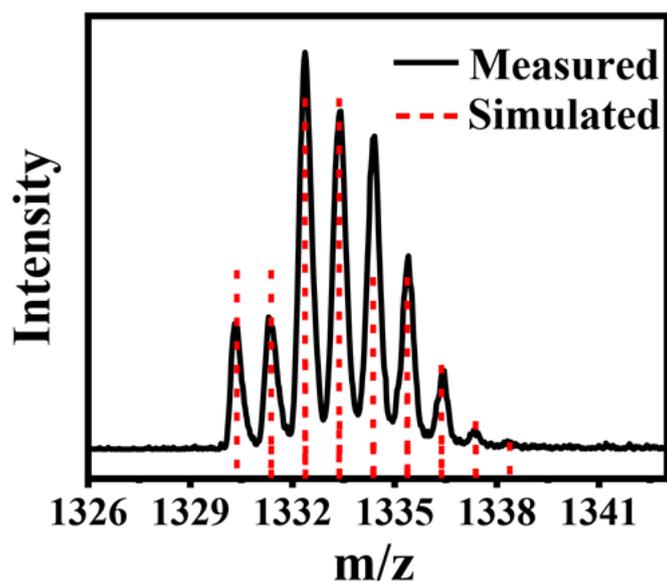


Figure S1. HR-MS (MALDI-TOF) and simulated data for compound 4a.

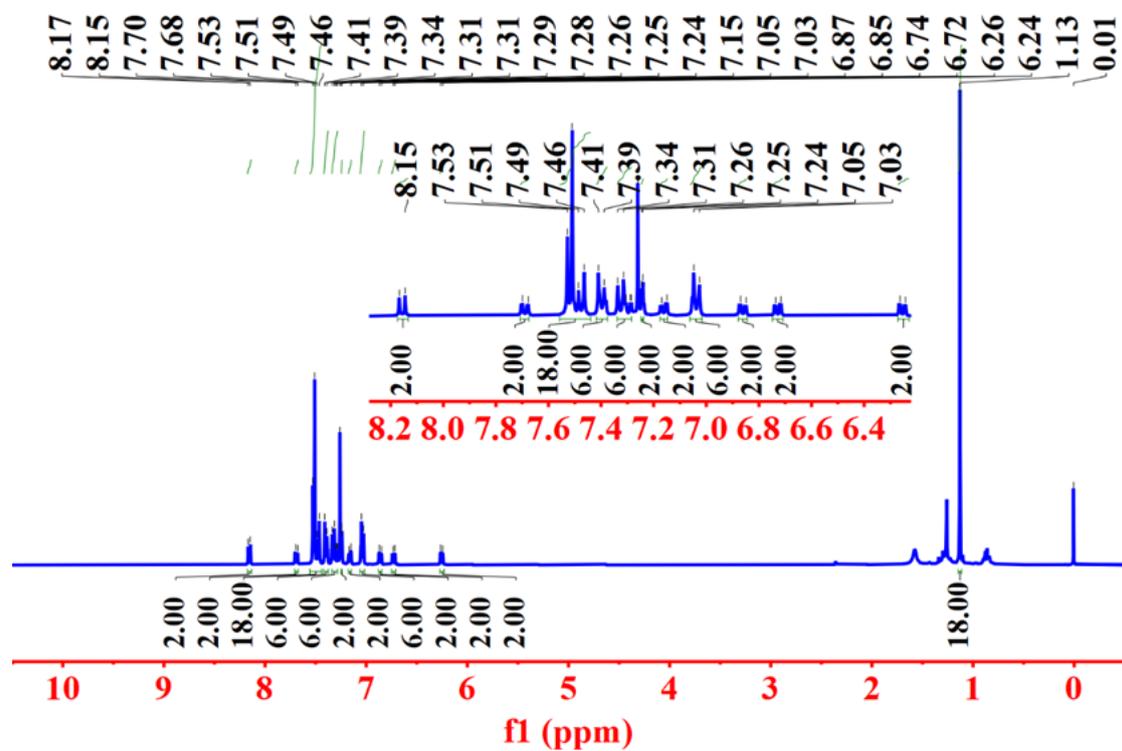


Figure S2. ¹H NMR spectrum of compound 4a in CDCl₃.

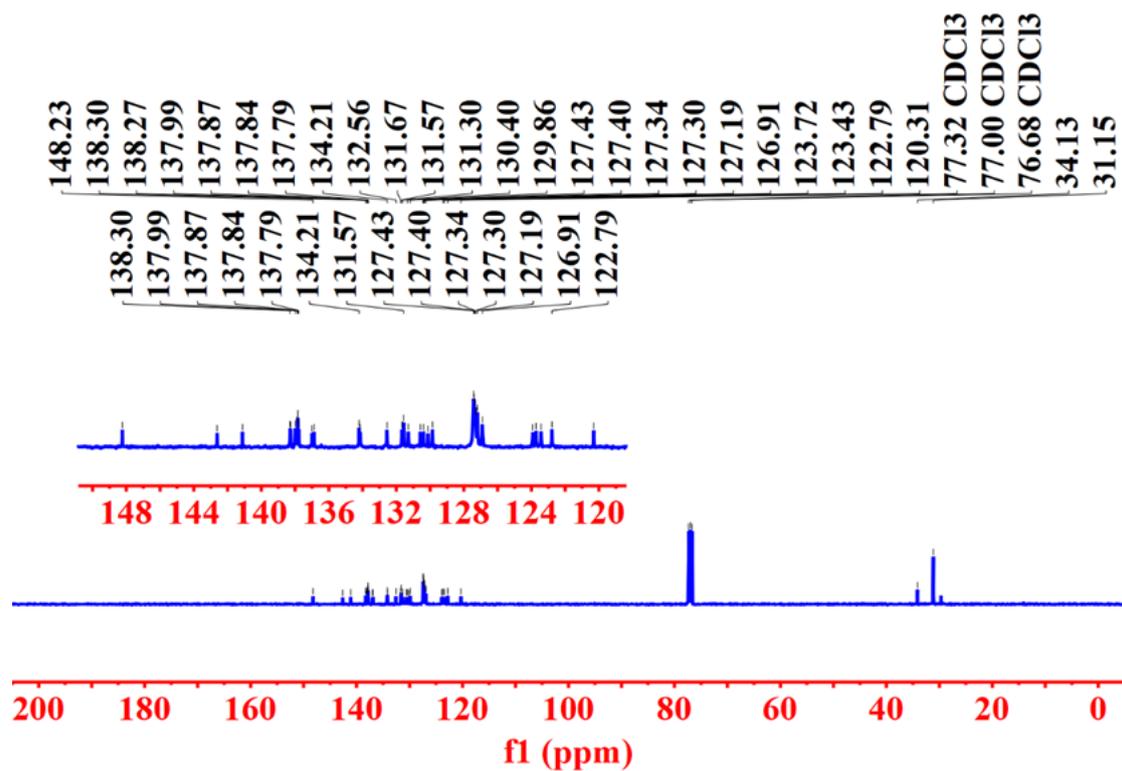


Figure S3. ^{13}C NMR spectrum of compound **4a** in CDCl_3 .

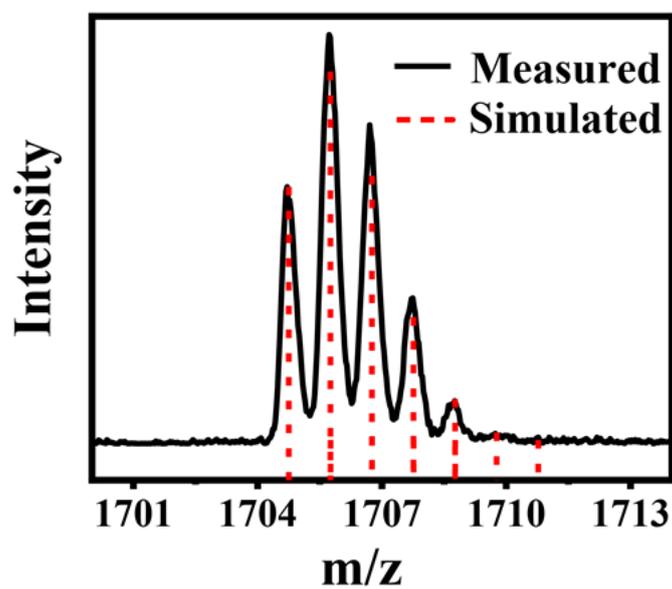


Figure S4. HR-MS (MALDI-TOF) and simulated data for **1a**.

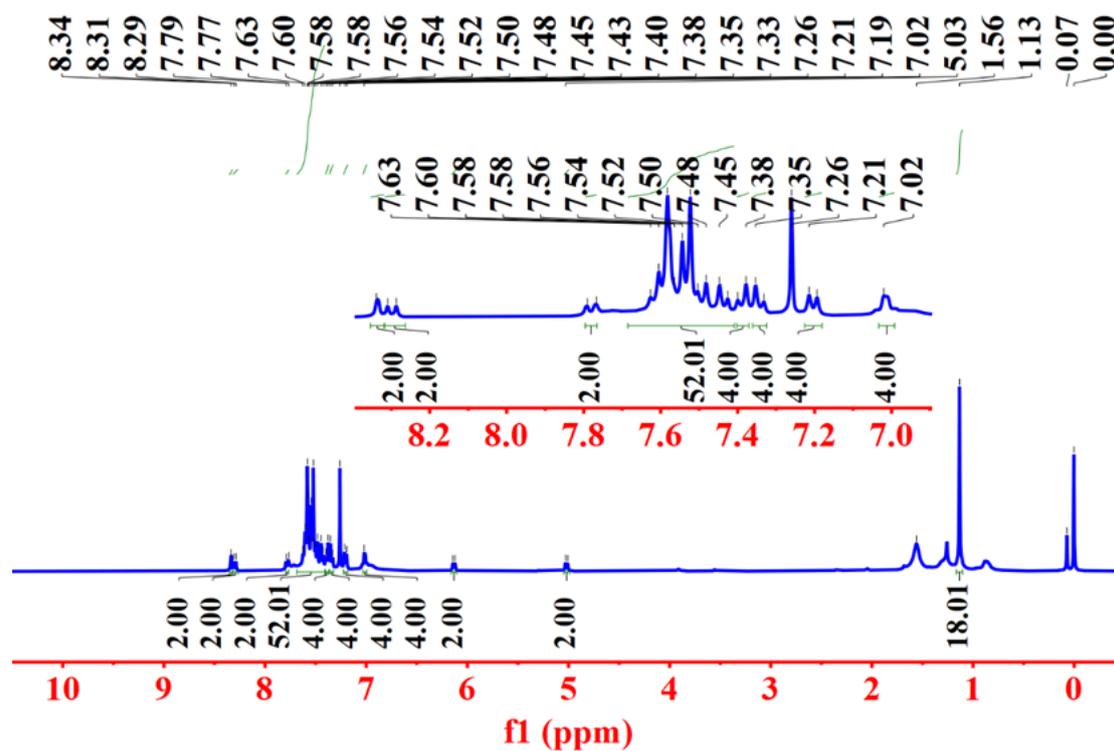


Figure S5. ^1H NMR spectrum (400 MHz, CDCl_3) of **1a** in CDCl_3 .

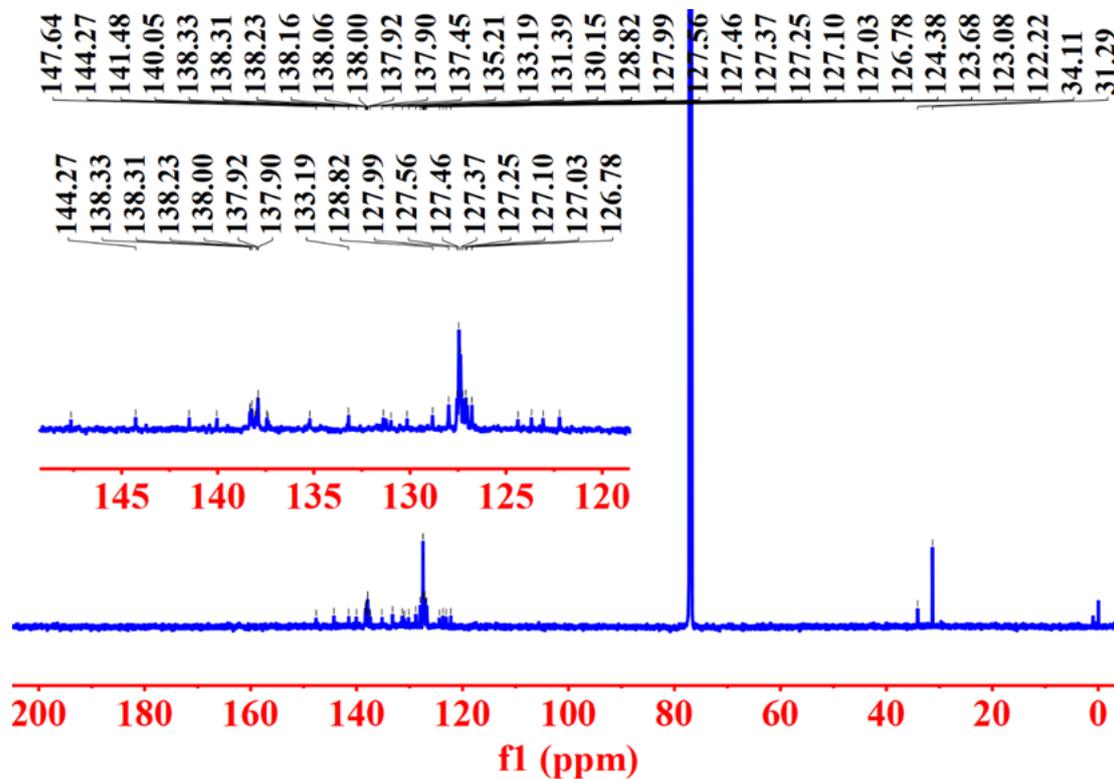


Figure S6. ^{13}C NMR spectrum (400 MHz, CDCl_3) of **1a** in CDCl_3 .

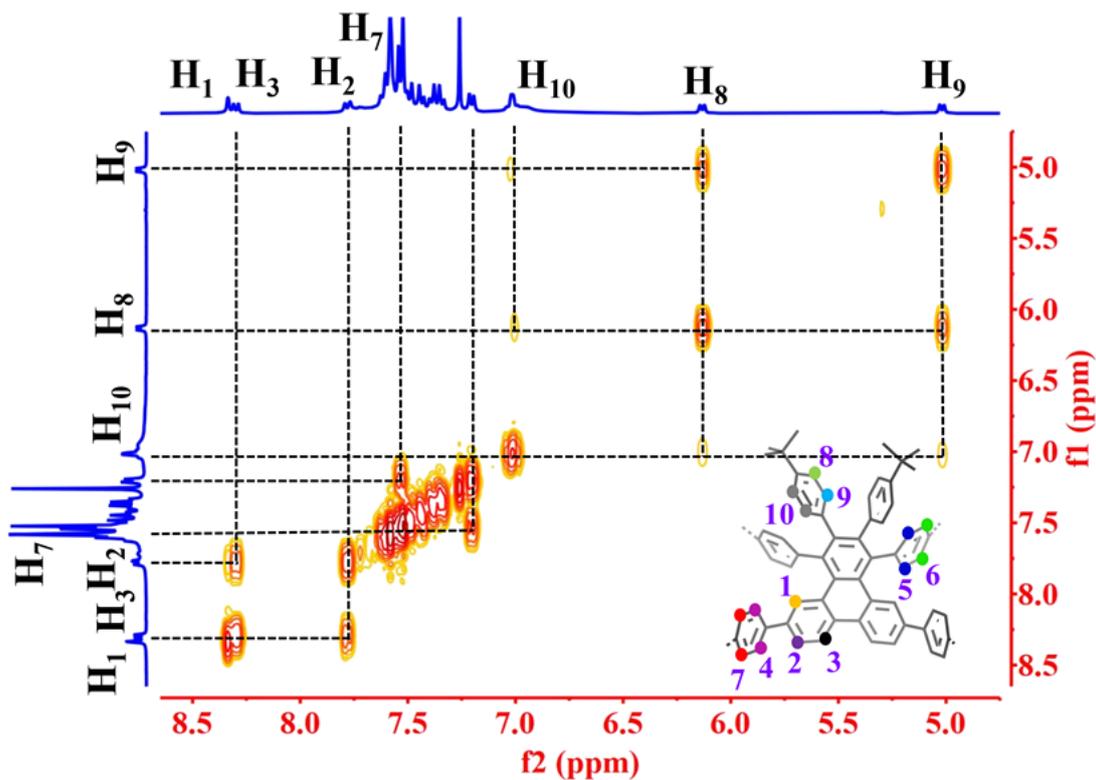


Figure S7. Expanded 2D ^1H - ^1H COSY NMR spectrum (400 MHz, CDCl_3) of **1a**.

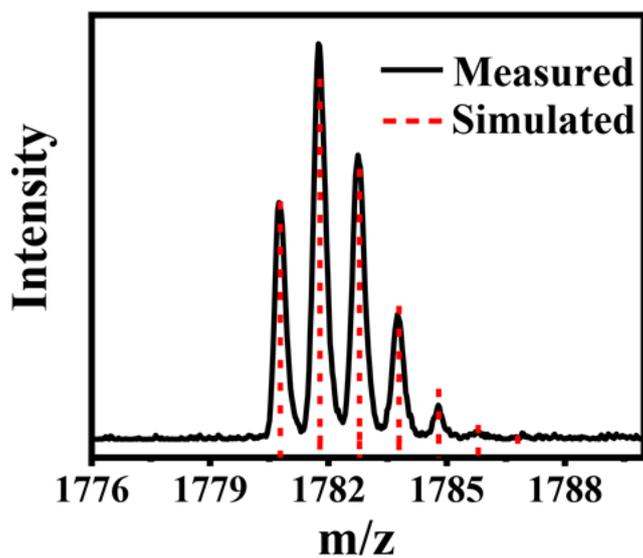


Figure S8. HR-MS (MALDI-TOF) and simulated data for **1b**.

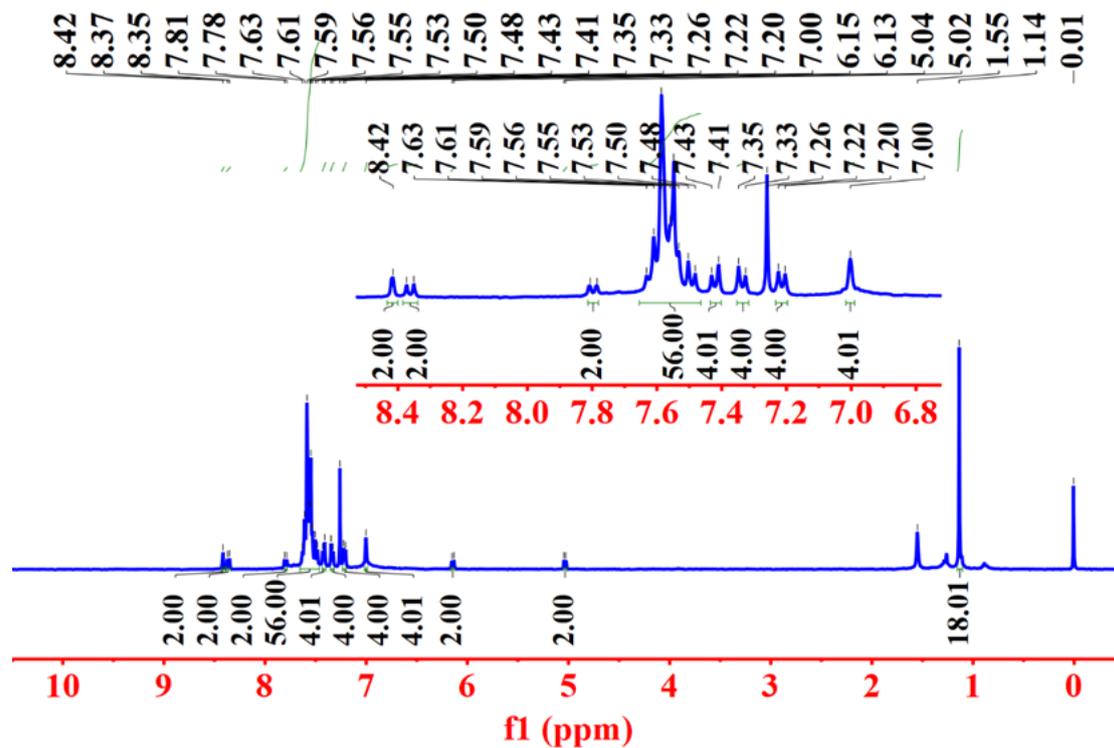


Figure S9. ^1H NMR spectrum (400 MHz, CDCl_3) of **1b** in CDCl_3 .

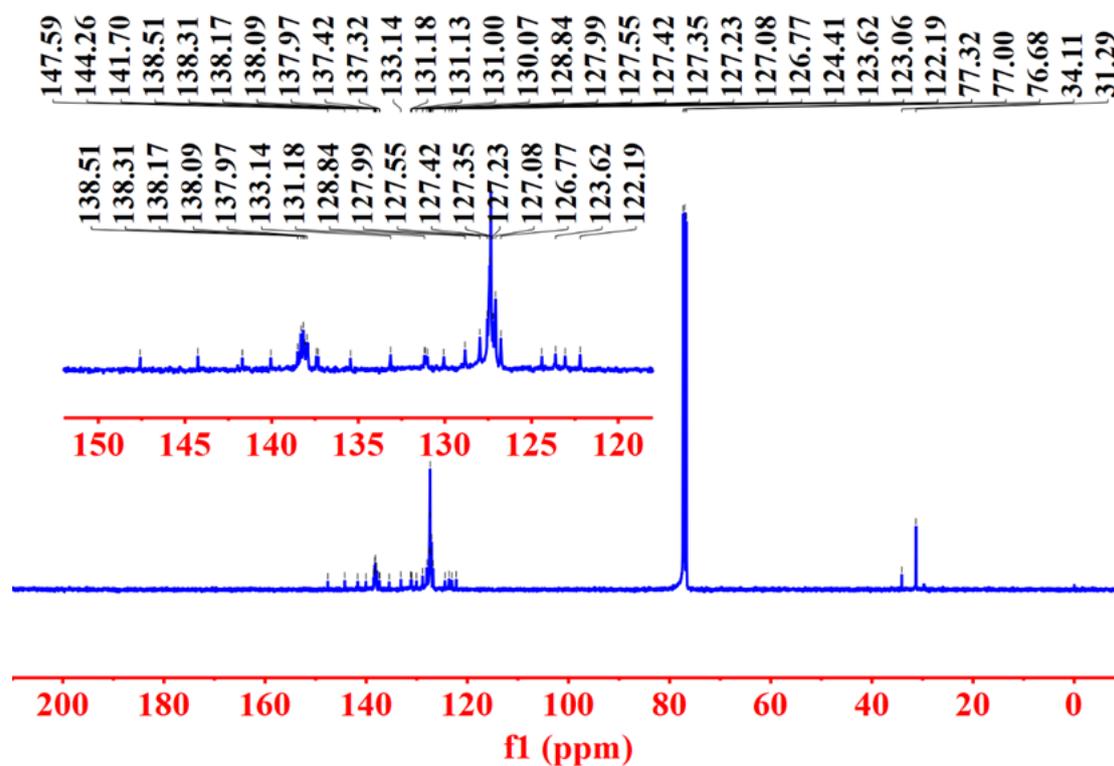


Figure S10. ^{13}C NMR spectrum (400 MHz, CDCl_3) of **1b** in CDCl_3 .

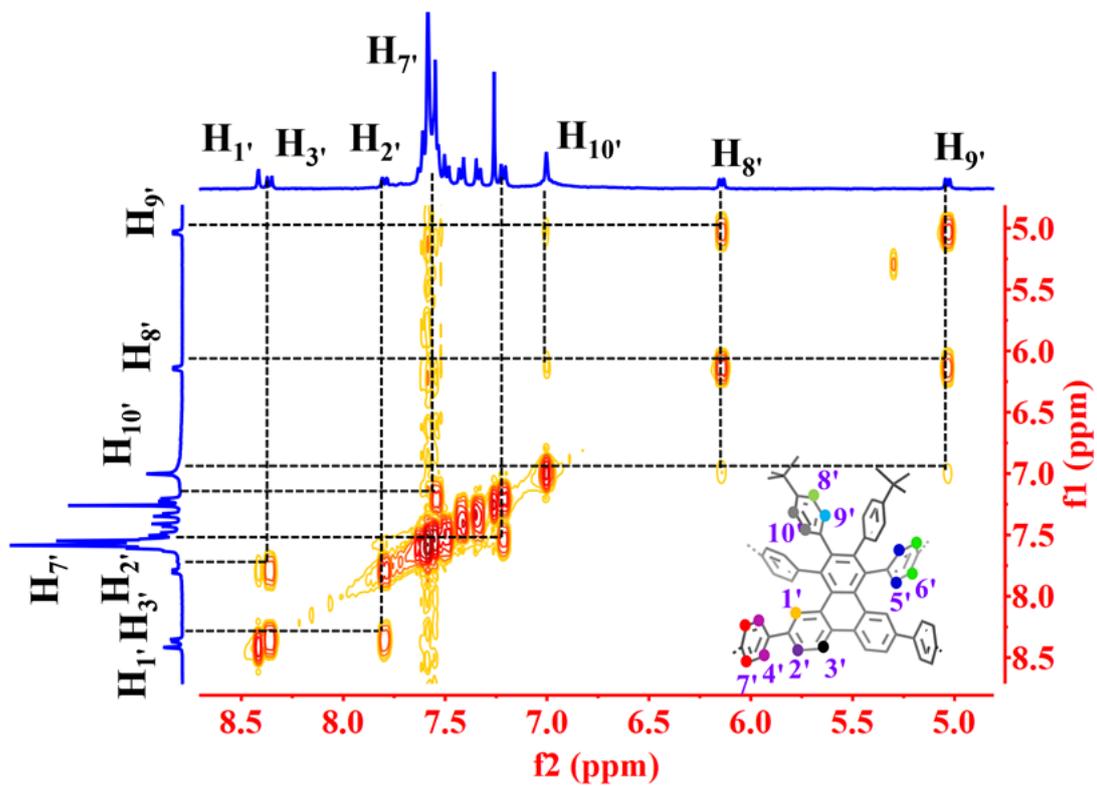


Figure S11. Expanded 2D ^1H - ^1H COSY NMR spectrum (400 MHz, CDCl_3) of **1b**.

X-ray Crystallography.

Crystalline blocks of $C_{60}@(\mathbf{1a})_2$ and $C_{70}@(\mathbf{1a})_2$ were obtained by slow liquid diffusion of hexane into a chlorobenzene solution containing **1a** and excess C_{60} or C_{70} afforded black single crystals suitable for X-ray measurements. Crystalline blocks of $3C_{60}@(\mathbf{1b})_2$ were obtained by slow evaporation of a toluene solution containing **1b** and excess C_{60} . Single crystal XRD measurements of $C_{60}@(\mathbf{1a})_2$ and $C_{70}@(\mathbf{1a})_2$ were conducted at 100 K at a Rigaku Oxford SuperNova Diffractometer using Cu $K\alpha$ radiation ($\lambda = 1.54184 \text{ \AA}$). Single crystal XRD measurements of $3C_{60}@(\mathbf{1b})_2$ was conducted at 173 K at the Bruker D8 Venture MetalJet X-ray diffractometer equipped with a Photon II detector using Ga $K\alpha$ radiation ($\lambda = 1.34138 \text{ \AA}$). The crystal structures were solved with the ShelXT structure solution program using Direct Methods, later refined with the ShelXL refinement package embedded within OLEX2. CCDC-2191567 ($C_{60}@(\mathbf{1a})_2$), CCDC-2191568 ($C_{70}@(\mathbf{1a})_2$), and CCDC-2161639 ($3C_{60}@(\mathbf{1b})_2$) contain the supplementary crystallographic data for this paper. These data can also be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data and structure refinement for $C_{60}@(\mathbf{1a})_2$

| Complex | $C_{60}@(\mathbf{1a})_2$ |
|--|---|
| Formular | $C_{176}H_{107}Cl_2$ |
| Formular weight | 2292.51 |
| Temperature/K | 100(10) |
| Crystal system | triclinic |
| Space group | P1 |
| a / Å | 15.9267(3) |
| b / Å | 20.9291(4) |
| c / Å | 22.0491(5) |
| α / deg | 90.828(2) |
| β / deg | 108.688(2) |
| γ / deg | 93.047(2) |
| Volume/Å ³ | 6948.5(3) |
| Z | 2 |
| $\rho_{\text{calc}}/\text{cm}^3$ | 1.096 |
| μ/mm^{-1} | 0.817 |
| F(000) | 2394 |
| Crystal size/mm ³ | 0.1 × 0.08 × 0.07 |
| Radiation | Cu K α ($\lambda = 1.54184$) |
| 2 Θ range for data collection/° | 5.868 to 139.278 |
| Index ranges | -17 ≤ h ≤ 19, -25 ≤ k ≤ 25, -26 ≤ l ≤ 26 |
| Reflections collected | 84249 |
| Independent reflections | 25463[R _{int} = 0.0495, R _{sigma} = 0.0502] |
| Data/restraints/parameters | 25463/891/1910 |
| Goodness-of-fit on F ² | 1.028 |
| Final R indexes [I ≥ 2 σ (I)] | R ₁ = 0.1178, wR ₂ = 0.3410 |
| Final R indexes [all data] | R ₁ = 0.1311, wR ₂ = 0.3518 |

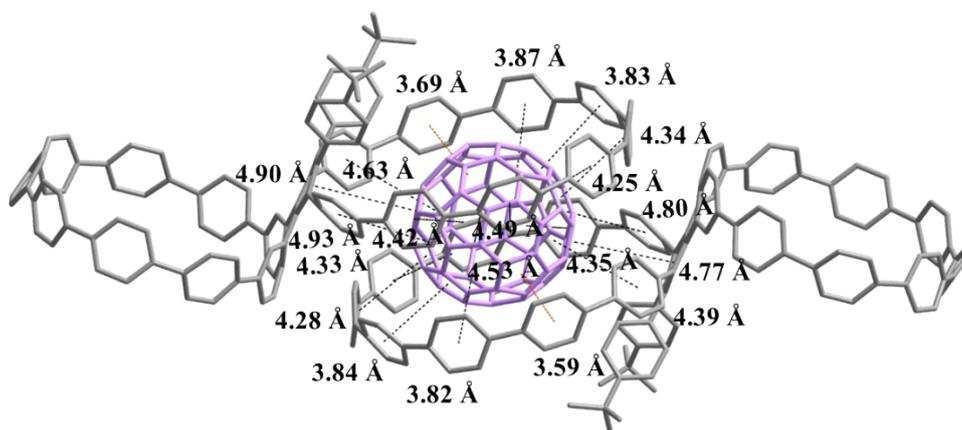


Figure S12. Side-views of a $C_{60}@(\mathbf{1a})_2$ complex highlighting the π - π interactions between the guests and cavities. Hydrogen atoms and disordered solvent molecules are omitted for clarity.

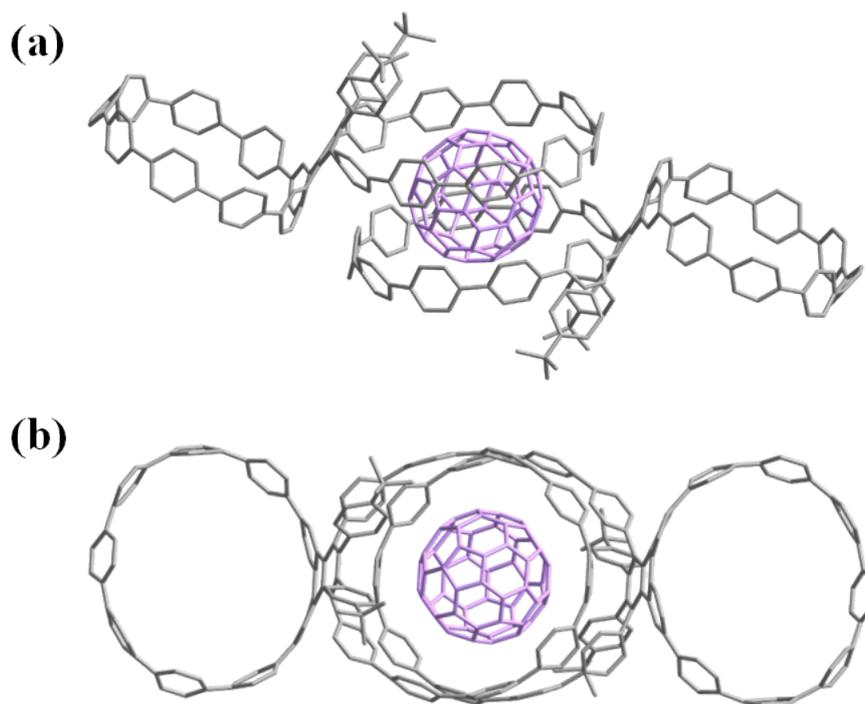


Figure S13. Side view (a) and top view (b) of the X-ray crystal structure of $C_{60}@(\mathbf{1a})_2$. Hydrogen atoms and disordered solvent molecules are omitted for clarity.

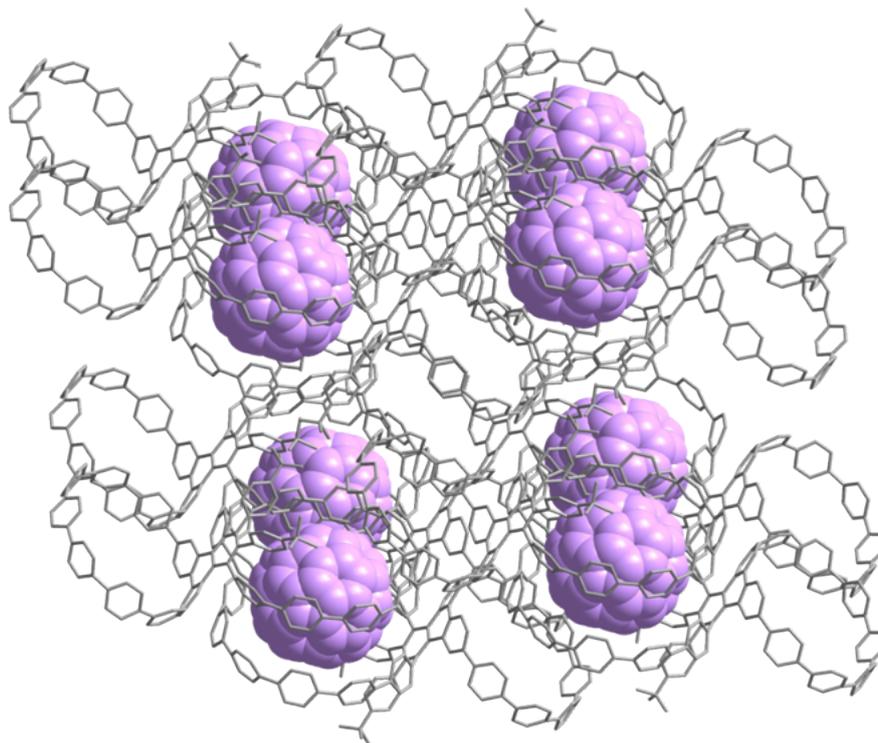


Figure S14. Packing structure of $C_{60}@(\mathbf{1a})_2$. Hydrogen atoms and solvent molecules are omitted for clarity.

Table S2. Crystal data and structure refinement for $C_{70}@(\mathbf{1a})_2$

| Complex | $C_{70}@(\mathbf{1a})_2$ |
|-----------------------|--------------------------|
| Formular | $C_{315}H_{110}$ |
| Formular weight | 3894.02 |
| Temperature/K | 100(2) |
| Crystal system | monoclinic |
| Space group | P21/c |
| a / Å | 20.6555(2) |
| b / Å | 38.6556(5) |
| c / Å | 25.2345(3) |
| α / deg | 90 |
| β / deg | 105.3310(10) |
| γ / deg | 90 |
| Volume/Å ³ | 19431.5(4) |

| | |
|--|--|
| Z | 4 |
| $\rho_{\text{calc}}/\text{cm}^3$ | 1.331 |
| μ/mm^{-1} | 0.584 |
| F(000) | 8000 |
| Crystal size/ mm^3 | $0.06 \times 0.05 \times 0.05$ |
| Radiation | Cu K α ($\lambda = 1.54184$) |
| 2 Θ range for data collection/ $^\circ$ | 4.99 to 139.218 |
| Index ranges | $-21 \leq h \leq 25, -45 \leq k \leq 46, -30 \leq l \leq 30$ |
| Reflections collected | 128766 |
| Independent reflections | 35548 [$R_{\text{int}} = 0.0541, R_{\text{sigma}} = 0.0563$] |
| Data/restraints/parameters | 35548/3508/3790 |
| Goodness-of-fit on F^2 | 1.063 |
| Final R indexes [$I \geq 2\sigma(I)$] | $R_1 = 0.1406, wR_2 = 0.4175$ |
| Final R indexes [all data] | $R_1 = 0.1629, wR_2 = 0.4408$ |

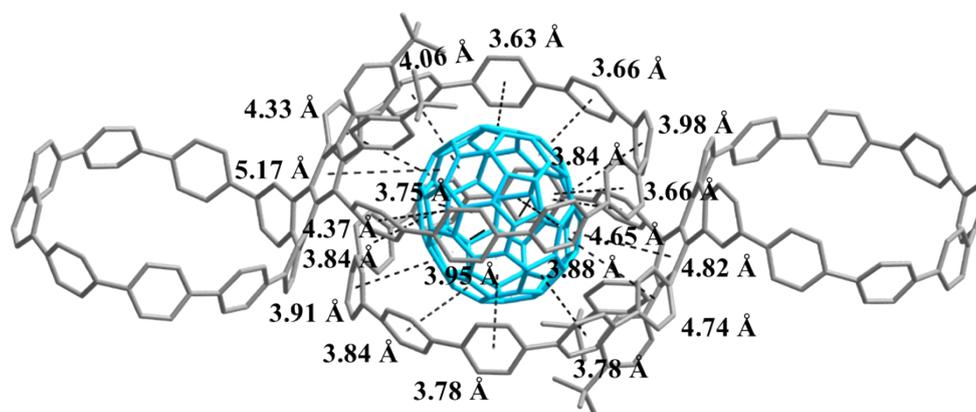


Figure S15. Side-views of a $C_{70}@(1a)_2$ complex highlighting the π - π interactions between the guests and cavities. Hydrogen atoms and disordered solvent molecules are omitted for clarity.

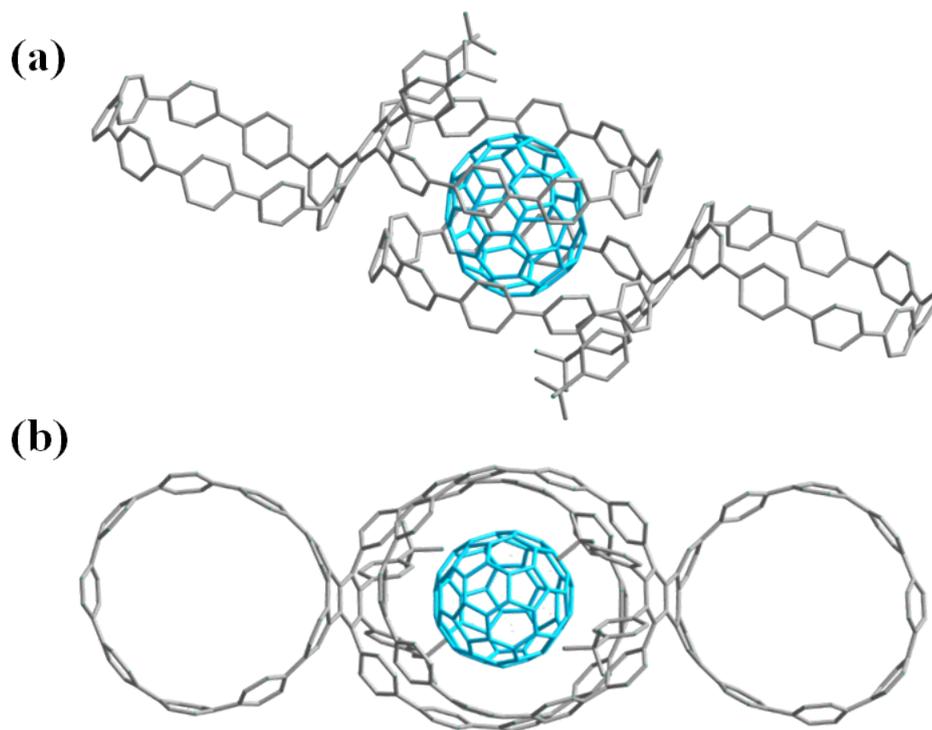


Figure S16. Side view (a) and top view (b) of the X-ray crystal structure of $C_{70}@(\mathbf{1a})_2$. Hydrogen atoms and disordered solvent molecules are omitted for clarity.

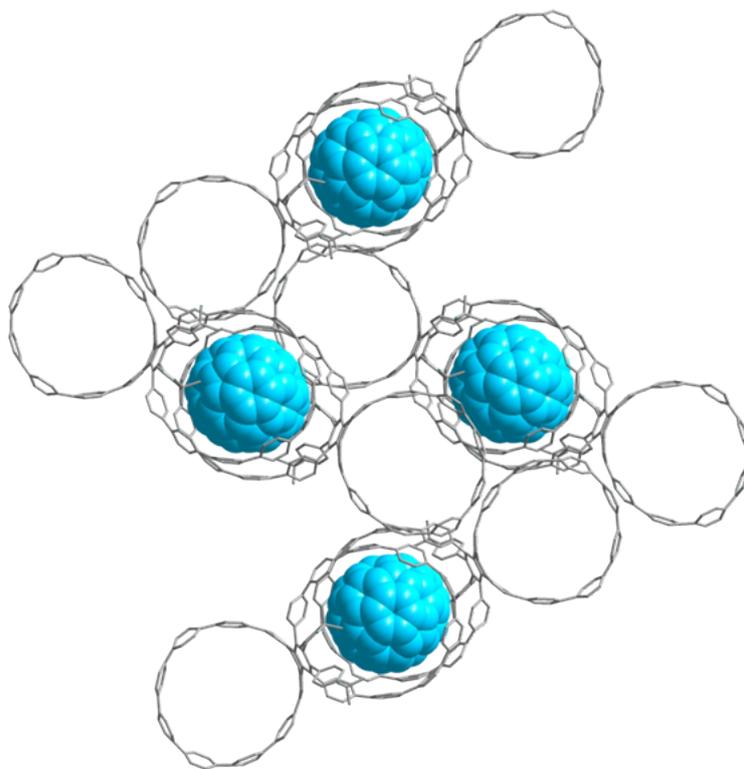


Figure S17. Packing structure of $C_{70}@(\mathbf{1a})_2$. Hydrogen atoms and solvent molecules are omitted for clarity.

Table S3. Crystal data and structure refinement for 3C₆₀@(1b)₂

| Complex | 3C ₆₀ @(1b) ₂ |
|------------------------------------|---|
| Formular | C ₁₁₅₈ H ₆₇₂ |
| Formular weight | 14584.92 |
| Temperature/K | 173(2) |
| Crystal system | monoclinic |
| Space group | P21/n |
| a / Å | 20.8830(7) |
| b / Å | 27.5133(9) |
| c / Å | 33.7675(11) |
| α / deg | 90 |
| β / deg | 97.309(2) |
| γ / deg | 90 |
| Volume/Å ³ | 19243.8(11) |
| Z | 1 |
| ρ _{calc} /cm ³ | 1.259 |
| μ/mm ⁻¹ | 0.350 |
| F(000) | 7620.0 |
| Crystal size/mm ³ | 0.340 × 0.210 × 0.170 |
| Radiation | Ga Kα (λ = 1.34138) |
| 2θ range for data collection/° | 6.042 to 106.074 |
| Index ranges | -24 ≤ h ≤ 20, -32 ≤ k ≤ 32, -40 ≤ l ≤ 40 |
| Reflections collected | 195069 |
| Independent reflections | 33959[R _{int} = 0.0495, R _{sigma} = 0.0407] |
| Data/restraints/parameters | 33959/2201/3350 |
| Goodness-of-fit on F ² | 1.039 |
| Final R indexes [I ≥ 2σ (I)] | R ₁ = 0.0904, wR ₂ = 0.2630 |
| Final R indexes [all data] | R ₁ = 0.1055, wR ₂ = 0.2790 |

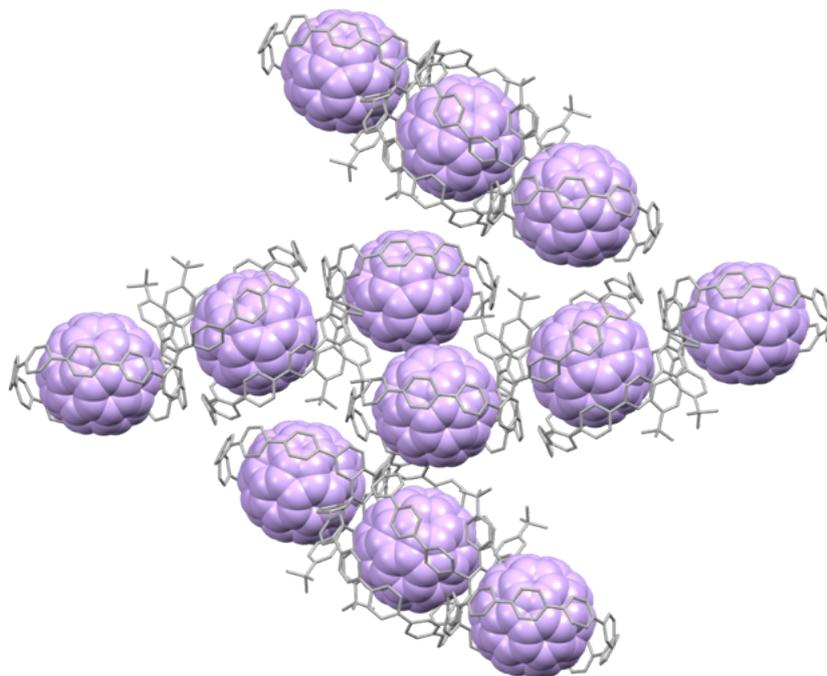


Figure S20. Packing structure of $3C_{60}@(1b)_2$. Hydrogen atoms and solvent molecules are omitted for clarity.

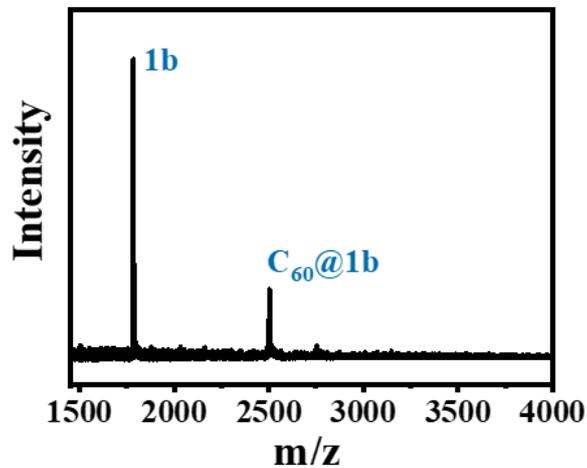


Figure S21. HR-MS (MALDI-TOF) data for $C_{60}@1b$ complex.

Fluorescence Quenching Experiments.

Fluorescence quenching was studied by the addition of C_{60} to **1b**. To a solution of **1b** (3.33×10^{-6} M) in toluene was added a solution of the C_{60} in toluene at 25 °C. The

concentrations of C_{60} range from 0 to 1.0×10^{-5} M. The changes in the fluorescence intensity of **1b** were measured at 474 nm. The binding constant (K_a) was determined by using equation:^{S2, S3}

$$F/F_0 = (1 + (k_f/k_s)K_a[\text{guest}])/(1 + K_a[\text{guest}])$$

F: fluorescence intensity of **1b**

F_0 : fluorescence intensity of **1b** before the addition of C_{60}

k_f : the proportionality constant of the complex

k_s : the proportionality constant of the host

[guest]: concentration of C_{60}

K_a : binding constant

Data points of fluorescence quenching experiments at 438 nm, 450 nm, 474 nm, and 485nm were fitted by the open access web portal Supramolecular.org (<http://supramolecular.org>). Links to all the fittings of the data are provided below:

1:1

<http://app.supramolecular.org/bindfit/view/3bd45da6-ec97-4de5-a79a-a729d09f9006>

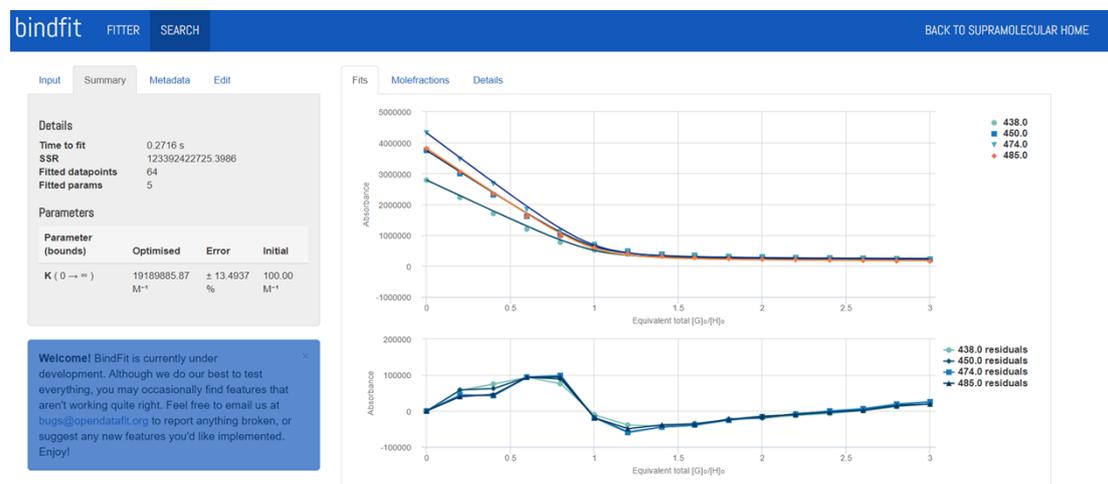


Figure S22. Screenshot from the result window of *supramolecular.org* from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/3bd45da6-ec97-4de5-a79a-a729d09f9006> which was fitted to 1:1 fluorescence quenching data.

1:2 full

<http://app.supramolecular.org/bindfit/view/be2cffe8-ec0e-47f1-8901-f8cd76c59e9d>

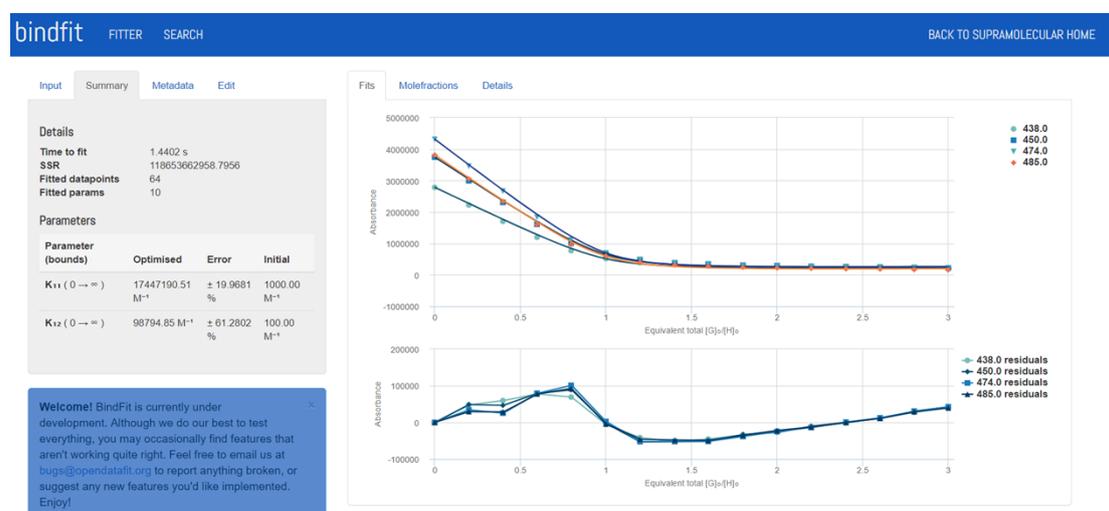


Figure S23. Screenshot from the result window of *supramolecular.org* from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/be2cffe8-ec0e-47f1-8901-f8cd76c59e9d> which was fitted to 1:2 full fluorescence quenching data.

1:2 additive

<http://app.supramolecular.org/bindfit/view/03e7c184-a79a-46c9-ba91-e7bc0aef0e58>

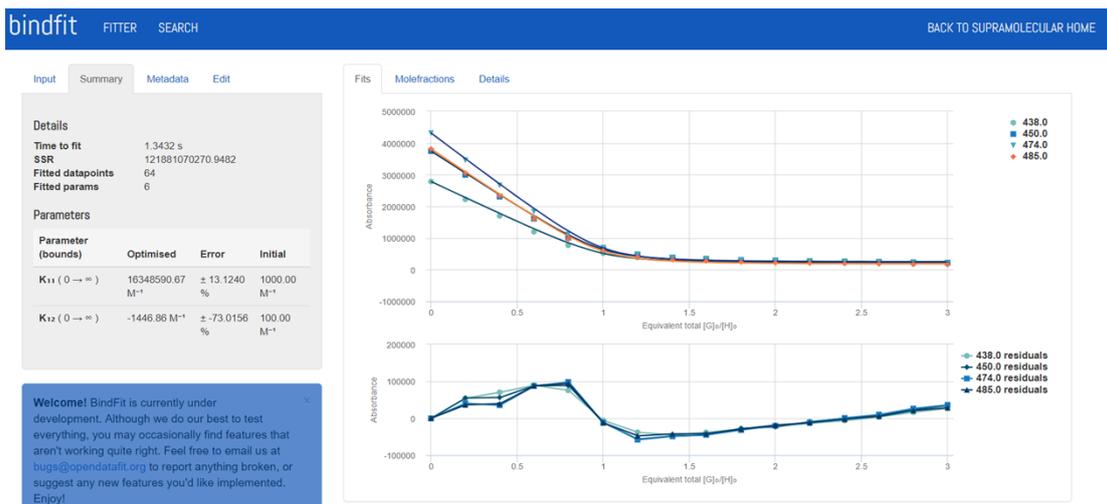


Figure S24. Screenshot from the result window of *supramolecular.org* from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/03e7c184-a79a-46c9-ba91-e7bc0aef0e58> which was fitted to 1:2 additive fluorescence quenching data.

1:2 non-cooperative

<http://app.supramolecular.org/bindfit/view/442de229-7fe8-4bc5-9958-744f573cde59>

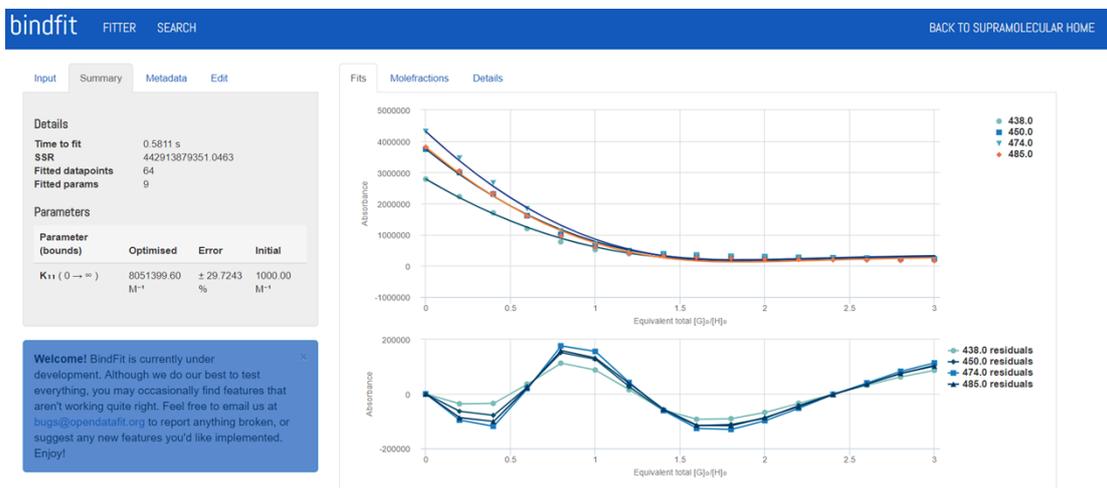


Figure S25. Screenshot from the result window of *supramolecular.org* from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/442de229-7fe8-4bc5-9958-744f573cde59> which was fitted to 1:2 non-cooperative fluorescence quenching data.

1:2 statistical

<http://app.supramolecular.org/bindfit/view/1ec97175-692d-47e1-bc84-950104d43590>

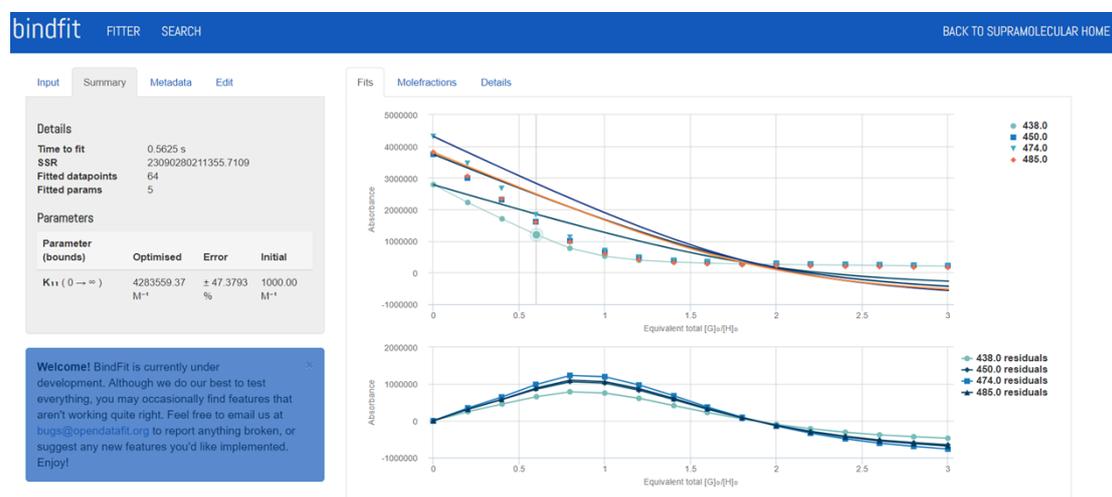


Figure S26. Screenshot from the result window of *supramolecular.org* from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/1ec97175-692d-47e1-bc84-950104d43590> which was fitted to 1:2 statistical fluorescence quenching data.

Computational Details.

Density functional theory calculations were used to identify the performed by using Gaussian 09 software.^{S4} Geometrical optimization were carried out at the theoretical level of B3LYP/6-31G(d,p), where DFT-D3(BJ)^{S5} and Polarizable continuum model (PCM)^{S6} methodologies can be used to correct dispersion force and solvent effect of dichloromethane. The resultant structures were further validated by frequency analysis without imaginary frequency. The strain energy (SE) was calculated using the reported computational methods.^{S7, S8} Moreover, time-dependent density functional theory (TD-DFT) with PBE0/6-31G(d,p)//PCM were used to simulate the UV spectra. The

S25

interaction between fullerene and bismacrocycle is typically evaluated following the formula: $E_{\text{int}} = E(\text{fullerene@bismacrocycle}) - E(\text{bismacrocycle}) - E(\text{fullerene})$, where $E(\text{fullerene@bismacrocycle})$, $E(\text{bismacrocycle})$ and $E(\text{fullerene})$ are the energy of optimized molecule, respectively.

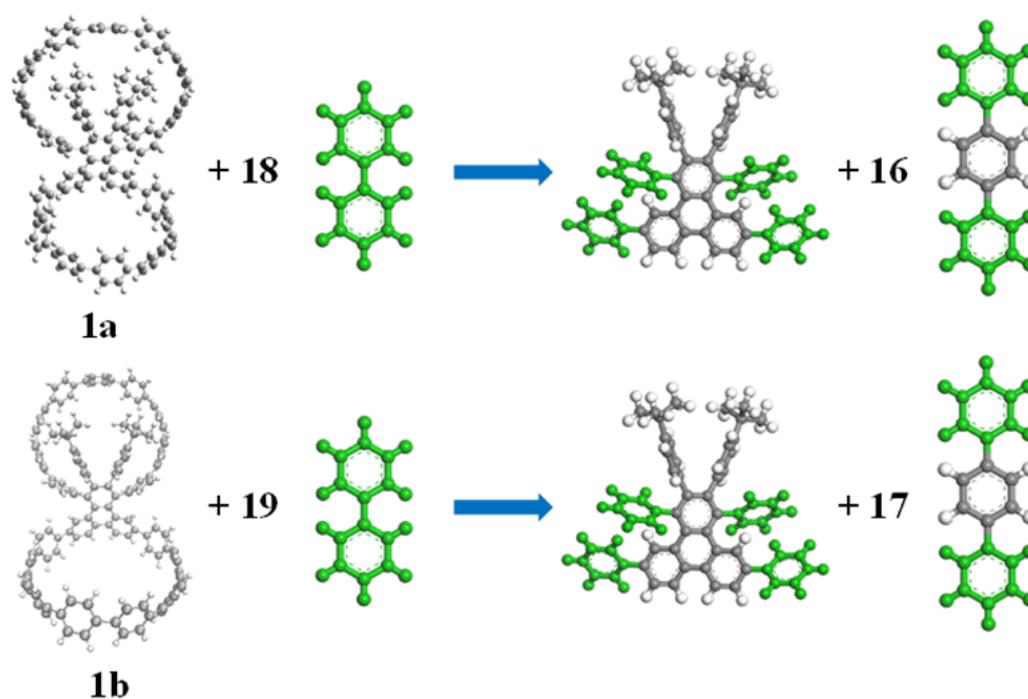


Figure S27. The calculation scheme of strain energy of **1a** and **1b**.

Table S4. Energy and strain energy for [9]CPP, [10]CPP, **1a**, and **1b**

| [9]CPP | |
|--------------------------|---------------|
| Biphenyl | -463.3704144 |
| Triphenyl | -694.4619375 |
| [9]CPP | -2079.7205796 |
| strain energy (kcal/mol) | 64.71 |

| [10]CPP | |
|--|---------------|
| Biphenyl | -463.3704144 |
| Triphenyl | -694.4619375 |
| [10]CPP | -2310.820458 |
| strain energy (kcal/mol) | 59.47 |
| 1a | |
| Biphenyl | -463.3704144 |
| Triphenyl | -694.4619375 |
| 1a | -5164.9571664 |
| Bridging phenyl with tert-Butylbenzene | -2394.397954 |
| strain energy (kcal/mol) | 103.12 |
| 1b | |
| Biphenyl | -463.3704144 |
| Triphenyl | -694.4619375 |
| 1b | -5396.048569 |
| Bridging phenyl with tert-Butylbenzene | -2394.397954 |
| strain energy (kcal/mol) | 103.19 |

Table S5. energy level (unit: eV) of frontier molecular orbitals for **1a**, **1b**, $C_{60}@(\mathbf{1a})_2$, $C_{70}@(\mathbf{1a})_2$, and $3C_{60}@(\mathbf{1b})_2$

| Molecule | 1a | 1b | $C_{60}@(\mathbf{1a})_2$ | $C_{70}@(\mathbf{1a})_2$ | $3C_{60}@(\mathbf{1b})_2$ |
|----------|-----------|-----------|--------------------------|--------------------------|---------------------------|
| LUMO+3 | -1.39922 | -1.49391 | -2.05338 | -2.47489 | -2.93558 |
| LUMO+2 | -1.52085 | -1.51840 | -3.17450 | -2.96007 | -3.02729 |
| LUMO+1 | -1.70317 | -1.71052 | -3.20634 | -3.03817 | -3.05150 |
| LUMO | -1.81936 | -1.84385 | -3.21913 | -3.05803 | -3.06919 |
| HOMO | -5.19795 | -5.22054 | -5.16503 | -5.19006 | -5.22000 |
| HOMO-1 | -5.32340 | -5.26816 | -5.17782 | -5.21673 | -5.22081 |

| | | | | | |
|-----------|----------|----------|----------|----------|----------|
| HOMO-2 | -5.47279 | -5.49483 | -5.33374 | -5.34490 | -5.31741 |
| HOMO-3 | -5.60123 | -5.52776 | -5.35796 | -5.39932 | -5.33537 |
| HOMO-LUMO | 3.37859 | 3.37668 | 1.94590 | 2.13202 | 2.15080 |

Table S6. Oscillator strengths and transitions of **1a** and **1b** from DFT calculations

| $\lambda_{\text{Exp.}}$ | λ_{DFT} | f_{osc} | Transitions |
|-------------------------|------------------------|------------------|--|
| 1a | | | |
| 346.5 | 380.9 | 0.52 | HOMO-1 → LUMO (47%) |
| | 372.9 | 1.14 | HOMO-2 → LUMO (44%) |
| | 367.67 | 0.92 | HOMO → LUMO+2 (47%) |
| | 364.8 | 0.38 | HOMO-2 → LUMO+1 (26%) |
| | 358.7 | 0.52 | HOMO → LUMO+3 (23%) |
| | 355.7 | 0.24 | HOMO → LUMO+3 (37%) |
| | 354.9 | 0.57 | HOMO-5 → LUMO (23%) |
| | 348.5 | 0.27 | HOMO → LUMO+4 (78%) |
| | 318.5 | 0.36 | HOMO-2 → LUMO+5 (28%) |
| 1b | | | |
| 346 | 367.67 | 1.2357 | HOMO-1 → LUMO+1 (30%) HOMO-1 → LUMO (19%) HOMO-3 → LUMO (17%) HOMO → LUMO+2 (15%) |
| | 362.12 | 2.8321 | HOMO-2 → LUMO (26%) HOMO-1 → LUMO+3 (15%) HOMO-2 → LUMO+1 (12%) |
| | 361.53 | 1.2074 | HOMO → LUMO+1 (23%) HOMO-1 → LUMO (14%) |
| | 345.14 | 0.7481 | HOMO-4 → LUMO (25%) HOMO → LUMO+4 (16%) HOMO-5 → LUMO (12%) |

| | | | |
|--|--------|--------|---|
| | 340.79 | 0.2570 | HOMO-3 → LUMO (28%) HOMO-1 → LUMO+2 (13%) |
| | 323.19 | 0.4924 | HOMO-3 → LUMO+2 (18%) HOMO-2 → LUMO+3 (18%) HOMO-3 → LUMO+1 (16%) |
| | 317.37 | 0.2263 | HOMO → LUMO+5 (33%) HOMO-2 → LUMO+3 (16%) |
| | 308.84 | 0.2080 | HOMO-6 → LUMO (30%) HOMO → LUMO+6 (26%) |

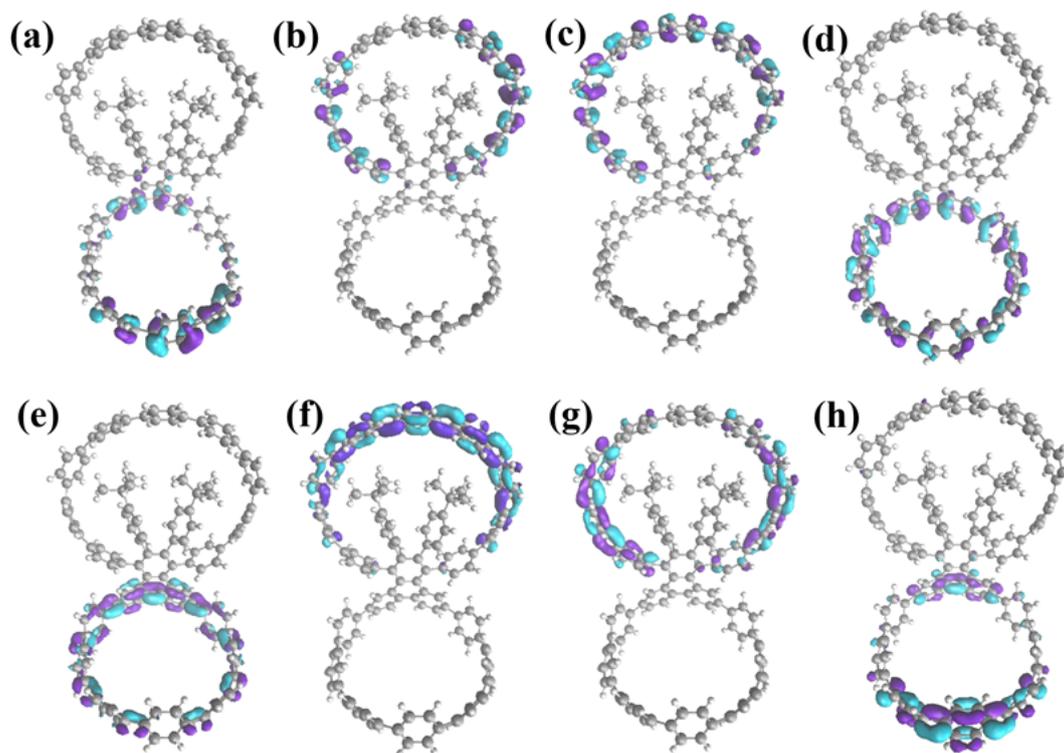


Figure S28. Frontier molecular orbitals of **1a**: HOMO-3 (a), HOMO-2 (b), HOMO-1 (c), HOMO (d), LUMO (e), LUMO+1 (f), LUMO+2 (g), LUMO+3 (h).

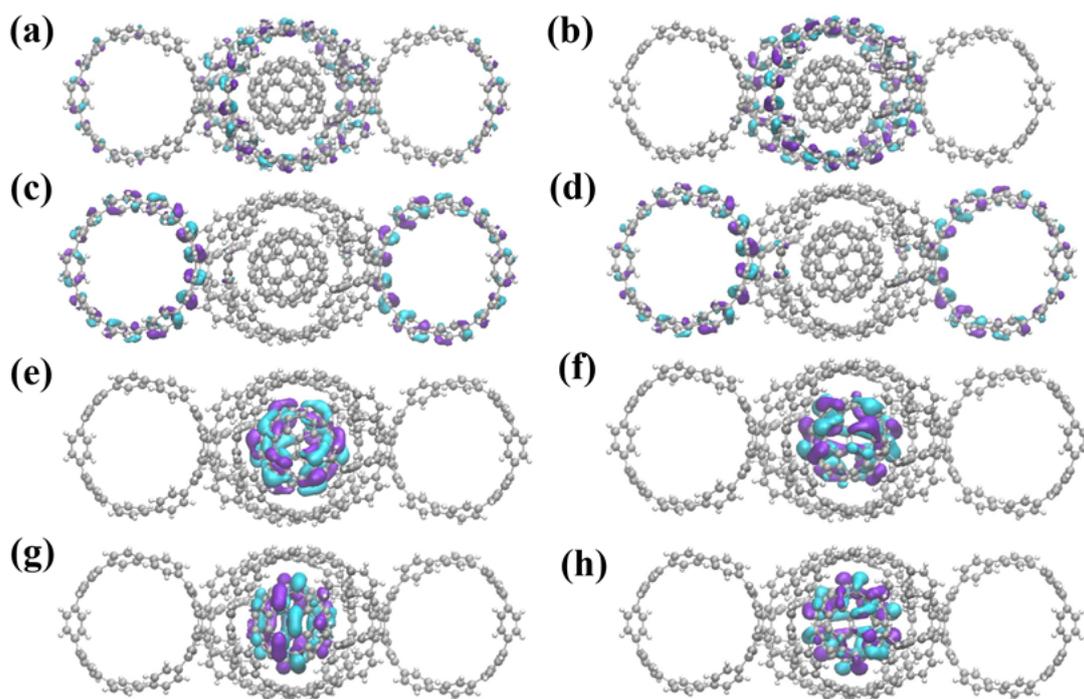


Figure S29. Frontier molecular orbitals of $C_{60}@(\mathbf{1a})_2$: HOMO-3 (a), HOMO-2 (b), HOMO-1 (c), HOMO (d), LUMO (e), LUMO+1 (f), LUMO+2 (g), LUMO+3 (h).

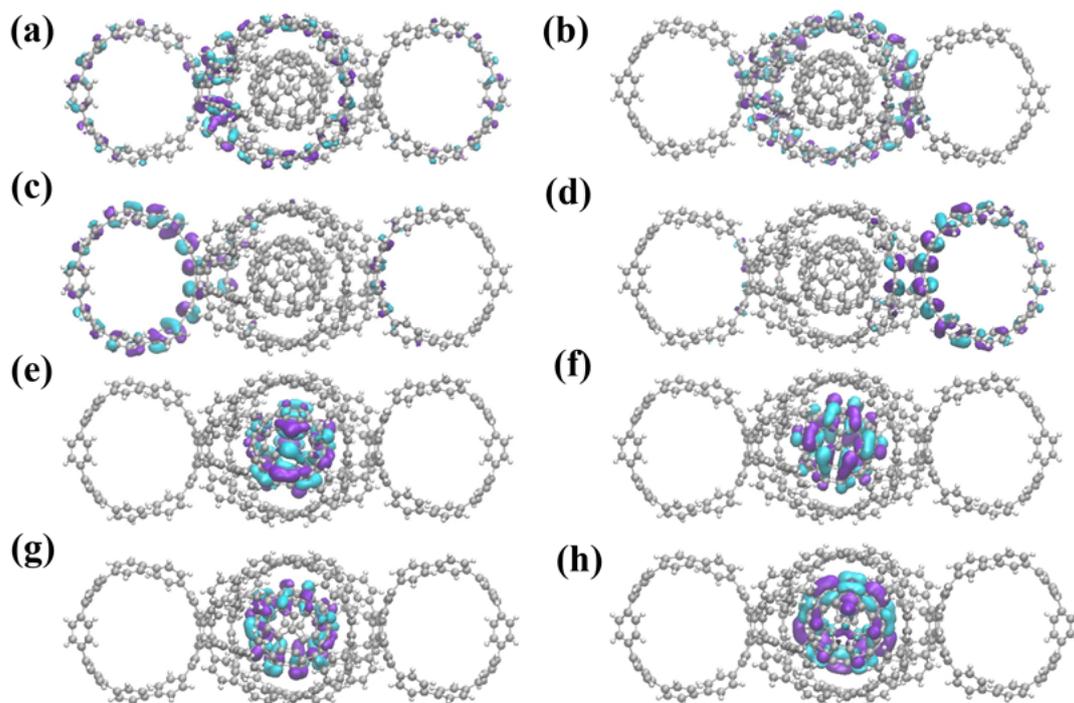


Figure S30. Frontier molecular orbitals of $C_{70}@(\mathbf{1a})_2$: HOMO-3 (a), HOMO-2 (b), HOMO-1 (c), HOMO (d), LUMO (e), LUMO+1 (f), LUMO+2 (g), LUMO+3 (h).

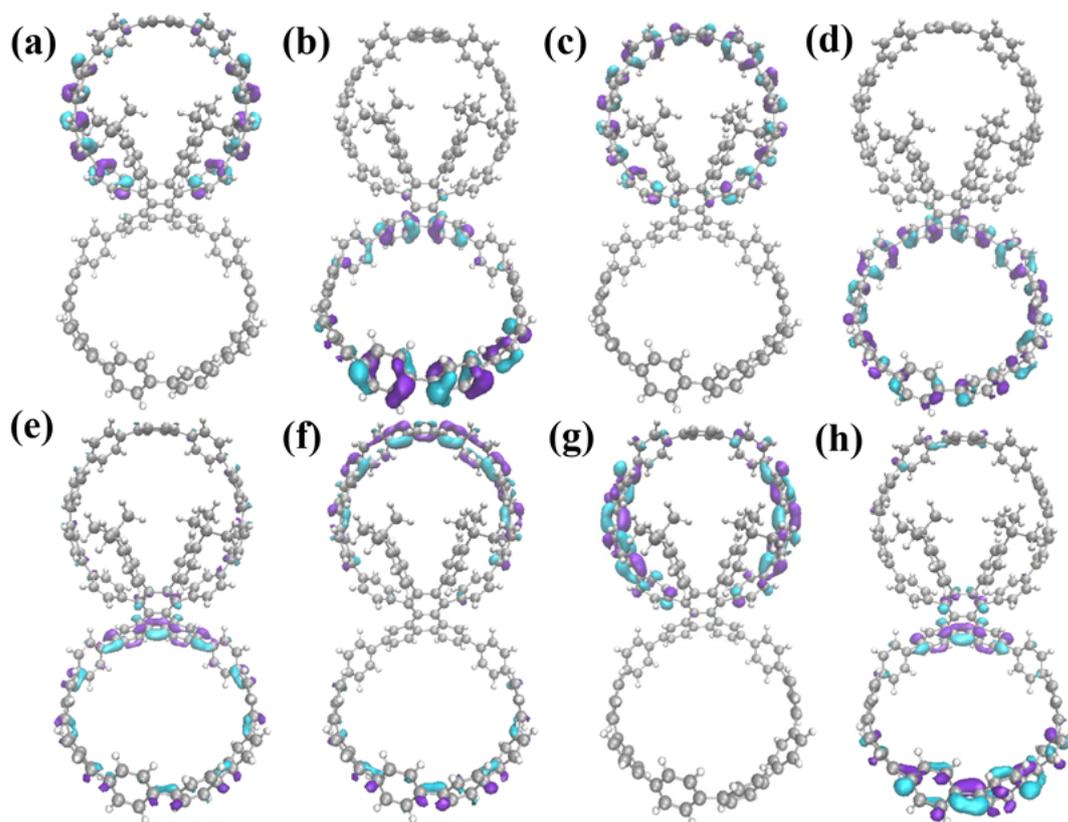


Figure S31. Frontier molecular orbitals of **1b**: HOMO-3 (a), HOMO-2 (b), HOMO-1 (c), HOMO (d), LUMO (e), LUMO+1 (f), LUMO+2 (g), LUMO+3 (h).

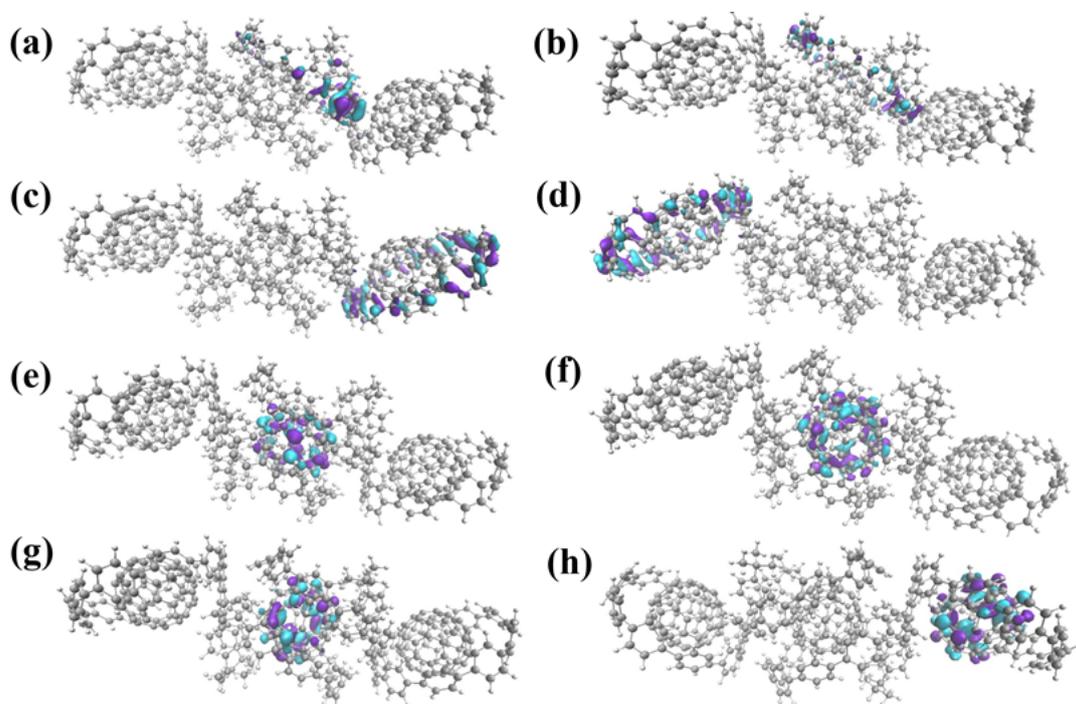


Figure S32. Frontier molecular orbitals of $3C_{60}@(\mathbf{1b})_2$: HOMO-3 (a), HOMO-2 (b), HOMO-1 (c), HOMO (d), LUMO (e), LUMO+1 (f), LUMO+2 (g), LUMO+3 (h).

Table S7. Relaxed structures of **1a**, **1b**, $C_{60}@(\mathbf{1a})_2$, $C_{70}@(\mathbf{1a})_2$, and $3C_{60}@(\mathbf{1b})_2$

| 1a | | | | | | | |
|-----------|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -0.312325 | -3.856037 | -2.963445 | C | 9.704870 | -4.332325 | 4.341429 |
| C | 0.487880 | -1.692691 | -1.966768 | C | 11.062103 | -4.042499 | 2.384923 |
| C | -0.977164 | -5.059291 | -2.749391 | C | 8.588418 | -6.518258 | 0.025418 |
| C | -1.629674 | 1.217387 | -0.793022 | C | 9.660445 | 5.047893 | 3.423498 |
| C | -0.661996 | 3.119944 | -3.110937 | C | 11.451498 | 1.827785 | 4.236273 |
| C | 0.279715 | -3.171523 | -1.895754 | C | -6.542338 | -2.268836 | 0.530609 |
| C | 2.479076 | -1.803827 | -3.494605 | C | 4.051759 | 4.963876 | -2.890965 |
| C | -0.484792 | -0.937154 | -1.291735 | C | 6.804417 | 4.948923 | -3.239246 |
| C | 0.180422 | 4.703340 | -0.991430 | C | 10.296018 | -3.212217 | 4.916730 |
| C | -10.983859 | -0.275193 | 0.826489 | C | 4.863411 | 5.736995 | -2.068267 |
| C | -4.213118 | 7.412448 | -0.278081 | C | 12.601465 | -0.310795 | 4.051876 |
| C | 1.482686 | 0.377293 | -2.849078 | C | 10.409615 | -0.225218 | 5.023348 |
| C | 1.473477 | -1.042854 | -2.746792 | C | 10.261890 | 4.065755 | 4.203670 |
| C | 0.386843 | -3.843276 | -0.671479 | C | 12.594469 | 1.073401 | 3.915538 |
| C | 0.506927 | 1.129822 | -2.150516 | C | 5.995010 | 4.174290 | -4.060733 |
| C | -1.629947 | -1.565069 | -0.559125 | C | 10.402653 | 1.157005 | 4.887254 |
| C | 2.467249 | 1.001389 | -3.742016 | C | -6.173678 | 1.810309 | 1.370797 |
| C | -0.239867 | -5.066203 | -0.470535 | C | -4.931999 | 3.779072 | 2.276072 |
| C | 2.921852 | 2.314307 | -3.544145 | C | -5.903047 | 3.891100 | -0.016725 |
| C | 0.294035 | 2.613440 | -2.224921 | H | -0.361449 | -3.379666 | -3.937712 |
| C | 3.087579 | -1.224847 | -4.636656 | H | -1.549881 | -5.480106 | -3.567956 |
| C | -10.630657 | -2.515516 | 1.851754 | H | -1.028535 | 2.486258 | -3.912083 |
| C | 2.950497 | -3.045221 | -3.038951 | H | 0.518236 | 5.309846 | -0.156895 |
| C | -0.916201 | 5.127794 | -1.760768 | H | -10.972727 | -0.752566 | -0.147282 |
| C | -1.262253 | 4.353728 | -2.879672 | H | 0.887822 | -3.355844 | 0.159026 |
| C | -5.922105 | 7.668404 | 1.566575 | H | -0.180971 | -5.519596 | 0.512071 |
| C | -10.812519 | 1.773871 | 2.126212 | H | 2.627388 | 2.829003 | -2.645781 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -5.609250 | 7.556165 | 0.198815 | H | 2.642276 | -3.382139 | -2.061348 |
| C | -1.047465 | -5.640119 | -1.469527 | H | -2.102007 | 4.654588 | -3.497191 |
| C | -0.473576 | 0.472459 | -1.388098 | H | -5.168972 | 8.020631 | 2.264254 |
| C | -10.435063 | 3.204983 | 2.130525 | H | -1.067763 | -0.784540 | 1.361150 |
| C | -3.936569 | 2.387177 | 0.387639 | H | -2.506271 | -2.474303 | -2.301622 |
| C | -8.578656 | -6.093485 | 0.726522 | H | -2.988690 | 0.515658 | -2.303595 |
| C | -1.825175 | -1.324973 | 0.803174 | H | -11.705506 | 3.815619 | 0.497213 |
| C | -2.630087 | -2.265344 | -1.245855 | H | -8.612340 | 6.387022 | -0.873368 |
| C | 3.070268 | 0.230621 | -4.771669 | H | -10.567167 | 5.952641 | 0.115144 |
| C | -2.890880 | 1.092958 | -1.390291 | H | -11.795342 | -2.818518 | 0.059631 |
| C | -10.901401 | -1.066030 | 1.984830 | H | -4.519967 | 8.007828 | -2.333200 |
| C | -10.877426 | 4.098889 | 1.139674 | H | -2.680608 | -7.166491 | -3.140790 |
| C | 9.022580 | 5.797192 | 1.087903 | H | -7.317697 | 7.246740 | 3.131702 |
| C | -7.888020 | 6.792103 | -0.175151 | H | -4.977324 | 1.520612 | -1.293325 |
| C | -10.232199 | 5.311549 | 0.924609 | H | -8.683787 | -5.359204 | -1.297404 |
| C | -11.055151 | -3.246795 | 0.727958 | H | 1.534640 | 3.102906 | -0.534551 |
| C | -3.856595 | 7.505831 | -1.635709 | H | -0.573750 | 2.068112 | 0.871521 |
| C | -2.986806 | -7.147249 | -2.100375 | H | -4.546044 | -3.200061 | -1.172085 |
| C | -7.144037 | 7.228702 | 2.060264 | H | -10.807349 | -4.994966 | -0.484579 |
| C | -4.015811 | 1.659084 | -0.809674 | H | -3.496502 | 6.753037 | 1.646741 |
| C | -4.030264 | -2.359423 | 0.747969 | H | -2.552975 | 3.092523 | 1.883444 |
| C | -8.166614 | -6.025027 | -0.614803 | H | -6.634623 | -6.447231 | -2.040416 |
| C | 0.764497 | 3.460696 | -1.212104 | H | -10.903886 | 1.684472 | -0.024409 |
| C | -1.536799 | 1.958307 | 0.384356 | H | -1.499294 | 5.665535 | 0.796043 |
| C | -3.794834 | -2.663732 | -0.601519 | H | -9.065572 | 2.994621 | 3.782109 |
| C | -2.137874 | -6.588454 | -1.125148 | H | -6.477732 | 7.145631 | -1.733177 |
| C | 3.868762 | 2.919637 | -4.367686 | H | -10.797595 | 1.473010 | 4.262743 |
| C | -10.499735 | -4.483070 | 0.422068 | H | -4.928281 | -7.915214 | -2.573879 |
| C | -3.267012 | 6.841768 | 0.591280 | H | -8.445798 | -4.810634 | 3.096946 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -2.670032 | 2.534923 | 0.961718 | H | -9.406399 | -2.629625 | 3.624509 |
| C | -7.000762 | -6.647513 | -1.039172 | H | -3.125385 | -1.461240 | 2.489243 |
| C | -9.108581 | 5.680683 | 1.685451 | H | -2.494646 | 6.927502 | -3.185532 |
| C | -10.943697 | 1.110493 | 0.895367 | H | 5.004795 | -3.884615 | -5.595170 |
| C | -6.191857 | -7.363699 | -0.140225 | H | 4.333679 | -1.670573 | -6.351224 |
| C | -4.751779 | -7.499875 | -0.461138 | H | 4.270533 | 0.367337 | -6.567270 |
| C | -9.499517 | -5.049086 | 1.230792 | H | -10.885125 | -0.976677 | 4.141835 |
| C | -1.861072 | 6.157468 | -1.270844 | H | -6.151301 | -8.209076 | 1.846604 |
| C | -8.109101 | 6.664145 | 1.206348 | H | -8.213544 | -7.110780 | 2.595258 |
| C | -2.122489 | 6.224639 | 0.107238 | H | 4.918559 | 2.694093 | -6.252275 |
| C | -9.429995 | 3.654464 | 3.001490 | H | -7.925544 | 5.114774 | 3.398528 |
| C | -6.664555 | 7.227803 | -0.668131 | H | 3.040603 | -5.514774 | -1.746066 |
| C | -10.841994 | 0.989389 | 3.291610 | H | 7.283477 | 5.357624 | 2.284123 |
| C | -4.267982 | -7.582139 | -1.778629 | H | 10.485654 | 6.408190 | -0.378818 |
| C | -9.206936 | -4.399710 | 2.442201 | H | 8.878322 | 6.624191 | -2.218046 |
| C | 3.922361 | -3.775334 | -3.718886 | H | 5.686908 | 5.577135 | 0.457553 |
| C | -9.755509 | -3.157690 | 2.743265 | H | -1.932218 | -6.336204 | 1.013834 |
| C | -5.361037 | -2.752516 | 1.400899 | H | 11.278629 | 4.459779 | 0.505631 |
| C | 9.953896 | 5.166547 | 2.052962 | H | 7.949996 | -5.456294 | -2.326416 |
| C | -3.004443 | -1.706422 | 1.440833 | H | -4.141902 | -7.120055 | 1.570655 |
| C | -2.706631 | 6.890700 | -2.121283 | H | 4.475125 | -6.568368 | -0.060073 |
| C | 4.318401 | -3.301990 | -4.988846 | H | 12.332023 | 2.742235 | 1.871112 |
| C | -5.215067 | 2.964339 | 1.004702 | H | 6.527993 | -4.404164 | -4.000897 |
| C | 4.674531 | -4.812333 | -2.976596 | H | 5.743683 | -5.456717 | 1.528198 |
| C | 3.920992 | -2.050757 | -5.423674 | H | -4.769856 | -2.515398 | 3.501505 |
| C | 3.871147 | 0.908531 | -5.717027 | H | -6.508243 | -2.416075 | 3.203155 |
| C | -10.888981 | -0.399545 | 3.222354 | H | 12.361257 | -2.348731 | 2.373701 |
| C | -6.711125 | -7.597535 | 1.145590 | H | 7.333014 | -4.879816 | 3.281991 |
| C | -7.879394 | -6.972580 | 1.571305 | H | -4.591450 | -4.654844 | 2.140560 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.253912 | 2.224926 | -5.533639 | H | -5.336530 | -4.765852 | 0.544926 |
| C | 7.159841 | 6.050140 | -1.043228 | H | 10.551447 | -6.393499 | 0.873531 |
| C | -8.781973 | 4.864035 | 2.782848 | H | 8.949872 | -4.878483 | 4.898808 |
| C | 4.117776 | -5.504606 | -1.884503 | H | 11.326016 | -4.307432 | 1.366689 |
| C | 7.640249 | 5.687866 | 1.314334 | H | 8.951422 | -6.968019 | -0.893814 |
| C | 9.431843 | 6.231611 | -0.185720 | H | 8.901405 | 5.685688 | 3.866289 |
| C | 8.520243 | 6.354632 | -1.229033 | H | -6.501392 | -1.184707 | 0.389351 |
| C | 6.729750 | 5.812383 | 0.272892 | H | -7.493038 | -2.519317 | 1.010174 |
| C | -2.548829 | -6.723688 | 0.212446 | H | 2.975835 | 4.986075 | -2.745766 |
| C | 11.018059 | 4.395116 | 1.556635 | H | 7.881588 | 4.876675 | -3.346325 |
| C | 6.872858 | -5.520264 | -2.213961 | H | 9.991176 | -2.904022 | 5.912303 |
| C | -3.819086 | -7.176546 | 0.537326 | H | 4.405742 | 6.350841 | -1.298187 |
| C | 4.931551 | -6.102180 | -0.928167 | H | 13.473075 | -0.871319 | 3.727640 |
| C | 11.619240 | 3.415191 | 2.335700 | H | 9.517269 | -0.718622 | 5.393604 |
| C | 6.061575 | -4.919739 | -3.168166 | H | 9.960855 | 3.954053 | 5.240968 |
| C | 11.211473 | -2.424460 | 4.195903 | H | 13.460730 | 1.568656 | 3.487360 |
| C | 10.002842 | -4.712034 | 3.020222 | H | 6.462619 | 3.519166 | -4.788148 |
| C | 4.610735 | 4.087969 | -3.840948 | H | 9.505088 | 1.704272 | 5.155038 |
| C | 6.265455 | 5.672339 | -2.162469 | H | -5.712445 | 1.139654 | 2.102546 |
| C | 6.788913 | -5.714399 | 1.393654 | H | -6.436807 | 1.213396 | 0.493212 |
| C | 11.183585 | 3.160937 | 3.646979 | H | -4.261131 | 4.616807 | 2.069367 |
| C | -5.526526 | -2.144224 | 2.803031 | H | -4.486605 | 3.161978 | 3.063222 |
| C | 7.225344 | -6.194171 | 0.147518 | H | -6.813922 | 4.315110 | 0.411526 |
| C | 11.652950 | -2.924805 | 2.959529 | H | -6.180947 | 3.352739 | -0.927260 |
| C | 6.333402 | -6.039669 | -1.025499 | H | -7.102242 | 2.204617 | 1.796922 |
| C | 7.695376 | -5.386174 | 2.393662 | H | -5.868583 | 4.191376 | 2.660647 |
| C | 9.079210 | -5.524950 | 2.194063 | H | -5.242642 | 4.713923 | -0.299530 |
| C | -5.415521 | -4.286288 | 1.521634 | H | -5.465659 | -1.051975 | 2.778663 |
| C | 9.495750 | -6.191686 | 1.027696 | H | -6.358106 | -4.605009 | 1.972559 |

| | | | | | | | |
|--------------------------|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | 11.465719 | -0.999602 | 4.514597 | H | -6.539020 | -2.740020 | -0.455756 |
| $C_{60}@(\mathbf{1a})_2$ | | | | | | | |
| C | 7.422181 | 2.792427 | 0.738721 | C | -7.403608 | 1.139493 | -4.636681 |
| C | 9.732780 | 3.204938 | -2.670492 | C | -19.780074 | -0.744083 | -2.012358 |
| C | 8.406738 | 0.638163 | -0.222011 | C | -18.865017 | -4.153228 | 1.076538 |
| C | 8.386038 | -0.776038 | -0.149991 | C | -19.497230 | -3.692371 | -1.583290 |
| C | 8.792958 | -0.928786 | -2.604667 | C | -18.240438 | -4.936543 | 0.091490 |
| C | 8.796357 | -1.541909 | -1.327313 | C | -20.404607 | -1.412975 | -0.946359 |
| C | 7.584541 | -0.654318 | 2.153608 | C | -18.655392 | -4.744809 | -1.238761 |
| C | 7.720890 | 3.840700 | 1.618364 | C | -19.961601 | -2.787164 | -0.612167 |
| C | 6.319279 | 2.944338 | -0.113962 | C | -6.620996 | 1.458976 | -5.748723 |
| C | 8.797902 | 0.527494 | -2.682113 | C | -15.444485 | 6.693215 | 1.480451 |
| C | 9.321699 | 2.581234 | -1.496274 | C | -21.193025 | -0.638583 | -0.076333 |
| C | 13.000335 | 5.823627 | -1.905431 | C | -14.337004 | 6.342112 | 0.687796 |
| C | 6.729653 | -4.794239 | 2.241145 | C | -5.295422 | 1.882962 | -5.608380 |
| C | 3.979168 | -5.495151 | 3.279191 | C | -19.778540 | 0.642859 | -2.087527 |
| C | 10.667729 | 4.348613 | -2.569686 | C | -2.817283 | -1.328322 | 1.717971 |
| C | 7.959356 | 1.404662 | 0.884988 | C | -16.742358 | 6.426679 | 1.057246 |
| C | 8.811809 | 1.272035 | -1.476390 | C | -20.401537 | 1.424407 | -1.100198 |
| C | 5.568547 | -4.941165 | 1.468206 | C | 1.963454 | -2.677582 | -1.269485 |
| C | 7.892565 | -1.418654 | 1.015263 | C | -14.598327 | 5.903208 | -0.620979 |
| C | 7.615391 | -3.745275 | 2.004865 | C | -19.706340 | -3.103138 | 0.732741 |
| C | 6.833467 | 4.902178 | 1.782971 | C | -2.522166 | -2.312764 | -0.946651 |
| C | 10.688798 | 5.204545 | -1.452594 | C | -16.988215 | 5.796135 | -0.175881 |
| C | 5.424431 | -4.123399 | 0.334483 | C | -21.191568 | 0.750299 | -0.151668 |
| C | 7.359905 | -2.812780 | 0.992082 | C | -3.539414 | -3.583327 | -6.429124 |
| C | 9.303439 | -2.846408 | -1.204242 | C | -0.431471 | -3.095625 | -1.694372 |
| C | 7.642309 | 0.761768 | 2.091811 | C | -1.626494 | -2.367788 | -2.093410 |
| C | 9.021147 | -1.755116 | -3.727841 | C | -15.894339 | 5.635483 | -1.042814 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | 10.655250 | -4.717825 | -2.077897 | C | -5.582849 | -5.000817 | -6.687643 |
| C | 5.657624 | 1.728552 | 3.229545 | C | -3.267253 | -1.160798 | -0.700453 |
| C | 6.308433 | -3.079748 | 0.101442 | C | 0.818687 | -2.697127 | -2.169012 |
| C | 7.775963 | 2.033511 | 4.300522 | C | -18.230608 | 5.035461 | -0.448771 |
| C | 9.464793 | 2.537773 | -3.888560 | C | -3.239043 | 1.189924 | -0.787492 |
| C | 11.759718 | 4.411826 | -3.450354 | C | -19.489320 | 3.619686 | -1.979631 |
| C | 7.037547 | 1.533306 | 3.225282 | C | -2.028626 | -2.526208 | 1.464721 |
| C | 5.638558 | 4.957361 | 1.051906 | C | 1.809806 | -3.059029 | 0.065844 |
| C | 4.474505 | 5.761397 | 1.488093 | C | 0.930311 | -1.552497 | -3.063057 |
| C | 15.456994 | 6.376054 | -2.192528 | C | -19.700061 | 3.284854 | 0.386457 |
| C | 9.720455 | -3.591898 | -2.303077 | C | -3.409482 | 0.795668 | 0.602464 |
| C | 4.388032 | -5.692396 | 1.950412 | C | -19.955729 | 2.825773 | -0.916479 |
| C | 12.901267 | 5.133278 | -3.124804 | C | -18.856847 | 4.364411 | 0.614964 |
| C | 11.832876 | 5.924787 | -1.126841 | C | -0.215177 | -0.853100 | -3.446099 |
| C | 3.613975 | 6.415136 | 0.594253 | C | -1.885051 | -3.008474 | 0.161428 |
| C | 1.791044 | -6.453014 | 2.807162 | C | -3.151422 | -0.017729 | -1.590393 |
| C | 9.024819 | 1.228071 | -3.887778 | C | -18.645551 | 4.701653 | -1.750648 |
| C | 6.886014 | -1.231800 | 3.345634 | C | 2.161827 | 0.570724 | -2.770050 |
| C | 5.745093 | 2.863761 | 5.374262 | C | 2.144401 | -0.824686 | -2.718887 |
| C | 2.352287 | 6.842944 | 0.998236 | C | 0.504569 | -3.472704 | 0.561100 |
| C | 0.358797 | -6.488709 | 3.176627 | C | -1.519661 | -1.269078 | -2.950030 |
| C | -2.257713 | -5.673212 | 3.919559 | C | -4.349862 | 2.102412 | -6.793765 |
| C | 3.522978 | -6.393763 | 1.096745 | C | -5.060457 | 1.936308 | -8.145621 |
| C | 4.075742 | 5.662566 | 2.830387 | C | -3.739526 | 3.518491 | -6.730003 |
| C | 5.019658 | 2.376877 | 4.281003 | C | -3.216045 | 1.054628 | -6.702745 |
| C | 5.444146 | 4.011149 | 0.032831 | C | 3.426254 | 0.663704 | -0.652582 |
| C | -3.399568 | -4.810425 | 4.293496 | C | 2.521259 | 2.315858 | 0.950083 |
| C | 0.469760 | 6.704199 | 2.684519 | C | 1.625581 | 2.370872 | 2.096839 |
| C | 14.611465 | 5.819586 | -0.017415 | C | -0.966887 | -1.297946 | 3.171415 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | 9.457742 | -3.058421 | -3.586514 | C | -0.819576 | 2.700232 | 2.172456 |
| C | 2.813187 | 6.080309 | 3.230222 | C | 1.567264 | -2.245319 | 2.266440 |
| C | 7.138409 | 2.689765 | 5.350659 | C | 3.238172 | -1.186837 | 0.790935 |
| C | 2.706948 | -5.863742 | 3.695251 | C | 2.027747 | 2.529311 | -1.461299 |
| C | -3.310773 | 5.176377 | 3.934410 | C | -1.810693 | 3.062121 | -0.062416 |
| C | 1.898842 | 6.621059 | 2.310027 | C | 2.464287 | -2.298632 | 1.119865 |
| C | 2.251288 | -6.772320 | 1.517848 | C | 0.355142 | -2.970966 | 1.921195 |
| C | -1.349853 | -6.161694 | 4.876866 | C | 1.884159 | 3.011572 | -0.158005 |
| C | 11.748110 | -4.876131 | -2.945521 | C | 2.302172 | 0.073073 | 2.697788 |
| C | -5.106069 | -2.574209 | 4.660186 | C | 2.781159 | -1.521527 | -1.609604 |
| C | -5.354666 | -3.508583 | 3.640237 | C | 1.518750 | 1.272164 | 2.953463 |
| C | -4.439741 | 4.941101 | 3.129225 | C | -0.884161 | -2.507441 | 2.364359 |
| C | 10.675079 | -5.448126 | -0.874898 | H | -8.590665 | -3.771742 | -2.259777 |
| C | 5.584065 | -1.726493 | 3.199492 | H | -6.080477 | -2.151041 | 0.809754 |
| C | -0.068464 | -6.557918 | 4.514329 | H | -9.516357 | -3.068666 | 0.549236 |
| C | 17.000814 | 5.661150 | -0.449821 | H | -6.891595 | 5.448225 | -3.091457 |
| C | -1.892211 | -5.789295 | 2.570157 | H | -4.622673 | 4.939669 | -3.952295 |
| C | -5.606776 | 1.633906 | 4.540963 | H | -8.443467 | 3.578285 | -2.686117 |
| C | 0.052005 | 6.874590 | 4.015962 | H | -7.025745 | -5.650013 | -2.547496 |
| C | -5.629786 | -1.191999 | 4.641828 | H | -9.824995 | -5.250091 | 0.790945 |
| C | 16.754833 | 6.154813 | -1.743803 | H | -4.543058 | 4.216740 | 0.288737 |
| C | -0.612849 | -6.190900 | 2.209750 | H | -9.492598 | 3.226197 | 0.211419 |
| C | -5.774197 | -0.430314 | 5.813456 | H | -8.911110 | 1.342924 | 4.724977 |
| C | 14.349582 | 6.114467 | -1.365874 | H | -5.075841 | -1.363826 | -2.397164 |
| C | 12.888895 | -5.558877 | -2.543084 | H | -6.110204 | 2.378687 | 0.700264 |
| C | -5.676703 | 0.871419 | 3.366114 | H | -8.852464 | -1.899814 | -4.319957 |
| C | 15.907399 | 5.597153 | 0.430118 | H | -9.677465 | -3.033306 | 4.830770 |
| C | -0.512357 | 6.354733 | 1.745722 | H | -11.777126 | -3.777036 | 4.324354 |
| C | -4.087243 | -2.867698 | 5.580831 | H | -15.295413 | -6.692375 | 3.215215 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | -5.763054 | 0.960033 | 5.763813 | H | -13.778340 | -5.041283 | 3.751429 |
| C | -4.516270 | -4.606101 | 3.463034 | H | -11.842551 | -6.521986 | 0.214664 |
| C | -4.023587 | 3.336736 | 5.352588 | H | -3.923163 | -6.564596 | 0.434667 |
| C | -5.297773 | 3.874492 | 3.385305 | H | -8.906859 | -0.719379 | 4.834423 |
| C | -1.796615 | 6.003254 | 2.139335 | H | -1.698150 | -7.320350 | -0.274219 |
| C | 5.070566 | 3.549643 | 6.568692 | H | -3.839989 | 6.618879 | -0.081167 |
| C | 12.986586 | -6.113532 | -1.256193 | H | -4.713393 | -5.137630 | -3.531280 |
| C | -5.057053 | 3.004014 | 4.462056 | H | -3.942654 | -2.490132 | -4.238648 |
| C | -5.688609 | -0.514001 | 3.415777 | H | -4.533512 | -4.036146 | 0.555649 |
| C | -2.156041 | 5.989828 | 3.495349 | H | -13.781454 | -5.617972 | -0.657335 |
| C | -3.251774 | -3.959267 | 5.400622 | H | -9.675131 | 3.645075 | 4.472316 |
| C | -3.168531 | 4.396835 | 5.093681 | H | -2.488276 | -5.882727 | -4.246761 |
| C | 4.808715 | -2.043568 | 4.302981 | H | -7.740515 | -3.059741 | -6.174915 |
| C | 11.818537 | -6.129354 | -0.472156 | H | -2.384570 | 5.594135 | -4.692513 |
| C | -1.233819 | 6.527156 | 4.411694 | H | -1.599698 | 7.289835 | -0.821463 |
| C | 5.415490 | 2.775751 | 7.859735 | H | 1.628482 | 6.176213 | -5.924482 |
| C | 7.404655 | -1.139579 | 4.637196 | H | -11.768885 | 4.331771 | 3.886244 |
| C | 19.781158 | 0.740086 | 2.007990 | H | 6.178052 | 3.354688 | -2.952545 |
| C | 18.866093 | 4.148408 | -1.081817 | H | 4.627213 | -5.565599 | -2.263104 |
| C | 19.499071 | 3.688308 | 1.577960 | H | -9.813591 | 5.417998 | 0.217079 |
| C | 18.242095 | 4.932272 | -0.096837 | H | -5.170464 | 1.845998 | -2.208099 |
| C | 20.405531 | 1.408405 | 0.941539 | H | -0.631220 | 6.874366 | -5.283831 |
| C | 18.657445 | 4.740885 | 1.233342 | H | 2.555267 | 5.427258 | -1.797733 |
| C | 19.962829 | 2.782608 | 0.607004 | H | -0.755118 | -7.230110 | -4.757647 |
| C | 6.621966 | -1.458614 | 5.749322 | H | -17.583268 | -6.304289 | 2.423498 |
| C | 15.442380 | -6.697409 | -1.480536 | H | 0.324160 | 6.127538 | -1.168969 |
| C | 21.193430 | 0.633465 | 0.071532 | H | 5.813768 | 0.935577 | -6.775801 |
| C | 14.335258 | -6.345704 | -0.687647 | H | -13.769305 | 5.527678 | 3.179623 |
| C | 5.296183 | -1.881989 | 5.609116 | H | 5.575062 | -1.356455 | -2.406531 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | 19.779250 | -0.646828 | 2.083672 | H | -16.053167 | -5.228261 | -1.443063 |
| C | 2.816411 | 1.331414 | -1.714539 | H | 0.234146 | -6.205771 | -0.710987 |
| C | 16.740465 | -6.431056 | -1.057868 | H | 3.863796 | 2.162280 | -6.370110 |
| C | 20.401697 | -1.428921 | 1.096427 | H | 5.794090 | -1.524915 | -6.687443 |
| C | -1.964336 | 2.680681 | 1.272918 | H | 4.703523 | 5.287803 | -2.636207 |
| C | 14.597135 | -5.906372 | 0.620873 | H | 3.807428 | -2.671874 | -6.183612 |
| C | 19.707205 | 3.098178 | -0.737930 | H | 6.135841 | -3.684411 | -2.718662 |
| C | 16.986903 | -5.800103 | 0.174934 | H | 2.473966 | -5.590971 | -1.397232 |
| C | 21.191599 | -0.755389 | 0.147380 | H | 5.599232 | 1.078632 | -2.494636 |
| C | 3.539426 | 3.583100 | 6.426601 | H | 2.393910 | 4.081889 | -6.054710 |
| C | 0.430577 | 3.098712 | 1.697799 | H | 2.304381 | -4.537942 | -5.729572 |
| C | 15.893360 | -5.638830 | 1.042173 | H | -3.795312 | 2.393646 | -4.137195 |
| C | 5.582357 | 5.001180 | 6.686067 | H | -11.830772 | 6.619976 | -0.494201 |
| C | 3.266300 | 1.163884 | 0.703899 | H | 1.512103 | -6.615156 | -5.456383 |
| C | 18.229586 | -5.039647 | 0.447113 | H | -5.071324 | -1.738529 | -7.793604 |
| C | 1.488179 | -1.083735 | 3.039018 | H | -6.493180 | -2.757481 | -8.047142 |
| C | 0.195796 | -0.600167 | 3.502624 | H | -8.412913 | 0.769435 | -4.783494 |
| C | 19.489187 | -3.623617 | 1.977005 | H | -19.165348 | -1.306319 | -2.707241 |
| C | -0.931199 | 1.555598 | 3.066503 | H | -18.575137 | -4.271922 | 2.115072 |
| C | 19.699215 | -3.289745 | -0.389283 | H | -19.742415 | -3.529490 | -2.628476 |
| C | 3.408637 | -0.792581 | -0.599032 | H | -18.259150 | -5.384694 | -2.021398 |
| C | 19.955446 | -2.830234 | 0.913391 | H | -7.054510 | 1.338990 | -6.734322 |
| C | 18.855640 | -4.369168 | -0.617091 | H | -15.284128 | 7.114300 | 2.468395 |
| C | 0.214282 | 0.856189 | 3.449542 | H | -21.758584 | -1.126545 | 0.711731 |
| C | 0.590579 | 3.494204 | 0.304349 | H | -19.162637 | 1.125346 | -2.839001 |
| C | 3.150504 | 0.020817 | 1.593839 | H | -17.572328 | 6.645947 | 1.722108 |
| C | 18.645056 | -4.705450 | 1.748721 | H | -13.770286 | 5.626399 | -1.264910 |
| C | -2.162709 | -0.567635 | 2.773485 | H | -20.049958 | -2.431650 | 1.512368 |
| C | -2.145278 | 0.827778 | 2.722322 | H | -21.756107 | 1.321781 | 0.578881 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -0.505451 | 3.475782 | -0.557678 | H | -3.115886 | -2.575745 | -6.370530 |
| C | 4.350698 | -2.101267 | 6.794597 | H | -3.099663 | -4.080368 | -7.299249 |
| C | 3.216989 | -1.053359 | 6.703735 | H | -16.042278 | 5.156700 | -2.004935 |
| C | 3.740165 | -3.517268 | 6.730856 | H | -5.131141 | -5.498459 | -7.552745 |
| C | 5.061453 | -1.935288 | 8.146382 | H | -6.669067 | -5.035268 | -6.809526 |
| C | 0.966003 | 1.301026 | -3.167978 | H | -19.734539 | 3.345196 | -3.001191 |
| C | -1.568154 | 2.248402 | -2.263011 | H | -20.045105 | 2.702299 | 1.234021 |
| C | -1.489076 | 1.086815 | -3.035585 | H | -18.567017 | 4.594246 | 1.634691 |
| C | -0.196690 | 0.603250 | -3.499187 | H | -18.247869 | 5.252303 | -2.597765 |
| C | -2.465170 | 2.301720 | -1.116434 | H | -5.466251 | 0.927020 | -8.266549 |
| C | -0.356027 | 2.974036 | -1.917769 | H | -4.351112 | 2.107964 | -8.961027 |
| C | -2.303077 | -0.069993 | -2.694346 | H | -3.057061 | 3.678533 | -7.571743 |
| C | -0.591468 | -3.491121 | -0.300929 | H | -3.170841 | 3.668566 | -5.808644 |
| C | -2.782011 | 1.524613 | 1.613028 | H | -2.635608 | 1.172115 | -5.783357 |
| C | 0.883278 | 2.510517 | -2.360930 | H | -2.530674 | 1.153552 | -7.551858 |
| C | -7.420705 | -2.793645 | -0.739263 | H | -4.933715 | -3.241234 | -8.727597 |
| C | -9.732373 | -3.207728 | 2.668736 | H | -3.224373 | -4.132322 | -5.537048 |
| C | -8.405847 | -0.639772 | 0.221737 | H | -5.328616 | -5.578392 | -5.793138 |
| C | -8.385669 | 0.774464 | 0.150155 | H | 8.593283 | 3.771443 | 2.257766 |
| C | -8.793562 | 0.926224 | 2.604747 | H | 6.080122 | 2.148203 | -0.807910 |
| C | -8.796728 | 1.539782 | 1.327592 | H | 9.517566 | 3.066707 | -0.550858 |
| C | -7.583364 | 0.653675 | -2.153217 | H | 6.890153 | -5.448730 | 3.092220 |
| C | -7.718780 | -3.841399 | -1.619740 | H | 4.620772 | -4.938235 | 3.953505 |
| C | -6.318646 | -2.946259 | 0.114414 | H | 8.443043 | -3.579705 | 2.686387 |
| C | -8.798068 | -0.530084 | 2.681703 | H | 7.028438 | 5.649813 | 2.545594 |
| C | -9.320969 | -2.583501 | 1.494911 | H | 9.826556 | 5.247997 | -0.793504 |
| C | -12.999013 | -5.826957 | 1.901554 | H | 4.540956 | -4.215417 | -0.286828 |
| C | -6.731012 | 4.793902 | -2.240269 | H | 9.491951 | -3.228186 | -0.210766 |
| C | -3.981160 | 5.496528 | -3.277849 | H | 8.909689 | -1.346269 | -4.724790 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -10.667024 | -4.351578 | 2.567163 | H | 5.078500 | 1.362629 | 2.395888 |
| C | -7.957753 | -1.405818 | -0.885283 | H | 6.109076 | -2.378341 | -0.698926 |
| C | -8.811318 | -1.274194 | 1.475712 | H | 8.853882 | 1.900448 | 4.320213 |
| C | -5.570257 | 4.941571 | -1.466927 | H | 9.677032 | 3.029718 | -4.832437 |
| C | -7.892171 | 1.417609 | -1.014802 | H | 11.777061 | 3.773148 | -4.327058 |
| C | -7.616187 | 3.744403 | -2.004278 | H | 15.296547 | 6.687896 | -3.220183 |
| C | -6.831313 | -4.902846 | -1.784278 | H | 13.778806 | 5.037079 | -3.755296 |
| C | -10.687482 | -5.207101 | 1.449746 | H | 11.844642 | 6.519577 | -0.218394 |
| C | -5.426167 | 4.124073 | -0.333004 | H | 3.923885 | 6.562292 | -0.435250 |
| C | -7.360488 | 2.812105 | -0.991361 | H | 8.905864 | 0.715976 | -4.834937 |
| C | -9.304255 | 2.844134 | 1.204816 | H | 1.700013 | 7.319895 | 0.274577 |
| C | -7.640399 | -0.762448 | -2.091791 | H | 3.838091 | -6.618556 | 0.082860 |
| C | -9.022405 | 1.752077 | 3.728132 | H | 4.716459 | 5.138571 | 3.531379 |
| C | -10.656971 | 4.714799 | 2.078674 | H | 3.943883 | 2.489656 | 4.236558 |
| C | -5.655748 | -1.729009 | -3.230586 | H | 4.533785 | 4.033929 | -0.554571 |
| C | -6.309614 | 3.079883 | -0.100264 | H | 13.783583 | 5.615349 | 0.653270 |
| C | -7.774564 | -2.033113 | -4.300814 | H | 9.672985 | -3.648591 | -4.471580 |
| C | -9.464974 | -2.540965 | 3.887156 | H | 2.492067 | 5.884791 | 4.247658 |
| C | -11.759309 | -4.415388 | 3.447422 | H | 7.740788 | 3.060777 | 6.174261 |
| C | -7.035629 | -1.533478 | -3.225626 | H | 2.382337 | -5.591866 | 4.693686 |
| C | -5.636960 | -4.958459 | -1.052363 | H | 1.597600 | -7.288826 | 0.823171 |
| C | -4.472475 | -5.761975 | -1.488327 | H | -1.631115 | -6.172686 | 5.925191 |
| C | -15.455605 | -6.380213 | 2.187617 | H | 11.766678 | -4.335795 | -3.885979 |
| C | -9.721879 | 3.589102 | 2.303776 | H | -6.180063 | -3.350737 | 2.953489 |
| C | -4.389950 | 5.693228 | -1.948962 | H | -4.624696 | 5.569771 | 2.264164 |
| C | -12.900556 | -5.137019 | 3.121208 | H | 9.812271 | -5.420104 | -0.215778 |
| C | -11.831258 | -5.927523 | 1.123331 | H | 5.170847 | -1.844902 | 2.208864 |
| C | -3.612342 | -6.416156 | -0.594399 | H | 0.628459 | -6.871932 | 5.285072 |
| C | -1.793195 | 6.454736 | -2.805767 | H | -2.556646 | -5.423591 | 1.798150 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -9.025278 | -1.231165 | 3.887030 | H | 0.758816 | 7.229968 | 4.759271 |
| C | -6.885087 | 1.231818 | -3.345071 | H | 17.584552 | 6.299391 | -2.429110 |
| C | -5.744409 | -2.863480 | -5.375724 | H | -0.325757 | -6.125111 | 1.169949 |
| C | -2.350209 | -6.843139 | -0.997910 | H | -5.814750 | -0.931312 | 6.776007 |
| C | -0.361033 | 6.491001 | -3.175473 | H | 13.766968 | -5.532048 | -3.179591 |
| C | 2.255727 | 5.676748 | -3.919027 | H | -5.575547 | 1.361344 | 2.407203 |
| C | -3.524922 | 6.394477 | -1.095158 | H | 16.055443 | 5.225228 | 1.438361 |
| C | -4.072941 | -5.661978 | -2.830303 | H | -0.232252 | 6.209683 | 0.712037 |
| C | -5.018430 | -2.377097 | -4.282626 | H | -3.864103 | -2.157181 | 6.369484 |
| C | -5.443408 | -4.012965 | -0.032448 | H | -5.794203 | 1.529181 | 6.688097 |
| C | 3.397949 | 4.814530 | -4.293149 | H | -4.705850 | -5.284223 | 2.637302 |
| C | -0.466858 | -6.702552 | -2.683269 | H | -3.806933 | 2.674983 | 6.184298 |
| C | -14.609503 | -5.822703 | 0.012993 | H | -6.134460 | 3.689397 | 2.719296 |
| C | -9.459394 | 3.055282 | 3.587117 | H | -2.472189 | 5.595700 | 1.398333 |
| C | -2.810036 | -6.079054 | -3.229677 | H | -5.600077 | -1.073611 | 2.494715 |
| C | -7.137670 | -2.689135 | -5.351470 | H | -2.394597 | -4.077149 | 6.054252 |
| C | -2.709089 | 5.865575 | -3.693933 | H | -2.302635 | 4.540096 | 5.730553 |
| C | 3.312936 | -5.173203 | -3.933309 | H | 3.795632 | -2.391821 | 4.138090 |
| C | -1.896103 | -6.620137 | -2.309280 | H | 11.829331 | -6.622427 | 0.495275 |
| C | -2.253350 | 6.773434 | -1.516258 | H | -1.508551 | 6.615976 | 5.458061 |
| C | 1.347457 | 6.164933 | -4.876097 | H | 8.414159 | -0.770009 | 4.783901 |
| C | -11.750170 | 4.872454 | 2.945988 | H | 19.166827 | 1.302755 | 2.702871 |
| C | 5.104926 | 2.578722 | -4.660056 | H | 18.575894 | 4.266819 | -2.120294 |
| C | 5.352996 | 3.512751 | -3.639656 | H | 19.744563 | 3.525725 | 2.623121 |
| C | 4.441812 | -4.937146 | -3.128223 | H | 18.261673 | 5.381177 | 2.015884 |
| C | -10.676623 | 5.445523 | 0.875927 | H | 7.055626 | -1.338811 | 6.734879 |
| C | -5.583470 | 1.727319 | -3.198781 | H | 15.281581 | -7.118828 | -2.468267 |
| C | 0.065966 | 6.560542 | -4.513250 | H | 21.758865 | 1.120973 | -0.716902 |
| C | -16.999049 | -5.665158 | 0.444638 | H | 19.163460 | -1.128862 | 2.835530 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | 1.890406 | 5.792550 | -2.569553 | H | 17.570155 | -6.650798 | -1.722923 |
| C | 5.606583 | -1.629362 | -4.540319 | H | 13.769385 | -5.629093 | 1.264974 |
| C | -0.048676 | -6.873702 | -4.014477 | H | 20.050350 | 2.426304 | -1.517433 |
| C | 5.628684 | 1.196544 | -4.641660 | H | 21.755729 | -1.327303 | -0.583147 |
| C | -16.753359 | -6.159210 | 1.738527 | H | 16.041746 | -5.159717 | 2.004060 |
| C | 0.610944 | 6.193521 | -2.208838 | H | 19.734825 | -3.348801 | 2.998376 |
| C | 5.773292 | 0.434736 | -5.813166 | H | 20.044125 | -2.707605 | -1.237186 |
| C | -14.347992 | -6.117993 | 1.361434 | H | 18.565403 | -4.599316 | -1.636631 |
| C | -12.891028 | 5.555002 | 2.543419 | H | 18.247517 | -5.255671 | 2.596183 |
| C | 5.676049 | -0.866674 | -3.365559 | H | 2.636411 | -1.170762 | 5.784430 |
| C | -15.905353 | -5.600505 | -0.434903 | H | 3.629992 | -0.039555 | 6.707657 |
| C | 0.514693 | -6.351583 | -1.744460 | H | 2.531722 | -1.152228 | 7.552936 |
| C | 4.086517 | 2.872490 | -5.581063 | H | 4.522065 | -4.282359 | 6.775134 |
| C | 5.762645 | -0.955606 | -5.763268 | H | 3.171368 | -3.667226 | 5.809544 |
| C | 4.514376 | 4.610048 | -3.462342 | H | 3.057763 | -3.677248 | 7.572659 |
| C | 4.024541 | -3.333355 | -5.351803 | H | 5.467465 | -0.926082 | 8.267256 |
| C | 5.299154 | -3.870045 | -3.384502 | H | 5.882393 | -2.650308 | 8.261243 |
| C | 1.798836 | -5.999596 | -2.138043 | H | 4.352149 | -2.106790 | 8.961857 |
| C | -5.070604 | -3.549414 | -6.570519 | H | 4.932732 | 3.241478 | 8.725719 |
| C | -12.988455 | 6.110103 | 1.256700 | H | 6.492708 | 2.758279 | 8.046028 |
| C | 5.057765 | -2.999816 | -4.461315 | H | 5.071357 | 1.738792 | 7.791848 |
| C | 5.687587 | 0.518728 | -3.415515 | H | 3.116213 | 2.575388 | 6.367985 |
| C | 2.158626 | -5.987104 | -3.493969 | H | 3.224611 | 4.131817 | 5.534282 |
| C | 3.250815 | 3.963874 | -5.400748 | H | 3.099142 | 4.080152 | 7.296451 |
| C | 3.170188 | -4.393995 | -5.092729 | H | 5.328301 | 5.578778 | 5.791532 |
| C | -3.427135 | -0.660612 | 0.656023 | H | 6.668520 | 5.035931 | 6.808355 |
| C | -4.808188 | 2.044849 | -4.302198 | H | 5.130199 | 5.498633 | 7.551042 |
| C | -11.820152 | 6.126554 | 0.473054 | H | -5.881534 | 2.651160 | -8.260544 |
| C | 1.237018 | -6.525729 | -4.410158 | H | -4.521529 | 4.283473 | -6.774392 |

| | | | | | | | |
|--------------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -5.415880 | -2.775361 | -7.861361 | H | -3.628952 | 0.040780 | -6.706696 |
| $C_{70}@(\mathbf{1a})_2$ | | | | | | | |
| C | -6.343235 | -3.059075 | 0.013524 | C | 1.931282 | 6.623499 | -2.605364 |
| C | -7.968368 | -1.497793 | 1.016804 | C | -3.344972 | 5.254098 | -4.021211 |
| C | -5.441841 | -4.100948 | 0.180408 | C | 4.369376 | -5.621545 | -1.600231 |
| C | -7.058669 | 1.336030 | 3.335472 | C | -2.242959 | -5.568326 | -3.676541 |
| C | -6.421664 | 2.882719 | 0.066017 | C | 3.922947 | -5.200711 | -2.863230 |
| C | -7.402019 | -2.876665 | 0.917561 | C | -3.993566 | -2.672239 | -5.267511 |
| C | -8.797477 | -1.507804 | -1.353368 | C | -0.637412 | -6.181016 | -1.960217 |
| C | -7.671193 | -0.791762 | 2.192779 | C | -5.800424 | -0.393645 | -5.671641 |
| C | -6.813936 | 4.736282 | 2.097038 | C | 2.415565 | 6.915474 | -1.316994 |
| C | 5.650120 | -0.592176 | 3.356409 | C | -3.239442 | 4.417922 | -5.146240 |
| C | -1.862638 | 6.411142 | 2.469805 | C | 9.514221 | 3.534082 | 2.633343 |
| C | -8.482077 | 0.616874 | -0.119612 | C | -4.109593 | 3.358526 | -5.340001 |
| C | -8.443225 | -0.798498 | -0.122938 | C | 5.057724 | 2.054363 | -6.929482 |
| C | -7.623040 | -3.850940 | 1.897652 | C | 17.852503 | -5.096313 | 0.231822 |
| C | -8.055884 | 1.328540 | 1.031873 | C | 7.176273 | 1.321209 | -5.650464 |
| C | -6.948140 | -1.411303 | 3.347997 | C | 3.550389 | -6.472840 | -0.846937 |
| C | -8.857353 | 1.315467 | -1.348679 | C | 9.252237 | 2.971496 | 3.905874 |
| C | -6.712897 | -4.893432 | 2.072140 | C | 5.354029 | -3.385108 | -6.565611 |
| C | -9.353005 | 2.629143 | -1.301581 | C | 10.437828 | 4.680315 | 2.435490 |
| C | -7.500558 | 2.716042 | 0.945867 | C | 8.844120 | 1.655839 | 4.016444 |
| C | -8.786085 | -0.824255 | -2.595478 | C | 8.821578 | -1.325103 | 4.141837 |
| C | 5.033333 | -2.682709 | 4.520698 | C | -5.808991 | 0.996917 | -5.670637 |
| C | -9.254782 | -2.835571 | -1.308586 | C | 0.077627 | 6.786037 | -4.312669 |
| C | -5.663810 | 4.817810 | 1.301131 | C | -1.229171 | 6.465891 | -4.654347 |
| C | -5.522401 | 3.925218 | 0.227774 | C | 9.208419 | -2.651714 | 4.143821 |
| C | 0.006976 | 6.757953 | 4.119573 | C | 13.981704 | -6.304303 | 1.524948 |
| C | 5.602199 | 1.514151 | 4.552911 | C | -3.142338 | -3.746012 | -5.072318 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -0.423647 | 6.560625 | 2.795656 | C | 10.422516 | 5.450532 | 1.257187 |
| C | -5.569985 | -4.985091 | 1.264914 | C | 15.498659 | -5.686566 | -0.271776 |
| C | -7.725824 | 0.625661 | 2.197921 | C | 16.392126 | -6.391934 | 1.849539 |
| C | 5.073700 | 2.898121 | 4.507146 | C | 15.100038 | -6.621904 | 2.316342 |
| C | -5.637995 | 2.531843 | 5.465458 | C | 14.210043 | -5.916337 | 0.193552 |
| C | 2.275665 | -5.823736 | 3.615344 | C | 4.049603 | 5.519876 | -3.088467 |
| C | -7.410634 | -1.294487 | 4.658734 | C | 18.432689 | -4.288368 | 1.224658 |
| C | -5.658204 | -1.913577 | 3.140241 | C | 12.698552 | 5.463439 | 2.856858 |
| C | -8.819372 | 0.636953 | -2.592935 | C | 2.794389 | 5.955007 | -3.493965 |
| C | -5.673780 | 1.472213 | 3.280756 | C | 11.561057 | 6.137351 | 0.843950 |
| C | 5.581979 | -1.305641 | 4.558972 | C | 19.268530 | -3.231482 | 0.886781 |
| C | 5.370608 | 3.805201 | 3.474950 | C | 11.563697 | 4.776513 | 3.269856 |
| C | -16.924596 | 5.562552 | 0.049123 | C | 19.603098 | 2.681476 | -0.696734 |
| C | 1.841674 | 5.908692 | 2.207200 | C | 17.936598 | 4.917295 | -0.194794 |
| C | 4.527579 | 4.888525 | 3.223018 | C | 10.362274 | -4.501266 | 2.825995 |
| C | 5.398929 | -3.646550 | 3.567408 | C | 12.646671 | -6.010833 | 2.110918 |
| C | -2.417223 | 6.796333 | 1.239149 | C | 14.309138 | 5.795456 | -0.305895 |
| C | -3.551179 | -6.478477 | 0.835934 | C | 19.556704 | -2.940266 | -0.457428 |
| C | 1.311158 | 6.454113 | 4.491632 | C | 5.865310 | 1.733466 | -8.203661 |
| C | -4.972329 | 2.054905 | 4.330576 | C | 14.088685 | 6.298987 | 0.987582 |
| C | -5.264396 | -2.040535 | 5.536536 | C | 19.320076 | 3.090312 | 0.617599 |
| C | 1.933425 | -5.928930 | 2.260860 | C | 12.749088 | 6.080482 | 1.595450 |
| C | -7.734941 | 3.704332 | 1.909053 | C | 15.593243 | 5.504284 | -0.748919 |
| C | -7.740472 | 1.822345 | 4.452571 | C | 16.707083 | 5.705852 | 0.083934 |
| C | -4.831288 | -2.213481 | 4.212400 | C | 4.548147 | 3.514398 | -7.014591 |
| C | -4.362856 | -5.731765 | 1.702387 | C | 16.500430 | 6.371142 | 1.305767 |
| C | -9.728999 | 3.317478 | -2.449815 | C | 20.019526 | 1.270564 | -0.912472 |
| C | 4.576095 | -4.749759 | 3.327230 | C | 18.355631 | 4.610227 | -1.501701 |
| C | -2.653775 | 5.652931 | 3.350948 | C | 18.502774 | 4.186328 | 0.863637 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -7.037692 | 2.418772 | 5.498240 | C | 15.212938 | 6.662751 | 1.750194 |
| C | 0.654318 | -6.330827 | 1.883679 | C | 18.275290 | -4.908511 | -1.096288 |
| C | 3.371379 | 5.097452 | 3.995518 | C | 19.996311 | -1.559875 | -0.791996 |
| C | 5.656785 | 0.792805 | 3.353147 | C | 3.849038 | 1.082859 | -6.857519 |
| C | -0.325110 | -6.623215 | 2.843206 | C | 10.332322 | -5.368140 | 1.717202 |
| C | -1.763018 | -6.530939 | 2.488737 | C | 12.607879 | -5.288390 | 3.315479 |
| C | 3.373007 | -4.917331 | 4.033324 | C | 19.174332 | 3.510592 | -1.748527 |
| C | -4.454666 | 5.565646 | 1.730473 | C | 11.457558 | -6.108910 | 1.365343 |
| C | 2.223702 | 5.929621 | 3.556463 | C | 20.844164 | 0.581617 | -0.005296 |
| C | -3.928365 | 5.238623 | 2.990276 | C | 19.314340 | 0.513326 | -1.863297 |
| C | 3.989567 | 3.182259 | 5.353214 | C | 19.112561 | -3.848138 | -1.435249 |
| C | 0.538854 | 6.222416 | 1.834871 | C | 20.832732 | -0.809961 | 0.053946 |
| C | 5.718549 | 0.802296 | 5.759268 | C | 11.486170 | -4.547758 | 3.667206 |
| C | -2.271968 | -6.878990 | 1.225913 | C | 19.302961 | -0.874695 | -1.804228 |
| C | 3.066030 | -3.997828 | 5.051872 | C | 5.893725 | -2.676574 | -7.833505 |
| C | -9.609038 | -3.533721 | -2.458001 | C | 5.714470 | -4.891102 | -6.601905 |
| C | 3.880183 | -2.904220 | 5.291364 | C | 3.814940 | -3.247979 | -6.554751 |
| C | -4.269124 | -2.250599 | 6.684964 | H | 6.047885 | 2.266354 | 0.791335 |
| C | -18.149208 | 4.782005 | 0.368969 | H | 4.512227 | 4.139724 | 0.370722 |
| C | -6.579977 | -1.607620 | 5.737765 | H | 6.017687 | -2.184878 | 0.911423 |
| C | -3.697223 | 6.375319 | 0.873383 | H | 6.959825 | -5.570338 | -2.560172 |
| C | -9.359954 | -2.917661 | -3.707833 | H | -5.813381 | 1.511727 | -2.330568 |
| C | -4.883274 | 3.148073 | 6.651126 | H | 8.555152 | 3.567593 | -2.422572 |
| C | -10.510268 | -4.703987 | -2.303963 | H | 7.021306 | 5.458285 | -2.852320 |
| C | -8.974342 | -1.591031 | -3.768807 | H | 9.319978 | -3.163999 | 0.801883 |
| C | -9.037757 | 1.397168 | -3.764476 | H | 9.365038 | 3.196753 | 0.532766 |
| C | 5.703591 | -0.591126 | 5.762374 | H | 4.422994 | -4.020805 | 0.532777 |
| C | 0.083726 | -6.708171 | 4.187945 | H | 0.712326 | -6.598040 | -5.038032 |
| C | 1.361991 | -6.320455 | 4.565582 | H | 8.804538 | 0.562747 | -4.470158 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -9.466318 | 2.709818 | -3.700908 | H | 5.431212 | 2.025870 | -2.280217 |
| C | -14.313710 | 6.124660 | -0.895136 | H | 5.212332 | -1.164499 | -2.416033 |
| C | 3.155372 | 4.259021 | 5.102539 | H | -6.292361 | -3.352486 | -2.861622 |
| C | -10.472120 | -5.524695 | -1.160958 | H | -2.616044 | -5.490141 | -1.555548 |
| C | -15.805221 | 5.401822 | 0.883450 | H | -4.779494 | -5.266092 | -2.515499 |
| C | -16.727463 | 6.174365 | -1.201902 | H | -6.131287 | 3.821084 | -2.653071 |
| C | -15.443653 | 6.450494 | -1.666396 | H | 1.653851 | -7.471700 | -0.703308 |
| C | -14.524803 | 5.677907 | 0.420531 | H | 4.006703 | 6.670662 | 0.103996 |
| C | -3.891346 | -5.466468 | 2.998265 | H | -1.552938 | -5.897519 | -5.695060 |
| C | -18.718680 | 4.004305 | -0.653787 | H | 4.145421 | -2.185678 | -4.367446 |
| C | -12.758019 | -5.512242 | -2.746658 | H | -2.483685 | 6.002022 | -1.540372 |
| C | -2.614346 | -5.851806 | 3.379252 | H | 8.588342 | -3.768687 | -2.119702 |
| C | -11.593967 | -6.252205 | -0.772352 | H | 9.070837 | -2.036492 | -4.016116 |
| C | -19.528857 | 2.915851 | -0.356138 | H | 4.308970 | 2.582560 | -4.375841 |
| C | -11.639817 | -4.784844 | -3.135035 | H | -4.586835 | 5.692516 | -2.305531 |
| C | -19.710840 | -3.063240 | 0.968522 | H | 2.287164 | -5.115740 | -4.237780 |
| C | -17.991094 | -5.229969 | 0.355748 | H | 8.020927 | -3.130716 | -5.960661 |
| C | -10.662206 | 4.462232 | -2.293285 | H | -0.214057 | 6.611295 | -0.948409 |
| C | -12.976804 | 5.884467 | -1.500704 | H | -5.802888 | -0.929132 | -2.325021 |
| C | -14.342042 | -6.021682 | 0.405971 | H | 4.536611 | -4.507785 | -3.425489 |
| C | -19.801080 | 2.561541 | 0.976191 | H | -3.727087 | -1.903821 | -5.981492 |
| C | -4.942410 | -2.136074 | 8.068279 | H | -0.374307 | -6.182503 | -0.913101 |
| C | -14.118277 | -6.461808 | -0.909843 | H | -5.784204 | -0.932182 | -6.612206 |
| C | -19.427751 | -3.405530 | -0.364690 | H | 1.798180 | 7.467568 | -0.618885 |
| C | -12.787627 | -6.186261 | -1.514070 | H | -2.384620 | 4.514031 | -5.801881 |
| C | -15.629763 | -5.781720 | 0.868717 | H | -3.913201 | 2.656760 | -6.140177 |
| C | -16.744028 | -5.973251 | 0.034079 | H | 7.676399 | 1.097997 | -6.582693 |
| C | -3.609192 | -3.647106 | 6.567293 | H | 3.896264 | -6.837799 | 0.112848 |
| C | -16.529615 | -6.577678 | -1.217672 | H | 9.438720 | 3.555401 | 4.799233 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -20.160824 | -1.674349 | 1.249919 | H | 8.713078 | 1.226445 | 4.999484 |
| C | -18.407746 | -4.992695 | 1.677865 | H | 8.692293 | -0.813476 | 5.084935 |
| C | -18.584294 | -4.467661 | -0.665080 | H | -5.805920 | 1.534530 | -6.611682 |
| C | -15.238487 | -6.817631 | -1.682015 | H | 0.794088 | 7.003838 | -5.095468 |
| C | -18.558676 | 4.528902 | 1.690403 | H | -1.511468 | 6.443988 | -5.699729 |
| C | -20.206555 | 1.158269 | 1.253959 | H | 9.383246 | -3.161457 | 5.083710 |
| C | -3.179022 | -1.153056 | 6.577524 | H | -2.222280 | -3.799533 | -5.638879 |
| C | -10.644189 | 5.284137 | -1.150672 | H | 9.539509 | 5.445438 | 0.627298 |
| C | -12.931210 | 5.210619 | -2.732886 | H | 15.638714 | -5.247541 | -1.251869 |
| C | -19.252662 | -3.927050 | 1.979212 | H | 17.238703 | -6.580911 | 2.499694 |
| C | -11.784296 | 5.981938 | -0.760622 | H | 14.951406 | -6.986594 | 3.326313 |
| C | -21.009069 | -0.966651 | 0.379705 | H | 13.364811 | -5.652240 | -0.429942 |
| C | -19.466972 | -0.942627 | 2.228658 | H | 4.656968 | 4.919332 | -3.755270 |
| C | -19.370175 | 3.436813 | 1.989016 | H | 18.110854 | -4.403396 | 2.252282 |
| C | -21.031567 | 0.426048 | 0.381700 | H | 13.603950 | 5.396475 | 3.447342 |
| C | -11.794773 | 4.512820 | -3.122572 | H | 2.434643 | 5.677909 | -4.476903 |
| C | -19.489394 | 0.446519 | 2.230629 | H | 11.554214 | 6.665752 | -0.102585 |
| C | -5.233067 | 2.357879 | 7.937645 | H | 19.586654 | -2.538706 | 1.656055 |
| C | -5.306938 | 4.629646 | 6.807390 | H | 11.602640 | 4.185635 | 4.176618 |
| C | -3.352007 | 3.090662 | 6.453630 | H | 13.459009 | 5.494492 | -0.905566 |
| C | 1.008843 | -2.689042 | -2.545288 | H | 5.234290 | 1.901554 | -9.082963 |
| C | -1.903645 | -3.054623 | -0.266104 | H | 6.184089 | 0.685410 | -8.207270 |
| C | 0.236423 | -3.266313 | -1.507279 | H | 19.626236 | 2.459726 | 1.443165 |
| C | 3.398150 | -0.472973 | 0.909481 | H | 15.724843 | 4.981349 | -1.688152 |
| C | -0.893874 | 2.073697 | 2.892281 | H | 5.394146 | 4.208809 | -7.052596 |
| C | 1.121122 | 2.767887 | 1.918289 | H | 3.930283 | 3.764007 | -6.145828 |
| C | -1.222145 | -3.367059 | 0.985822 | H | 17.350662 | 6.599580 | 1.938252 |
| C | -1.841989 | -2.588796 | 2.053737 | H | 17.984695 | 5.199874 | -2.332231 |
| C | 1.236345 | 3.556765 | -0.364263 | H | 18.183152 | 4.393551 | 1.877403 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.176588 | 1.293129 | 3.506947 | H | 15.071338 | 7.114486 | 2.725394 |
| C | 3.147704 | 0.870367 | 1.363501 | H | 17.893311 | -5.560013 | -1.873920 |
| C | 2.158925 | -2.854578 | 0.016560 | H | 3.214319 | 1.314923 | -5.998678 |
| C | 3.503700 | 0.319524 | -1.364289 | H | 4.205355 | 0.052725 | -6.751753 |
| C | -1.218025 | -3.042620 | -1.506900 | H | 9.449612 | -5.399522 | 1.087705 |
| C | -2.328473 | 0.071870 | 2.943367 | H | 13.514425 | -5.188498 | 3.899502 |
| C | 2.647820 | 2.404687 | -2.007361 | H | 19.433970 | 3.253332 | -2.769070 |
| C | -0.301239 | 2.983904 | 1.919117 | H | 11.440484 | -6.715456 | 0.467003 |
| C | 1.878511 | 2.913175 | 0.727955 | H | 21.448558 | 1.143709 | 0.697422 |
| C | -0.187399 | 3.760084 | -0.364417 | H | 18.660383 | 1.021137 | -2.561437 |
| C | -2.888883 | -1.787614 | 1.435722 | H | 19.375436 | -3.682799 | -2.473832 |
| C | -0.658714 | 3.662269 | -1.742258 | H | 21.428296 | -1.320130 | 0.802337 |
| C | 1.426512 | 1.724258 | 2.892527 | H | 11.536428 | -3.883101 | 4.520776 |
| C | -1.793426 | -2.268448 | -2.545169 | H | 18.640286 | -1.429173 | -2.457198 |
| C | 2.932453 | 1.925833 | 0.441748 | H | 5.660842 | -1.607295 | -7.791280 |
| C | -3.123383 | -0.497131 | 1.869085 | H | 5.430802 | -3.106379 | -8.729165 |
| C | 2.822183 | -1.393393 | 1.882592 | H | 5.326299 | -5.390594 | -5.707576 |
| C | 2.793766 | -2.023786 | -0.941433 | H | 6.799727 | -5.029610 | -6.633132 |
| C | 0.145812 | -3.555027 | 0.985503 | H | 3.513009 | -2.195801 | -6.521305 |
| C | 1.656928 | 3.330112 | -1.742185 | H | 3.376114 | -3.765593 | -5.695444 |
| C | 0.891490 | -3.472224 | -0.265007 | H | -6.167351 | -2.307749 | -0.743851 |
| C | 3.434527 | -0.782056 | -0.474352 | H | -4.558423 | -4.144363 | -0.440717 |
| C | -1.309975 | -0.678218 | 3.524906 | H | -6.236764 | 2.117123 | -0.670550 |
| C | 2.417480 | 0.796138 | 2.622661 | H | -6.944707 | 5.432515 | 2.916824 |
| C | 3.042677 | 0.216007 | -2.741910 | H | 5.560887 | -1.123944 | 2.422779 |
| C | -2.109871 | 1.474780 | 2.613471 | H | -8.439332 | -3.724618 | 2.597504 |
| C | 1.026918 | -1.029228 | 3.534985 | H | -6.837777 | -5.586158 | 2.895836 |
| C | -0.932313 | 1.929165 | -3.986239 | H | -9.555863 | 3.066779 | -0.336398 |
| C | -0.022483 | -0.051064 | 3.815605 | H | -9.447358 | -3.279722 | -0.344298 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 2.513078 | 1.507759 | -3.146640 | H | -4.633861 | 3.963155 | -0.385888 |
| C | 0.383198 | -1.962930 | -3.648144 | H | -0.704251 | 7.094328 | 4.864942 |
| C | -0.988027 | 3.343874 | 0.729194 | H | -8.405119 | -0.908177 | 4.841559 |
| C | 2.222370 | -0.610350 | 2.956804 | H | -5.297809 | -2.044292 | 2.133246 |
| C | -1.061030 | -2.044940 | 3.072439 | H | -5.144987 | 1.113982 | 2.413112 |
| C | 3.258890 | 1.660523 | -0.912440 | H | 6.238884 | 3.639868 | 2.847850 |
| C | -2.664949 | -0.188937 | -3.188169 | H | 2.511394 | 5.495065 | 1.466786 |
| C | -2.932230 | -2.089989 | 0.013135 | H | 4.747939 | 5.551565 | 2.394374 |
| C | -0.679200 | 0.565190 | -4.444098 | H | 6.306472 | -3.514135 | 2.990530 |
| C | 2.437997 | -0.946310 | -3.177240 | H | -1.839144 | 7.413431 | 0.561623 |
| C | -2.825212 | -1.307099 | -2.266397 | H | -3.916833 | -6.732312 | -0.152156 |
| C | 2.273337 | -2.066460 | -2.260296 | H | 1.611809 | 6.555053 | 5.527857 |
| C | -1.531971 | -0.467943 | -4.058762 | H | -3.897867 | 2.123104 | 4.253271 |
| C | -3.561713 | 0.263409 | -0.478926 | H | 2.606572 | -5.550327 | 1.503409 |
| C | -3.308807 | 1.336261 | -1.371007 | H | -8.574464 | 3.606541 | 2.583306 |
| C | 0.485133 | 3.414359 | -2.606617 | H | -8.819087 | 1.725140 | 4.505494 |
| C | 1.402711 | 1.580926 | -3.981296 | H | -3.823870 | -2.552350 | 4.009933 |
| C | -3.306522 | -1.113328 | -0.945450 | H | 4.853306 | -5.461721 | 2.558666 |
| C | -2.900622 | 1.100696 | -2.751554 | H | -2.221045 | 5.309738 | 4.282606 |
| C | 0.969409 | -3.003904 | 2.055133 | H | -7.585510 | 2.786236 | 6.358082 |
| C | 0.354972 | 2.558620 | -3.698647 | H | 0.374265 | -6.261610 | 0.844193 |
| C | 2.215074 | -2.557232 | 1.445347 | H | 5.568578 | 1.321046 | 2.416900 |
| C | 1.279277 | -0.887374 | -4.058187 | H | -4.489993 | 4.567606 | 3.628350 |
| C | -2.021050 | 2.185130 | -3.158909 | H | 3.728928 | 2.473083 | 6.128773 |
| C | 0.385903 | -2.262501 | 3.076731 | H | 0.226100 | 6.032736 | 0.819532 |
| C | -0.983871 | -1.755161 | -3.644429 | H | 5.740114 | 1.344881 | 6.697561 |
| C | -3.420475 | 0.549873 | 0.903186 | H | -1.658662 | -7.446405 | 0.536533 |
| C | -1.876976 | 3.072534 | -2.013479 | H | 2.119731 | -4.083668 | 5.570022 |
| C | -2.674974 | 2.544483 | -0.916398 | H | 3.566868 | -2.142929 | 5.994656 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | -2.797544 | 1.765137 | 1.360382 | H | -6.959859 | -1.473409 | 6.741018 |
| C | 0.764781 | 0.348885 | -4.443070 | H | -4.108908 | 6.662584 | -0.087390 |
| C | -2.286106 | 2.711237 | 0.439579 | H | -9.539748 | -3.469407 | -4.622787 |
| C | 6.287912 | 2.998551 | 0.034867 | H | -8.856978 | -1.120144 | -4.734770 |
| C | 7.949977 | 1.384280 | -0.799951 | H | -8.901305 | 0.933991 | -4.731835 |
| C | 5.425395 | 4.058490 | -0.202950 | H | 5.710341 | -1.131413 | 6.702174 |
| C | 7.203029 | -1.525205 | -3.083318 | H | -0.627667 | -7.023943 | 4.941825 |
| C | 6.249904 | -2.960095 | 0.197522 | H | 1.641183 | -6.332942 | 5.612494 |
| C | 7.398710 | 2.774515 | -0.792702 | H | -9.665020 | 3.257013 | -4.614659 |
| C | 8.672943 | 1.478340 | 1.605213 | H | 2.252045 | 4.379236 | 5.686517 |
| C | 7.738200 | 0.634519 | -1.965653 | H | -9.584743 | -5.530186 | -0.537293 |
| C | 6.774693 | -4.859794 | -1.763497 | H | -15.929433 | 4.920118 | 1.845462 |
| C | -5.852495 | 0.987199 | -3.269789 | H | -17.582144 | 6.371876 | -1.838782 |
| C | 1.793915 | -6.329643 | -2.528825 | H | -15.309324 | 6.859236 | -2.661391 |
| C | 8.343678 | -0.692135 | 0.454833 | H | -13.670007 | 5.406809 | 1.027789 |
| C | 8.337401 | 0.723762 | 0.397017 | H | -4.494817 | -4.857792 | 3.659911 |
| C | 7.699643 | 3.723292 | -1.777919 | H | -18.406519 | 4.169708 | -1.677509 |
| C | 7.974960 | -1.443475 | -0.692471 | H | -13.668484 | -5.437531 | -3.328344 |
| C | 7.190206 | 1.227405 | -3.223830 | H | -2.230688 | -5.535335 | 4.340840 |
| C | 8.661561 | -1.347330 | 1.723073 | H | -11.570438 | -6.822138 | 0.149476 |
| C | 6.826279 | 4.783272 | -2.027549 | H | -19.836941 | 2.249313 | -1.152212 |
| C | 9.116652 | -2.677617 | 1.742792 | H | -11.696318 | -4.155027 | -4.014269 |
| C | 7.393634 | -2.820972 | -0.602370 | H | -13.495343 | -5.727567 | 1.013850 |
| C | 8.641484 | 0.846995 | 2.873896 | H | -5.746522 | -2.871930 | 8.177746 |
| C | -5.134094 | 3.076925 | -4.419982 | H | -5.354382 | -1.132260 | 8.219110 |
| C | 9.153876 | 2.796295 | 1.511715 | H | -19.756588 | -2.746961 | -1.159093 |
| C | 5.561566 | -4.908844 | -1.064791 | H | -15.767598 | -5.304699 | 1.831195 |
| C | 5.352210 | -3.997075 | -0.018080 | H | -4.371681 | -4.432411 | 6.607663 |
| C | -0.018423 | -6.357814 | -4.274906 | H | -2.903564 | -3.795003 | 7.392776 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | -5.704748 | -1.113305 | -4.465012 | H | -17.378328 | -6.798381 | -1.854909 |
| C | 0.363497 | -6.384410 | -2.920180 | H | -18.015302 | -5.608980 | 2.478635 |
| C | 5.641817 | 4.923009 | -1.289080 | H | -18.267471 | -4.621014 | -1.689252 |
| C | 7.762629 | -0.783446 | -1.909062 | H | -15.092584 | -7.221699 | -2.677293 |
| C | -5.110538 | -2.472439 | -4.438925 | H | -18.185556 | 5.155058 | 2.492762 |
| C | 5.994396 | -2.748808 | -5.325391 | H | -2.454693 | -1.259491 | 7.393970 |
| C | -2.170105 | 6.093420 | -3.671383 | H | -3.641681 | -0.162649 | 6.636353 |
| C | 7.822995 | 1.018148 | -4.450398 | H | -9.756120 | 5.313490 | -0.528657 |
| C | 5.927290 | 1.832705 | -3.218946 | H | -13.840255 | 5.111577 | -3.313154 |
| C | 8.633608 | -0.612462 | 2.935008 | H | -19.510855 | -3.722453 | 3.011960 |
| C | 5.817757 | -1.597352 | -3.195061 | H | -11.774447 | 6.552833 | 0.160889 |
| C | -5.716365 | 1.712086 | -4.461544 | H | -21.605114 | -1.511959 | -0.343086 |
| C | -5.403643 | -3.451114 | -3.473545 | H | -18.795517 | -1.464422 | 2.899339 |
| C | 16.609519 | -5.836466 | 0.575825 | H | -19.621926 | 3.221749 | 3.021232 |
| C | -1.919523 | -5.781453 | -2.328864 | H | -21.644907 | 0.953894 | -0.339587 |
| C | -4.545985 | -4.536946 | -3.282273 | H | -11.835771 | 3.881455 | -4.001538 |
| C | -5.319429 | 3.976265 | -3.354179 | H | -18.835061 | 0.987799 | 2.902793 |
| C | 2.280000 | -6.826893 | -1.308062 | H | -6.304878 | 2.409592 | 8.150973 |
| C | 3.668946 | 6.466694 | -0.905314 | H | -4.687110 | 2.772972 | 8.792604 |
| C | -1.296356 | -5.961196 | -4.644469 | H | -4.787971 | 5.081954 | 7.660475 |
| C | 5.222010 | -2.188347 | -4.303452 | H | -6.385889 | 4.709545 | 6.972741 |
| C | 5.886223 | 1.861081 | -5.653886 | H | -3.010190 | 2.056421 | 6.342595 |
| C | -1.800243 | 6.278912 | -2.331077 | H | -2.861026 | 3.526238 | 7.330440 |
| C | 7.692788 | -3.837734 | -1.518412 | H | -4.195843 | -2.318442 | 8.848654 |
| C | 7.990331 | -2.088276 | -4.090569 | H | -3.058775 | -3.740500 | 5.626134 |
| C | 5.299230 | 2.152711 | -4.413565 | H | -2.649454 | -1.221958 | 5.624591 |
| C | 4.487158 | 5.723702 | -1.769848 | H | -4.955260 | 1.305819 | 7.815408 |
| C | 9.461118 | -3.324552 | 2.924078 | H | -5.052701 | 5.190607 | 5.901677 |
| C | -4.439721 | 5.042660 | -3.160050 | H | -3.041299 | 3.657789 | 5.570437 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|----------|-----------|-----------|
| C | 2.657165 | -5.545513 | -3.315360 | H | 6.749286 | 2.375574 | -8.283348 |
| C | 7.391825 | -2.701315 | -5.189772 | H | 3.940849 | 3.645499 | -7.917508 |
| C | -0.494293 | 6.617698 | -1.990463 | H | 3.247263 | 1.162114 | -7.770658 |
| C | -3.370947 | -4.676657 | -4.043506 | H | 6.978898 | -2.790377 | -7.914468 |
| C | -5.844623 | -0.401208 | -3.267012 | H | 5.276128 | -5.362483 | -7.489206 |
| C | 0.498916 | 6.767273 | -2.968949 | H | 3.408951 | -3.696903 | -7.467494 |

1b

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -0.301854 | -2.821291 | 1.498805 | C | 7.846441 | -7.163462 | 2.097903 |
| C | 0.155007 | -1.404522 | 1.357067 | H | 7.925657 | -7.424590 | 3.148721 |
| C | 0.176044 | 1.421135 | 1.371980 | C | -1.861988 | -2.266035 | -2.850848 |
| C | 1.629092 | -1.426714 | 3.393206 | C | -12.815412 | -0.668718 | -2.066811 |
| C | -0.461147 | -0.686376 | 0.320072 | C | 12.003649 | -4.603088 | -2.112445 |
| C | -12.818510 | 2.835874 | -0.749003 | C | -3.514351 | 6.291015 | -0.133769 |
| C | -0.122071 | -3.785491 | 0.498624 | C | 8.942641 | -6.758889 | -0.036921 |
| H | 0.616953 | -3.617434 | -0.277698 | C | -8.271178 | 7.073070 | 1.042588 |
| C | -5.824629 | -6.778506 | 0.290717 | C | 6.532233 | -6.528257 | 0.192264 |
| C | -0.438756 | 0.725262 | 0.319961 | H | 5.591933 | -6.211161 | -0.246383 |
| C | 1.979378 | -0.756295 | 4.593340 | C | -8.923677 | 5.804065 | -1.332950 |
| C | -13.262925 | 1.433840 | -0.926786 | C | -7.664802 | -6.221281 | -1.302867 |
| C | -13.885496 | 0.696741 | 0.096231 | C | 4.162798 | -6.240388 | 2.020452 |
| C | -0.282850 | 2.833450 | 1.547856 | H | 3.860005 | -6.811414 | 1.147923 |
| C | -1.227224 | -3.097121 | 2.514293 | C | 12.648856 | -3.428975 | -2.747326 |
| H | -1.357313 | -2.380009 | 3.318619 | C | 11.817933 | 4.657119 | -2.415803 |
| C | 1.990483 | 0.705007 | 4.603182 | C | -4.790235 | 6.729713 | -0.462901 |
| C | 0.905317 | -0.712673 | 2.340293 | C | 7.675283 | -6.533698 | -0.598456 |
| C | 2.809704 | -3.436115 | 4.158249 | C | 10.143823 | -6.283567 | -0.761100 |
| C | 1.641047 | 1.397436 | 3.415355 | C | 11.969654 | 4.853746 | -1.033628 |
| C | -12.838573 | -2.817746 | -0.823411 | H | 12.698129 | 4.261327 | -0.489554 |
| C | 3.603493 | -4.614608 | 3.743876 | C | 11.610232 | 2.653296 | -3.854742 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | 0.910473 | 0.706427 | 2.351562 | C | 13.099455 | 0.744734 | -3.580638 |
| C | -9.949633 | -5.942833 | -0.516020 | C | 11.991891 | -4.703571 | -0.710127 |
| C | -11.164377 | -5.100651 | -0.599774 | C | 9.985482 | 6.257951 | -2.369947 |
| C | -13.274086 | -1.408872 | -0.964451 | H | 9.223084 | 6.812925 | -2.907868 |
| C | -2.030913 | -5.057307 | 1.312983 | C | 8.990800 | -7.163597 | 1.308596 |
| C | -0.962409 | -4.891833 | 0.415146 | C | 12.422102 | 3.456501 | -3.037664 |
| H | -0.836446 | -5.584966 | -0.409930 | C | -7.618238 | 6.210897 | -1.097531 |
| C | -1.209358 | 3.070000 | 2.572825 | C | 11.090147 | -5.526605 | -0.051504 |
| H | -1.340148 | 2.321691 | 3.348012 | C | 11.177456 | -5.495641 | -2.820722 |
| C | 2.094412 | -2.736523 | 3.190844 | C | 13.193933 | -0.732686 | -3.498299 |
| H | 1.994918 | -3.168710 | 2.206144 | C | 10.864506 | 5.448134 | -3.080232 |
| C | -12.385271 | 3.261545 | 0.517824 | H | 10.771469 | 5.378609 | -4.159896 |
| C | -11.563150 | 4.372935 | 0.659797 | C | 11.937571 | 1.330196 | -4.113664 |
| C | -13.890647 | -0.694345 | 0.077981 | C | 12.123698 | -2.878240 | -3.929796 |
| C | -12.396713 | -3.273633 | 0.429747 | C | 13.617875 | -2.664455 | -2.073406 |
| C | 2.117886 | 2.705654 | 3.231796 | C | 12.403328 | -1.570395 | -4.305152 |
| H | 2.015271 | 3.156139 | 2.255740 | C | 10.262202 | -6.310616 | -2.161115 |
| C | -4.812757 | -6.633686 | -0.675901 | C | -4.130828 | -3.226566 | -3.490341 |
| C | -3.201281 | -5.911957 | 1.005454 | C | 13.870158 | -1.345562 | -2.428425 |
| C | -11.134035 | 5.103438 | -0.460145 | C | -3.857309 | 3.192875 | -3.754686 |
| C | -2.083518 | -4.185139 | 2.415436 | C | 13.662434 | 2.925901 | -2.644473 |
| C | -7.261806 | -6.775048 | -0.074896 | C | 13.997166 | 1.603263 | -2.918611 |
| C | -11.579116 | -4.391691 | 0.539545 | C | -3.163900 | 3.382521 | -5.112976 |
| C | -0.102869 | 3.835074 | 0.585649 | C | -5.504601 | -3.537106 | -2.874947 |
| C | 3.642810 | 4.562714 | 3.796596 | C | -3.536638 | -4.541966 | -4.036371 |
| C | -1.267731 | 1.434122 | -0.703746 | C | -4.403143 | 4.559960 | -3.294558 |
| C | 2.848754 | 3.381926 | 4.204122 | C | -4.333349 | -2.232617 | -4.654938 |
| C | -1.367615 | -1.373384 | -0.653106 | C | -5.034036 | 2.209533 | -3.943105 |
| C | -5.430203 | -6.663517 | 1.635802 | H | -14.318217 | 1.217587 | 0.944973 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -2.061453 | 4.163745 | 2.520259 | H | -12.579038 | 2.638784 | 1.384771 |
| H | -2.859223 | 4.233074 | 3.250818 | H | -11.136728 | 4.592946 | 1.633131 |
| C | -9.916295 | 5.938385 | -0.348558 | H | -14.326771 | -1.234284 | 0.912965 |
| C | 3.242319 | 5.402776 | 2.741286 | H | -12.579145 | -2.668818 | 1.311739 |
| H | 2.215780 | 5.368978 | 2.388105 | H | -5.039455 | -6.786234 | -1.725520 |
| C | -8.279770 | -7.070184 | 0.851484 | H | -2.882381 | -4.282567 | 3.141765 |
| C | -4.147773 | -6.259008 | 1.984581 | H | -11.144431 | -4.633538 | 1.503882 |
| C | 5.515556 | 6.233680 | 2.469709 | H | 0.634069 | 3.696959 | -0.198411 |
| C | 6.588469 | 6.702599 | 1.562558 | H | -6.161597 | -6.796173 | 2.425315 |
| C | 7.849738 | 7.115629 | 2.026733 | H | -8.035535 | -7.577360 | 1.779146 |
| H | 7.977285 | 7.369841 | 3.074626 | H | -3.907690 | -6.135313 | 3.035354 |
| C | -5.415593 | 6.643092 | 1.845863 | H | -6.153787 | 6.726558 | 2.636206 |
| C | -3.175217 | 5.951241 | 1.187328 | H | -2.967485 | 1.679224 | 0.591211 |
| C | 8.954959 | 7.134825 | 1.182135 | H | -0.811045 | 5.673990 | -0.245772 |
| H | 9.925899 | 7.405524 | 1.585665 | H | -2.836780 | -5.965301 | -1.120722 |
| C | -2.577534 | 1.831402 | -0.409192 | H | -9.211887 | -5.273904 | -2.427577 |
| C | -0.938927 | 4.948162 | 0.550415 | H | -12.973276 | -3.362301 | -2.908811 |
| C | -3.542076 | -6.192119 | -0.329406 | H | -10.336900 | -6.843906 | 1.406825 |
| C | -8.974471 | -5.816514 | -1.518581 | H | -4.538244 | -2.577081 | -0.799686 |
| C | -2.005104 | 5.082420 | 1.456385 | H | -11.520353 | -5.330407 | -2.716397 |
| C | -12.578753 | -3.638321 | -1.935721 | H | -11.466408 | 5.380540 | -2.574451 |
| C | 5.868066 | 5.529848 | 3.632893 | H | -12.321043 | 1.250914 | -2.857615 |
| H | 6.904436 | 5.516298 | 3.953685 | H | -4.387527 | 2.710112 | -1.114783 |
| C | 2.544394 | -1.528052 | 5.633139 | H | -3.888155 | 6.074901 | 3.224242 |
| H | 2.746237 | -1.069394 | 6.594385 | H | -1.182059 | 2.389258 | -3.960231 |
| C | 2.937776 | -2.837868 | 5.431176 | H | -12.931743 | 3.427474 | -2.822963 |
| H | 3.412984 | -3.383812 | 6.240030 | H | 0.025695 | -1.403936 | -2.290579 |
| C | 7.556352 | 6.495874 | -0.659810 | H | -10.336357 | 6.837243 | 1.567851 |
| H | 7.431502 | 6.183755 | -1.691082 | H | 0.229560 | 1.364098 | -2.240219 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -9.591194 | -6.657591 | 0.639734 | H | -1.527341 | -2.465486 | -3.864283 |
| C | -3.545190 | -2.326023 | -1.150618 | H | -12.331203 | -1.182958 | -2.890020 |
| C | -11.756800 | -4.754313 | -1.826906 | H | -2.807293 | 6.106724 | -0.934481 |
| C | 8.847955 | 6.738614 | -0.162875 | H | -8.040261 | 7.584999 | 1.971340 |
| C | 6.606511 | -6.751954 | 1.577220 | H | -9.147251 | 5.254759 | -2.241476 |
| C | -3.168708 | -2.606796 | -2.468789 | H | -6.926301 | -5.985288 | -2.058442 |
| C | 5.502585 | -6.281916 | 2.446129 | H | -5.019905 | 6.926074 | -1.504181 |
| C | 6.452587 | 6.479718 | 0.182425 | H | 7.601173 | -6.221935 | -1.635287 |
| H | 5.495217 | 6.157036 | -0.212824 | H | 10.644334 | 3.028374 | -4.176265 |
| C | -11.715877 | 4.786922 | -1.700129 | H | 12.605556 | -4.035419 | -0.117269 |
| C | 3.231607 | -5.425718 | 2.655743 | H | 9.946524 | -7.420679 | 1.755340 |
| H | 2.218436 | -5.372814 | 2.267992 | H | -6.862174 | 5.966199 | -1.834438 |
| C | -7.239975 | 6.782620 | 0.130292 | H | 11.028614 | -5.478516 | 1.030522 |
| C | -12.809692 | 0.719313 | -2.048234 | H | 11.207605 | -5.513004 | -3.905516 |
| C | -5.806251 | 6.808980 | 0.505292 | H | 11.211260 | 0.713006 | -4.629449 |
| C | 2.578450 | 1.452081 | 5.648542 | H | 11.400721 | -3.440164 | -4.511135 |
| H | 2.787732 | 0.974022 | 6.598643 | H | 14.120044 | -3.074045 | -1.203446 |
| C | 4.160884 | 6.219691 | 2.091792 | H | 11.926151 | -1.171410 | -5.193881 |
| H | 3.836123 | 6.813281 | 1.242566 | H | 9.592988 | -6.937784 | -2.742661 |
| C | -3.376125 | 2.419800 | -1.380609 | H | 14.524034 | -0.755790 | -1.795290 |
| C | -2.664712 | -1.713574 | -0.262938 | H | 14.349264 | 3.540253 | -2.069808 |
| H | -2.985128 | -1.506667 | 0.752201 | H | 14.945874 | 1.218174 | -2.558730 |
| C | -4.127470 | 6.243489 | 2.179605 | H | -2.317178 | 4.072614 | -5.041542 |
| C | 5.821632 | -5.604862 | 3.634913 | H | -3.873389 | 3.799409 | -5.834409 |
| H | 6.845698 | -5.609746 | 3.992577 | H | -2.799803 | 2.433152 | -5.517507 |
| C | 10.015734 | 6.303646 | -0.964460 | H | -6.008071 | -2.630023 | -2.527110 |
| C | -1.593108 | 2.245790 | -2.968198 | H | -5.419586 | -4.224338 | -2.029446 |
| C | -12.543993 | 3.679148 | -1.840636 | H | -6.148801 | -4.003516 | -3.627622 |
| C | -0.977161 | -1.661005 | -1.963658 | H | -4.204750 | -4.981726 | -4.785007 |

| | | | | | | | |
|---------------------------|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | 2.987622 | 2.759908 | 5.463985 | H | -3.402508 | -5.269447 | -3.230497 |
| H | 3.481891 | 3.285508 | 6.275008 | H | -2.563625 | -4.383223 | -4.509216 |
| C | 4.893255 | -4.790571 | 4.269985 | H | -4.916288 | 4.488811 | -2.333139 |
| H | 5.216295 | -4.182256 | 5.108132 | H | -5.112437 | 4.954851 | -4.030785 |
| C | 4.951369 | 4.712714 | 4.282899 | H | -3.589632 | 5.283964 | -3.183464 |
| H | 5.294231 | 4.082268 | 5.096672 | H | -3.390638 | -2.005294 | -5.160468 |
| C | -9.577799 | 6.653171 | 0.812836 | H | -4.751766 | -1.290297 | -4.287395 |
| C | -2.910353 | 2.624185 | -2.689871 | H | -5.023019 | -2.647980 | -5.398109 |
| C | -0.785147 | 1.660740 | -1.991994 | H | -5.595845 | 2.073134 | -3.015037 |
| C | 11.085568 | 5.656888 | -0.323282 | H | -4.667750 | 1.227835 | -4.259593 |
| H | 11.145147 | 5.670276 | 0.759837 | H | -5.726498 | 2.581420 | -4.706460 |
| $3C_{60}@(\mathbf{1b})_2$ | | | | | | | |
| C | -15.762221 | 3.196932 | -0.593857 | C | -4.217839 | -1.302358 | 5.496214 |
| C | -16.018608 | 3.192773 | 0.845127 | C | -5.286112 | -0.609074 | 4.898170 |
| C | -17.155037 | 2.306656 | 1.095077 | C | 7.772046 | -3.466536 | -0.806171 |
| C | -17.604314 | 1.768305 | -0.188646 | C | 6.241462 | 2.342229 | -1.395257 |
| C | -16.739346 | 2.318329 | -1.230615 | C | 9.397097 | -1.395666 | -4.326602 |
| C | -16.360587 | 1.521116 | -2.304339 | C | 8.498361 | 0.090270 | -2.014052 |
| C | -14.989639 | 1.566592 | -2.802059 | C | 9.700059 | 2.835351 | -4.312965 |
| C | -14.058164 | 2.404212 | -2.196289 | C | 9.207420 | -2.038466 | -3.077644 |
| C | -14.453821 | 3.238708 | -1.064227 | C | -4.020807 | 2.975470 | 5.275853 |
| C | -13.336722 | 3.282324 | -0.121768 | C | 10.361972 | 4.130730 | -4.033165 |
| C | -13.582408 | 3.275451 | 1.247029 | C | 8.597506 | -1.326277 | -1.955845 |
| C | -14.957420 | 3.232184 | 1.741408 | C | -1.139513 | 5.745763 | 3.961058 |
| C | -14.978806 | 2.385859 | 2.935464 | C | -2.386258 | 5.135208 | 4.487253 |
| C | -16.060770 | 1.545021 | 3.173406 | C | -4.299113 | 1.534311 | 5.511059 |
| C | -17.177273 | 1.506239 | 2.230506 | C | 5.921426 | 4.399776 | -0.140221 |
| C | -17.643707 | 0.123408 | 2.140420 | C | 7.256655 | 4.314954 | 0.290332 |
| C | -18.069588 | -0.389031 | 0.920446 | C | 6.850376 | -3.905885 | -1.772837 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -18.051777 | 0.455026 | -0.274984 | C | 9.192947 | 2.155617 | -3.213876 |
| C | -17.654592 | -0.382285 | -1.406336 | C | -4.050735 | -3.286828 | 3.980444 |
| C | -16.831157 | 0.140388 | -2.396212 | C | -3.285700 | -4.377785 | 3.579714 |
| C | -15.748340 | -0.668896 | -2.948813 | C | -5.325594 | 0.789690 | 4.903778 |
| C | -14.608676 | 0.213083 | -3.198970 | C | -4.100988 | 3.492464 | 3.976355 |
| C | -13.313785 | -0.238529 | -2.971024 | C | 9.813118 | -3.289621 | -2.862206 |
| C | -12.335929 | 0.640984 | -2.334336 | C | 3.844742 | 5.936578 | 2.582656 |
| C | -12.697644 | 1.930428 | -1.957440 | C | 4.913393 | 5.277232 | 0.504294 |
| C | -12.251382 | 2.473197 | -0.673288 | C | -2.332154 | -4.946842 | 4.436714 |
| C | -11.468431 | 1.694724 | 0.172173 | C | 5.451950 | 3.424950 | -1.033843 |
| C | -11.731446 | 1.687206 | 1.610406 | C | 1.354030 | 6.216896 | 2.680164 |
| C | -12.757031 | 2.460803 | 2.133862 | C | -3.295697 | 4.560682 | 3.589766 |
| C | -13.619705 | 1.908045 | 3.177578 | C | 7.983180 | -4.272848 | 0.320526 |
| C | -12.319296 | -0.194827 | 3.099497 | C | 11.484873 | -4.996462 | -3.417695 |
| C | -12.784985 | -1.579153 | 3.011497 | C | 7.100731 | -1.936791 | 1.507445 |
| C | -14.159630 | -1.622096 | 3.502494 | C | 10.542142 | -3.941018 | -3.847600 |
| C | -14.543619 | -0.265419 | 3.896104 | C | 7.372359 | 0.867590 | 1.542799 |
| C | -13.406970 | 0.617213 | 3.649143 | C | 2.626717 | 6.113600 | 0.515330 |
| C | -15.837982 | 0.187777 | 3.665425 | C | 6.001868 | -4.966819 | -1.497875 |
| C | -16.815490 | -0.690577 | 3.027146 | C | -1.197078 | -5.718361 | 3.872026 |
| C | -16.450965 | -1.978458 | 2.651271 | C | 11.195290 | -5.837010 | -2.327777 |
| C | -16.896456 | -2.516810 | 1.368893 | C | 0.163076 | 6.772835 | 2.177921 |
| C | -17.686971 | -1.743382 | 0.525038 | C | 3.758046 | 5.694542 | -0.177030 |
| C | -17.431841 | -1.738638 | -0.913521 | C | 13.554976 | -6.365557 | -2.063883 |
| C | -16.399078 | -2.510164 | -1.434717 | C | 14.677061 | -6.683113 | -1.149844 |
| C | -15.537191 | -1.961536 | -2.479938 | C | 15.982212 | -6.915573 | -1.616937 |
| C | -14.174587 | -2.434738 | -2.236822 | C | 2.354095 | -5.959822 | 0.480405 |
| C | -14.196071 | -3.275663 | -1.042455 | C | 4.774381 | -6.202140 | 0.304291 |
| C | -15.570219 | -3.322680 | -0.547838 | C | 17.076726 | -6.776269 | -0.769267 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -13.090633 | -1.596850 | -2.477537 | C | 5.846774 | -2.531668 | 1.318057 |
| C | -11.973696 | -1.558603 | -1.535818 | C | 7.100579 | -5.311330 | 0.615706 |
| C | -11.510738 | -0.174867 | -1.444895 | C | 4.957626 | 5.470826 | 1.894390 |
| C | -11.098450 | 0.337841 | -0.222864 | C | 0.062920 | 5.260500 | 4.504077 |
| C | -11.119902 | -0.503045 | 0.968515 | C | 6.017814 | -5.589517 | -0.231910 |
| C | -11.511542 | 0.328399 | 2.102041 | C | -3.303107 | 3.720215 | 6.233439 |
| C | -15.091487 | -2.459329 | 2.896336 | C | 13.820490 | -5.635617 | -3.233028 |
| C | -14.697493 | -3.294184 | 1.762848 | C | 9.577249 | 0.778410 | -5.574636 |
| C | -15.812893 | -3.329679 | 0.819779 | C | 9.815871 | 2.139651 | -5.533632 |
| C | -13.132787 | -3.241774 | -0.146047 | C | 15.590953 | -6.317709 | 1.070059 |
| C | -11.992090 | -2.362486 | -0.398110 | C | -1.062969 | 6.537295 | 2.802793 |
| C | -11.551560 | -1.821528 | 0.886335 | C | 5.595062 | 1.837635 | 2.862273 |
| C | -12.412761 | -2.371594 | 1.930510 | C | -2.493532 | 4.779593 | 5.845158 |
| C | -13.388813 | -3.251023 | 1.293721 | C | 16.901939 | -6.399590 | 0.573262 |
| C | -7.528058 | -2.642999 | 0.415577 | C | 13.048956 | 6.656451 | -1.911061 |
| C | -8.141705 | -1.283454 | 0.453282 | C | 6.494893 | 2.233132 | 3.855830 |
| C | -8.184579 | 1.530731 | 0.494900 | C | 12.046882 | 6.032015 | -2.805947 |
| C | -8.709730 | -1.339861 | 2.897790 | C | 14.499912 | -6.458260 | 0.225232 |
| C | -8.058104 | -0.565320 | -0.740013 | C | -2.330663 | -4.526786 | 5.779441 |
| C | 4.527570 | 3.061096 | -5.669624 | C | 9.858949 | 5.004069 | -3.052429 |
| C | -7.913440 | -3.648618 | -0.480387 | C | 1.114384 | -6.613812 | 2.503172 |
| C | -2.131529 | -5.855353 | -2.392869 | C | -3.236752 | -0.549966 | 6.165331 |
| C | -8.056653 | 0.852382 | -0.721908 | C | 2.337321 | -6.714028 | 1.661907 |
| C | -8.770085 | -0.672962 | 4.149511 | C | 10.004043 | -2.136240 | -5.369541 |
| C | 5.064989 | 1.703952 | -5.953607 | C | 12.213117 | -6.512507 | -1.666215 |
| C | 6.007940 | 1.073486 | -5.118594 | C | 5.162499 | -3.089006 | 2.388564 |
| C | -7.652075 | 2.921643 | 0.515438 | C | 6.024204 | 1.157832 | 1.726494 |
| C | -6.277874 | -2.737104 | 1.040059 | C | 3.549920 | -5.696146 | -0.169450 |
| C | -8.815820 | 0.789414 | 4.166243 | C | 12.505842 | 5.254460 | -3.882115 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -8.416914 | -0.605521 | 1.670741 | C | 17.992173 | -5.794667 | 1.373644 |
| C | -9.574613 | -3.379739 | 3.934780 | C | 6.938357 | -2.437768 | 3.870125 |
| C | -8.785364 | 1.493040 | 2.933799 | C | -3.097094 | -3.441034 | 6.181913 |
| C | 4.777085 | -2.480363 | -5.385461 | C | 8.290155 | 1.278876 | 2.514520 |
| C | -10.393410 | -4.585004 | 3.666945 | C | 10.563467 | -3.377990 | -5.143075 |
| C | -8.445076 | 0.807718 | 1.688674 | C | 11.675684 | 4.319688 | -4.488401 |
| C | 1.740458 | -5.175778 | -4.138829 | C | 12.803090 | -4.963112 | -3.899080 |
| C | 3.008656 | -4.517867 | -4.550743 | C | -1.305309 | -6.508363 | 2.714406 |
| C | 5.192086 | -1.114987 | -5.796410 | C | 5.683690 | -3.032964 | 3.691342 |
| C | -5.692154 | -4.626550 | -0.364169 | C | 7.644306 | -1.903403 | 2.790929 |
| C | -7.003048 | -4.631917 | -0.867659 | C | 18.900640 | -4.940900 | 0.727104 |
| C | -6.423212 | 3.068966 | 1.172956 | C | 14.268929 | 7.162380 | -2.391371 |
| C | -9.138513 | -2.673976 | 2.822490 | C | 7.855243 | 1.949585 | 3.655063 |
| C | 4.466480 | 3.475187 | -4.329827 | C | -3.276882 | 0.831209 | 6.173350 |
| C | 3.531560 | 4.413741 | -3.916573 | C | 18.353604 | 5.198788 | 2.149045 |
| C | 6.058467 | -0.316086 | -5.031596 | C | 4.737227 | -7.049537 | 1.424984 |
| C | 4.524305 | -2.695427 | -4.021590 | C | 15.255694 | 6.983482 | -0.176801 |
| C | -9.302376 | 2.799154 | 2.889508 | C | -0.166316 | -6.936771 | 2.031445 |
| C | -3.318639 | -5.595384 | -3.103603 | C | 12.909691 | 6.469222 | -0.526436 |
| C | -4.562333 | -5.309812 | -1.037393 | C | 0.090439 | -5.467127 | 4.379446 |
| C | 2.624689 | 4.974032 | -4.824789 | C | 1.276719 | 5.485394 | 3.878243 |
| C | -5.375763 | -3.714125 | 0.654426 | C | 10.689918 | 5.941605 | -2.450192 |
| C | -0.813032 | -5.788356 | -3.069329 | C | 19.085926 | 4.128850 | 2.865633 |
| C | 3.655397 | -3.701774 | -3.612729 | C | 19.523346 | -3.929127 | 2.845189 |
| C | -8.069494 | 3.920870 | -0.371376 | C | 3.539468 | -7.286964 | 2.103711 |
| C | -10.724885 | 4.575744 | 3.779735 | C | 13.993691 | 6.630153 | 0.326012 |
| C | -7.587141 | 1.513415 | -1.977979 | C | 16.450983 | 6.655116 | 0.634246 |
| C | -9.806620 | 3.437846 | 4.013297 | C | 19.653628 | -4.025601 | 1.449939 |
| C | -7.615971 | -1.246614 | -1.995400 | C | 19.013823 | -1.998558 | 4.302359 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -2.221044 | -5.966246 | -0.994852 | C | 20.150763 | 0.123673 | 3.956251 |
| C | -5.555450 | 4.082557 | 0.806804 | C | 18.417421 | 5.236498 | 0.745144 |
| C | 1.366639 | 5.559182 | -4.304326 | C | 17.973548 | -5.798738 | 2.779552 |
| C | -10.508250 | 5.484320 | 2.728580 | C | 15.354849 | 7.323739 | -1.537527 |
| C | 0.358222 | -6.323179 | -2.504074 | C | 19.944259 | -2.663150 | 3.489133 |
| C | -3.417498 | -5.714448 | -0.333585 | C | 1.223178 | -5.919172 | 3.716328 |
| C | -12.852251 | 6.133853 | 2.762425 | C | 17.489419 | 5.950871 | 0.004791 |
| C | -14.044511 | 6.579028 | 2.003108 | C | 17.400492 | 6.018312 | 2.780421 |
| C | -15.277021 | 6.840519 | 2.625642 | C | 19.980224 | 1.588237 | 3.781759 |
| C | -2.413953 | 6.267803 | -0.905737 | C | 18.724361 | -4.878580 | 3.504020 |
| C | -4.780611 | 5.697524 | -0.888407 | C | 19.114537 | -0.633460 | 4.529476 |
| C | -16.459418 | 6.840361 | 1.892112 | C | 18.538555 | 3.536965 | 4.016991 |
| C | -6.303909 | 2.073627 | -2.006850 | C | 20.193143 | 3.493133 | 2.278462 |
| C | -7.202842 | 4.957628 | -0.718101 | C | 18.989131 | 2.306200 | 4.476349 |
| C | -4.503783 | -5.305492 | -2.440707 | C | 16.462892 | 6.729562 | 2.036893 |
| C | 0.568749 | -4.712462 | -4.757764 | C | 6.021865 | 2.906755 | 5.151096 |
| C | -5.894197 | 4.993708 | -0.207495 | C | 20.614574 | 2.244733 | 2.711670 |
| C | 4.264845 | -3.409922 | -6.309015 | C | 4.886582 | -3.644651 | 4.850965 |
| C | -13.031356 | 5.324866 | 3.895815 | C | 21.078788 | -1.948238 | 3.071036 |
| C | -9.061898 | -1.446866 | 5.298685 | C | 21.183905 | -0.582880 | 3.309479 |
| C | -9.459858 | -2.768334 | 5.200897 | C | 5.482950 | -3.276719 | 6.225930 |
| C | -15.204213 | 6.462008 | -0.127841 | C | 4.495379 | 3.148078 | 5.150689 |
| C | 1.615695 | -6.014624 | -3.023543 | C | 6.735653 | 4.269274 | 5.324788 |
| C | -5.758399 | -1.889717 | -3.405714 | C | 4.908256 | -5.184643 | 4.689100 |
| C | 3.382940 | -4.406794 | -5.899783 | C | 6.368958 | 1.976574 | 6.341395 |
| C | -16.449438 | 6.576692 | 0.511714 | C | 3.426927 | -3.129665 | 4.805951 |
| C | -13.514030 | -6.751151 | 1.745833 | H | 6.493007 | -3.683280 | 6.343045 |
| C | -6.629889 | -2.399338 | -4.375227 | H | 4.853054 | -3.700031 | 7.015915 |
| C | -12.371698 | -6.259688 | 2.551256 | H | 5.520080 | -2.189100 | 6.354367 |

| | | | | | | | |
|---|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -14.025498 | 6.464965 | 0.603186 | H | 4.211799 | 3.649201 | 6.083002 |
| C | 2.806210 | 4.700617 | -6.191503 | H | 3.946507 | 2.202655 | 5.085982 |
| C | -10.083516 | -5.443372 | 2.597639 | H | 4.198863 | 3.780953 | 4.308262 |
| C | -1.107512 | 6.140683 | -3.049664 | H | 6.413518 | 4.746819 | 6.257308 |
| C | 4.336460 | 0.897782 | -6.845077 | H | 6.489932 | 4.930793 | 4.487852 |
| C | -2.387395 | 6.226002 | -2.309825 | H | 7.821964 | 4.142444 | 5.356599 |
| C | -9.168392 | 1.511042 | 5.332965 | H | 4.503085 | -5.477899 | 3.717580 |
| C | -11.553883 | 6.253927 | 2.233492 | H | 4.316190 | -5.659390 | 5.481812 |
| C | -5.709844 | 2.421612 | -3.209712 | H | 5.938860 | -5.551386 | 4.753420 |
| C | -6.246538 | -1.319960 | -2.236094 | H | 5.879024 | 1.005807 | 6.209808 |
| C | -3.593347 | 6.026217 | -0.210476 | H | 6.028375 | 2.424851 | 7.282181 |
| C | -12.638608 | -5.501523 | 3.703598 | H | 7.449249 | 1.812480 | 6.402408 |
| C | -17.658198 | 6.122473 | -0.215025 | H | 2.858325 | -3.549517 | 5.644847 |
| C | -7.675195 | 1.714791 | -4.391764 | H | 2.927149 | -3.416595 | 3.878562 |
| C | 3.750639 | 3.767278 | -6.607837 | H | 3.408027 | -2.037767 | 4.877967 |
| C | -8.500881 | -1.770806 | -2.939913 | H | -8.890697 | -3.603222 | -0.942239 |
| C | -9.658851 | 2.801392 | 5.265068 | H | 6.660757 | 1.663046 | -4.486213 |
| C | -11.663571 | -4.679226 | 4.255614 | H | -5.977386 | -1.954227 | 1.724888 |
| C | -11.984787 | 4.559758 | 4.397648 | H | -7.285042 | -5.354627 | -1.623960 |
| C | 1.309536 | 6.415350 | -3.192730 | H | -6.101404 | 2.289101 | 1.851438 |
| C | -6.364585 | 2.206401 | -4.432124 | H | -9.256223 | -3.124563 | 1.852073 |
| C | -8.283122 | 1.377206 | -3.180083 | H | 5.068397 | 2.969439 | -3.591149 |
| C | -18.572685 | 5.294188 | 0.455784 | H | 3.400271 | 4.605009 | -2.862531 |
| C | -14.721585 | -7.165921 | 2.332581 | H | 6.736152 | -0.780256 | -4.327431 |
| C | -8.008959 | -2.341166 | -4.112838 | H | 4.878671 | -1.974785 | -3.296201 |
| C | 4.403000 | -0.485122 | -6.772852 | H | -9.436877 | 3.268052 | 1.929794 |
| C | -19.052958 | -4.670030 | -1.684947 | H | -3.301229 | -5.561194 | -4.185478 |
| C | -4.777984 | 5.772645 | -2.291193 | H | -4.364404 | -3.672713 | 1.024774 |
| C | -15.904180 | -6.811216 | 0.237584 | H | 3.350902 | -3.747932 | -2.577997 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | 0.090875 | 6.706510 | -2.580345 | H | -9.025180 | 3.819482 | -0.871224 |
| C | -13.497579 | -6.520505 | 0.360608 | H | -1.328956 | -6.144313 | -0.409522 |
| C | 0.161824 | 5.043865 | -4.808768 | H | -4.544280 | 4.065672 | 1.178353 |
| C | -0.679998 | -5.004620 | -4.229953 | H | -9.529622 | 5.540131 | 2.265051 |
| C | -11.057809 | -6.271045 | 2.051926 | H | 0.293952 | -6.963390 | -1.632862 |
| C | -19.759912 | -3.507322 | -2.270025 | H | -3.445644 | -5.753665 | 0.747053 |
| C | -19.486262 | 4.516232 | -1.656249 | H | -15.311118 | 6.995113 | 3.697662 |
| C | -3.608730 | 6.054916 | -2.985052 | H | -1.491244 | 6.390203 | -0.353189 |
| C | -14.671166 | -6.549558 | -0.380277 | H | -17.404738 | 6.994601 | 2.398989 |
| C | -17.140337 | -6.348071 | -0.434844 | H | -5.763361 | 2.210589 | -1.083995 |
| C | -19.470625 | 4.506678 | -0.251617 | H | -7.507085 | 5.679733 | -1.466236 |
| C | -19.313330 | 2.683942 | -3.309711 | H | -5.368809 | -4.977632 | -3.002898 |
| C | -20.585837 | 0.634949 | -2.989689 | H | 0.656106 | -4.031609 | -5.595495 |
| C | -18.986672 | -4.779429 | -0.284939 | H | 4.495353 | -3.294537 | -7.361838 |
| C | -17.775540 | 6.240864 | -1.611387 | H | -14.027318 | 5.187980 | 4.297551 |
| C | -15.897244 | -7.196769 | 1.589883 | H | -9.044478 | -0.979811 | 6.273767 |
| C | -20.085012 | 3.349463 | -2.345283 | H | -9.737414 | -3.319144 | 6.091632 |
| C | -1.047320 | 5.322884 | -4.191867 | H | -15.170670 | 6.229938 | -1.184070 |
| C | -18.053717 | -5.601462 | 0.326034 | H | 2.501673 | -6.405144 | -2.539868 |
| C | -18.232943 | -5.522881 | -2.445375 | H | -4.689597 | -1.924882 | -3.551783 |
| C | -20.523433 | -0.848342 | -2.934689 | H | 2.925293 | -5.061299 | -6.632537 |
| C | -18.672174 | 5.448489 | -2.321130 | H | -13.093930 | 6.235662 | 0.103334 |
| C | -19.558066 | 1.354459 | -3.623687 | H | 2.161949 | 5.179777 | -6.919655 |
| C | -19.261242 | -2.874484 | -3.421472 | H | -9.093883 | -5.408994 | 2.155991 |
| C | -20.767404 | -2.840161 | -1.552779 | H | 3.597535 | 1.353475 | -7.491422 |
| C | -19.649228 | -1.583606 | -3.756982 | H | -9.127921 | 1.019476 | 6.295154 |
| C | -17.291105 | -6.344269 | -1.831705 | H | -11.379137 | 6.918486 | 1.395797 |
| C | -6.119252 | -2.974155 | -5.703980 | H | -4.707032 | 2.827633 | -3.192634 |
| C | -21.124146 | -1.536700 | -1.864733 | H | -5.566241 | -0.927392 | -1.497968 |

| | | | | | | | |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| C | -5.589249 | 2.417737 | -5.738877 | H | -3.578856 | 6.021749 | 0.871541 |
| C | -21.227243 | 2.694594 | -1.855324 | H | -13.652632 | -5.451743 | 4.080057 |
| C | -21.477333 | 1.366665 | -2.179924 | H | -8.222897 | 1.552174 | -5.309705 |
| C | -6.474995 | 2.209794 | -6.984362 | H | 3.834854 | 3.528682 | -7.661543 |
| C | -4.577449 | -2.928294 | -5.798260 | H | -9.567469 | -1.723479 | -2.757011 |
| C | -6.579079 | -4.445848 | -5.844384 | H | -9.984846 | 3.306276 | 6.166537 |
| C | -4.994787 | 3.846575 | -5.783023 | H | -11.926427 | -3.999785 | 5.057125 |
| C | -6.702629 | -2.129755 | -6.865619 | H | -12.178279 | 3.841575 | 5.184842 |
| C | -4.437472 | 1.377653 | -5.774775 | H | 2.224799 | 6.846769 | -2.803948 |
| C | -3.057773 | -1.339063 | 1.398216 | H | -9.279941 | 0.955214 | -3.174870 |
| C | -3.229709 | 1.495260 | 1.207820 | H | -18.482976 | 5.164160 | 1.526545 |
| C | -3.611661 | -0.721578 | 0.196092 | H | -14.744944 | -7.410396 | 3.388114 |
| C | -2.706260 | 0.907643 | 2.354795 | H | -8.710747 | -2.733170 | -4.839917 |
| C | -2.620649 | -0.548162 | 2.454399 | H | 3.720434 | -1.081301 | -7.365498 |
| C | -3.699028 | 0.661733 | 0.103205 | H | -5.672534 | 5.507573 | -2.840318 |
| C | 1.918410 | 2.835309 | -1.083647 | H | 0.068094 | 7.372662 | -1.725424 |
| C | 1.151143 | -1.153601 | -3.080118 | H | -12.584968 | -6.173641 | -0.106315 |
| C | -2.591629 | 2.679395 | 0.633222 | H | 0.198020 | 4.340596 | -5.631190 |
| C | 1.995300 | 2.937091 | 0.372940 | H | -1.553382 | -4.535135 | -4.662450 |
| C | -0.642050 | -1.999197 | 2.756011 | H | -10.817855 | -6.892105 | 1.196945 |
| C | -1.378548 | -0.885213 | 3.148751 | H | -3.628719 | 6.080671 | -4.066923 |
| C | -1.830521 | 1.047796 | -3.075828 | H | -14.654928 | -6.224080 | -1.412396 |
| C | 2.809957 | 1.831095 | 0.858364 | H | -20.067561 | 3.773773 | 0.276049 |
| C | -2.674049 | 2.582953 | -0.824112 | H | -18.425640 | 3.164279 | -3.699789 |
| C | 0.741485 | 3.160290 | -1.746444 | H | -19.574928 | -4.114010 | 0.331373 |
| C | -0.352158 | 3.689728 | 0.407493 | H | -17.120959 | 6.919698 | -2.145161 |
| C | -0.912882 | 2.602673 | 2.439137 | H | -16.830290 | -7.464191 | 2.071984 |
| C | 0.888670 | 3.352860 | 1.101720 | H | -1.944186 | 4.827379 | -4.539796 |
| C | -0.425438 | 3.594890 | -0.979129 | H | -17.934859 | -5.559097 | 1.400872 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| C | -1.183792 | 2.240439 | -2.765085 | H | -18.300669 | -5.507794 | -3.526567 |
| C | 1.324751 | 1.633565 | 2.823161 | H | -18.706920 | 5.510688 | -3.402606 |
| C | -3.343317 | 1.327438 | -1.147563 | H | -18.852576 | 0.840826 | -4.260778 |
| C | 0.328642 | -0.045432 | -3.569847 | H | -18.483681 | -3.355804 | -4.000991 |
| C | -1.465257 | 3.222467 | 1.234729 | H | -21.224578 | -3.320348 | -0.696780 |
| C | -1.056568 | -0.122930 | -3.492002 | H | -19.197104 | -1.115000 | -4.621093 |
| C | -1.616204 | 3.026306 | -1.610305 | H | -16.631935 | -6.951653 | -2.440990 |
| C | 2.480013 | 1.192223 | 2.048194 | H | -21.817281 | -1.021534 | -1.213743 |
| C | -2.940702 | 0.582024 | -2.248659 | H | -21.884449 | 3.212010 | -1.166034 |
| C | 0.543294 | 2.684347 | 2.353986 | H | -22.338032 | 0.875901 | -1.743886 |
| C | 2.689014 | 1.662760 | -1.495507 | H | -7.323716 | 2.902421 | -6.985092 |
| C | 2.866002 | -1.174707 | -1.302508 | H | -6.853118 | 1.182805 | -7.025178 |
| C | 3.236312 | 1.042663 | -0.293299 | H | -5.878973 | 2.389911 | -7.885483 |
| C | 2.338570 | -0.585091 | -2.447766 | H | -4.264052 | -3.355283 | -6.757109 |
| C | 2.254239 | 0.871094 | -2.551378 | H | -4.114029 | -3.505902 | -4.991473 |
| C | 3.329377 | -0.339981 | -0.197946 | H | -4.212680 | -1.897255 | -5.743879 |
| C | -2.279091 | -2.503535 | 0.982555 | H | -7.670110 | -4.520117 | -5.806568 |
| C | -1.516799 | 1.476240 | 2.985986 | H | -6.163701 | -5.049062 | -5.030474 |
| C | 2.230245 | -2.361091 | -0.729255 | H | -6.234162 | -4.858702 | -6.799349 |
| C | -2.359370 | -2.609318 | -0.472271 | H | -5.795233 | 4.592931 | -5.731500 |
| C | 0.274282 | 2.321069 | -2.850064 | H | -4.436762 | 3.989390 | -6.715612 |
| C | 1.010401 | 1.207433 | -3.243160 | H | -4.312447 | 4.009489 | -4.943820 |
| C | 1.462847 | -0.724763 | 2.979264 | H | -6.400322 | -1.083577 | -6.754037 |
| C | -3.178275 | -1.507489 | -0.957260 | H | -7.796015 | -2.173641 | -6.867809 |
| C | 2.305106 | -2.258116 | 0.727736 | H | -6.334625 | -2.506341 | -7.827063 |
| C | -1.108156 | -2.836246 | 1.649639 | H | -4.848998 | 0.365346 | -5.706868 |
| C | -0.014538 | -3.363435 | -0.505610 | H | -3.754813 | 1.523138 | -4.933047 |
| C | 0.547513 | -2.281613 | -2.535909 | H | -3.871876 | 1.473515 | -6.709367 |
| C | -1.256154 | -3.031021 | -1.201610 | H | 9.042610 | 3.116421 | 0.354919 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.058046 | -3.269872 | 0.881495 | H | -6.086385 | -1.155198 | 4.412579 |
| C | 0.814884 | -1.916407 | 2.669686 | H | 5.823206 | 1.537688 | -1.989166 |
| C | -1.691367 | -1.311563 | -2.920678 | H | 7.653633 | 5.068881 | 0.959692 |
| C | 2.984302 | -1.007444 | 1.055381 | H | 6.733890 | -3.351901 | -2.694743 |
| C | -0.696312 | 0.367515 | 3.475869 | H | 9.131494 | 2.683297 | -2.280091 |
| C | 1.099327 | -2.900384 | -1.331676 | H | -4.679385 | -2.784431 | 3.260545 |
| C | 0.689268 | 0.445028 | 3.394146 | H | -3.328351 | -4.700241 | 2.550445 |
| C | 1.248314 | -2.703366 | 1.514529 | H | -6.153975 | 1.295376 | 4.421250 |
| C | -2.850368 | -0.871183 | -2.148806 | H | -4.663960 | 2.952499 | 3.230835 |
| C | 2.576085 | -0.260956 | 2.153753 | H | 9.813434 | -3.694066 | -1.863855 |
| C | -0.909747 | -2.363196 | -2.453360 | H | 3.898863 | 6.047577 | 3.658276 |
| C | 15.848030 | -2.978089 | 1.245681 | H | 4.416391 | 3.441977 | -1.333865 |
| C | 16.281925 | -3.041716 | -0.148524 | H | -3.238669 | 4.831678 | 2.546539 |
| C | 17.370069 | -2.079964 | -0.323830 | H | 8.723494 | -3.978216 | 1.052408 |
| C | 17.612069 | -1.426238 | 0.962357 | H | 1.709062 | 6.284921 | -0.034337 |
| C | 16.667364 | -1.981460 | 1.929806 | H | 5.251270 | -5.234219 | -2.230043 |
| C | 16.096625 | -1.153405 | 2.889536 | H | 10.174658 | -5.914407 | -1.970253 |
| C | 14.681326 | -1.283610 | 3.219853 | H | 0.192739 | 7.377162 | 1.278429 |
| C | 13.900145 | -2.233533 | 2.569143 | H | 3.717650 | 5.610456 | -1.253577 |
| C | 14.497415 | -3.099969 | 1.556135 | H | 16.140291 | -7.154266 | -2.662097 |
| C | 13.513886 | -3.297226 | 0.492153 | H | 1.443702 | -5.487296 | 0.139076 |
| C | 13.927982 | -3.354446 | -0.833714 | H | 18.078927 | -6.906446 | -1.160564 |
| C | 15.347208 | -3.225877 | -1.160514 | H | 5.433031 | -2.591778 | 0.320015 |
| C | 15.453847 | -2.456641 | -2.401106 | H | 7.157624 | -5.782076 | 1.589203 |
| C | 16.490347 | -1.544463 | -2.568336 | H | 5.835585 | 5.158086 | 2.444927 |
| C | 17.473079 | -1.352655 | -1.503207 | H | 0.019981 | 4.600207 | 5.360438 |
| C | 17.817661 | 0.067622 | -1.458325 | H | -3.311682 | 3.400625 | 7.268934 |
| C | 18.046321 | 0.689528 | -0.236411 | H | 14.847206 | -5.477799 | -3.537836 |
| C | 17.942801 | -0.076613 | 1.006137 | H | 9.727217 | 0.252205 | -6.507065 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 17.343945 | 0.793269 | 2.017786 | H | 10.144008 | 2.661988 | -6.424199 |
| C | 16.444885 | 0.265512 | 2.936638 | H | 15.431480 | -6.001399 | 2.092426 |
| C | 15.242658 | 1.013397 | 3.294673 | H | -1.968600 | 6.954740 | 2.377825 |
| C | 14.151266 | 0.055201 | 3.469086 | H | 4.543851 | 2.046898 | 2.965861 |
| C | 12.865019 | 0.379960 | 3.054832 | H | -1.872662 | 5.281854 | 6.577991 |
| C | 12.044178 | -0.617594 | 2.370328 | H | 13.508538 | -6.248786 | 0.604177 |
| C | 12.547898 | -1.892800 | 2.133607 | H | -1.679037 | -5.018221 | 6.492164 |
| C | 12.309121 | -2.549651 | 0.848325 | H | 8.833794 | 4.898318 | -2.716240 |
| C | 11.579262 | -1.896311 | -0.139686 | H | -2.375511 | -1.057123 | 6.579349 |
| C | 12.020199 | -1.955729 | -1.532751 | H | 10.102010 | -1.693066 | -6.350706 |
| C | 13.160643 | -2.669566 | -1.869872 | H | 11.977076 | -7.121147 | -0.801501 |
| C | 14.103594 | -2.111043 | -2.838218 | H | 4.213654 | -3.573766 | 2.200483 |
| C | 12.646659 | -0.126071 | -3.071828 | H | 5.315299 | 0.859855 | 0.972599 |
| C | 12.990166 | 1.294706 | -3.029978 | H | 3.549914 | -4.996379 | -0.989718 |
| C | 14.409394 | 1.423147 | -3.352668 | H | 13.555719 | 5.284608 | -4.145423 |
| C | 14.942126 | 0.082142 | -3.597275 | H | 7.376178 | -2.379595 | 4.856982 |
| C | 13.853939 | -0.875802 | -3.425667 | H | -3.035333 | -3.091832 | 7.205724 |
| C | 16.228177 | -0.244492 | -3.180603 | H | 9.339418 | 1.067524 | 2.370618 |
| C | 17.047704 | 0.751465 | -2.494937 | H | 11.072479 | -3.897469 | -5.946037 |
| C | 16.541550 | 2.024939 | -2.260247 | H | 12.086416 | 3.632008 | -5.217418 |
| C | 16.779664 | 2.678104 | -0.975887 | H | 13.052160 | -4.297246 | -4.715720 |
| C | 17.514758 | 2.028797 | 0.010729 | H | -2.285324 | -6.767344 | 2.332808 |
| C | 17.081933 | 2.092509 | 1.404640 | H | 8.612659 | -1.446546 | 2.948857 |
| C | 15.936845 | 2.805723 | 1.740966 | H | 18.910351 | -4.899901 | -0.354495 |
| C | 14.994735 | 2.252122 | 2.711761 | H | 14.378501 | 7.373971 | -3.448577 |
| C | 13.641755 | 2.592009 | 2.272200 | H | 8.585270 | 2.245211 | 4.399812 |
| C | 13.748733 | 3.355477 | 1.031431 | H | -2.447413 | 1.384753 | 6.592993 |
| C | 15.166233 | 3.488297 | 0.704069 | H | 5.656033 | -7.483714 | 1.800926 |
| C | 12.603883 | 1.680887 | 2.440301 | H | -0.267267 | -7.508994 | 1.116324 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 11.626480 | 1.487594 | 1.373695 | H | 11.987878 | 6.054019 | -0.140031 |
| C | 11.284325 | 0.066780 | 1.328029 | H | 0.203319 | -4.826018 | 5.244464 |
| C | 11.058466 | -0.554398 | 0.107992 | H | 2.160128 | 4.992355 | 4.260540 |
| C | 11.167569 | 0.211034 | -1.130351 | H | 10.302430 | 6.571910 | -1.658415 |
| C | 11.759332 | -0.653611 | -2.145465 | H | 3.540747 | -7.889245 | 3.004737 |
| C | 15.190925 | 2.372183 | -2.701241 | H | 13.901004 | 6.337623 | 1.364022 |
| C | 14.594753 | 3.240964 | -1.687152 | H | 20.240035 | -3.283121 | 0.923768 |
| C | 15.576971 | 3.429322 | -0.621527 | H | 18.127095 | -2.525460 | 4.629528 |
| C | 12.812279 | 3.176411 | 0.017888 | H | 19.112600 | 4.593999 | 0.223282 |
| C | 11.722562 | 2.218361 | 0.193754 | H | 17.323425 | -6.491087 | 3.301388 |
| C | 11.485514 | 1.563467 | -1.092883 | H | 16.306079 | 7.658834 | -1.934324 |
| C | 12.424760 | 2.119569 | -2.062255 | H | 2.204674 | -5.649001 | 4.080686 |
| C | 13.244434 | 3.117236 | -1.377510 | H | 17.480743 | 5.850215 | -1.072759 |
| C | 7.525352 | 2.195937 | -0.859187 | H | 17.362974 | 6.061729 | 3.862216 |
| C | 8.064976 | 0.799557 | -0.863420 | H | 18.651794 | -4.855392 | 4.585178 |
| C | 8.149320 | -2.022159 | -0.800054 | H | 18.300533 | -0.136293 | 5.037174 |
| C | 8.915928 | 0.779667 | -3.235356 | H | 17.684114 | 3.995046 | 4.498646 |
| C | 7.815632 | 0.114813 | 0.328158 | H | 20.684193 | 3.946933 | 1.427013 |
| C | -3.885996 | -2.729895 | 5.256101 | H | 18.504317 | 1.863431 | 5.336561 |
| C | 8.046716 | 3.219531 | -0.056540 | H | 15.701928 | 7.309028 | 2.546654 |
| C | 2.625624 | 6.174404 | 1.918222 | H | 21.391181 | 1.738610 | 2.154350 |
| C | 7.781058 | -1.295577 | 0.343818 | H | 21.849357 | -2.455625 | 2.502207 |
| C | 9.220370 | 0.050989 | -4.415455 | H | 22.047158 | -0.050088 | 2.931248 |

REFERENCES

- (S1) S. Wang, X. Li, G. Zhuang, M. Chen, P. Huang, S. Yang, P. Du, *Chem. Commun.* **2021**, 57, 9104-9107.
- (S2) K. A. Connors, *Binding Constants*, Wiley, New York, **1987**.

- (S3) T. Iwamoto, Y. Watanabe, T. Sadahiro, T. Haino, S. Yamago, *Angew. Chem. Int. Ed.* **2011**, *50*, 8342-8344.
- (S4) Gaussian 09, Revision A.1, M. J. Frisch, et.al Gaussian, Inc., Wallingford CT, **2009**.
- (S5) Grimme S, Ehrlich S, Goerigk L. *J. Comp. Chem.* **2011**, *32*, 1456-1465.
- (S6) S. Miertuš, E. Scrocco, and J. Tomasi, *Chem. Phys.* **1981**, *55*, 117-129.
- (S7) Y. Segawa, H. Omachi, K. Itami, *Org. Lett.* **2010**, *12*, 2262-2265.
- (S8) H. Takaba, H. Omachi, Y. Yamamoto, J. Bouffard, K. Itami, *Angew. Chem. Int. Ed.* **2009**, *48*, 6112-6116.