Supplementary information

Cation recognition and pseudorotaxane formation of tris-dipyrrin BF₂ macrocycles

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Contents

- 1. General
- 2. Synthesis of 1 and 2
- 3. Absorption spectral changes of 1 upon addition of K^+ and Rb^+
- 4. Absorption spectral changes of **2** upon addition of K^+ , Rb^+ , and Cs^+
- 5. Absorption spectral changes of **2** upon addition of **3**
- 6. ¹H NMR spectral changes of **2** upon addition of Cs^+
- 7. ¹⁹F NMR spectral change of 1 upon addition of Cs^+
- 8. ¹¹B NMR spectral change of **1** upon addition of Cs^+
- 9. ¹H NMR spectral change of **2** upon addition of **3**
- 10. ¹H NMR spectra of **2+3** at low temperature
- 11. Fluorescence spectral changes of 2 upon addition of 3
- 12. Geometry optimized structures of 1 and 2
- 13. Electrostatic potential surface of 1, 2, and tetramethyl-BODIPY
- 14. NMR spectra of 1 and 2

1. General

All chemicals were reagent grade, and used without further purification. All reactions were performed under nitrogen atmosphere. Tris-dipyrrin macrocycles were prepared as previously described. Column chromatography was performed with Kanto Chemical silica gel 60 N (spherical, neutral) or Wako Chemical alumina (activated, about 200 mesh). ¹H NMR spectra were recorded on a Bruker ARX400 spectrometer at 400 MHz, or a Bruker AC300 spectrometer at 300 MHz. ¹³C NMR spectra were recorded on a Bruker ARX400 spectrometer at 100 MHz. In both NMR measurements, tetramethylsilane was used as an internal standard (0 ppm). ¹¹B NMR spectra were recorded on a Bruker ARX400 spectrometer at 128 MHz, boron trifluoride-diethyl etherate was used as an internal standard (0 ppm). ¹⁹F NMR spectra were recorded on a Bruker AVANCE500 spectrometer at 470 MHz, hexafluorobenzene was used as an internal standard (-162 ppm). UV-Vis spectra were recorded on JASCO V-660 spectrophotometer. Fluorescence spectra and absolute quantum yields were measured on a Hitachi F-4500 spectrometer and a Hamamatsu Photonics absolute PL quantum yield measurement system C9920-02, respectively. Mass spectra (ESI-TOF, positive mode) were recorded on an Applied Biosystems OStar Pulsar *i* spectrometer. Elemental analyses were performed at Chemical Analysis Center, University of Tsukuba. Geometry optimizations and surface potential calculations were performed with Spartan08 programs.¹ X-ray crystallographic analysis: Intensities of reflections were collected on a Rigaku Mercury CCD diffractometer with a graphite monochromated Mo-K α radiation ($\lambda = 0.71070$) using CrystalClear (Rigaku Corp.). The structure was solved by direct methods. The structure refinement was performed with SHELXL-97.

2. Synthesis of 1 and 2



1: To a stirred solution containing **5** (14.94 mg, 0.015 mmol) and trietylamine (0.5 mL, 3.6 mmol) in toluene (30 mL) was added boron trifluoride-diethyl etherate (0.5 mL, 4.0 mmol). After stirred for 48 h at 80 °C, the reaction mixture was washed with water (2 × 30 mL). The organic phase was dried over Na₂SO₄, filtered, evaporated to dryness. The obtained residue was purified by column chromatography on silica gel using chloroform as the eluent, and recrystallized from CH_2Cl_2 /hexane to give **1** (5.0 mg, >29%).

green powder, ¹H NMR (400 MHz, CDCl₃) δ 2.22 (s, 18H), 2.36 (s, 9H), 6.44 (d, J = 4.4 Hz, 6H), 6.47 (d, J = 4.4 Hz, 6H), 6.95 (s, 6H), 8.38 (s, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 20.1, 21.1, 121.7, 128.1, 129.0, 130.1, 130.3, 133.7, 136.8, 137.8, 138.5, 143.5, 158.1. MS(MALDI-TOF) observed m/z 1153.08 ([M+H]⁺), calcd for C₇₂H₅₈B₃F₆N₆ m/z 1153.49. Anal. Calcd for C₇₂H₅₇B₃F₆N₆•2H₂O: C, 72.75; H, 5.17; N, 7.07. Found: C, 72.54; H, 5.18; N, 6.82.

2: To a stirred solution containing **6** (40.3 mg, 0.038 mmol) and trietylamine (0.5 mL, 3.6 mmol) in toluene (40 mL) was added boron trifluoride-diethyl etherate (0.5 mL, 4.0 mmol). After stirred for 10h at 80 °C, the reaction mixture was added water (80 mL) and the organic layer separated. The aqueous phase was extracted with dichloromethane (3×80 mL). The combined organic phase was dried over Na₂SO₄, filtered, evaporated to dryness. The obtained residue was purified by column chromatography on silica gel using dichloromethane as the eluent, and recrystallized from CH₂Cl₂/hexane to give **2** (45.3 mg, >99%).

Green powder, mp > 300 °C. ¹H NMR (400 MHz, CDCl₃) δ 3.80 (s, 18H), 6.67 (d, *J* = 4.0 Hz, 6H), 6.88 (d, *J* = 4.0 Hz, 6H), 7.50-7.65 (m, 15H), 7.84 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 62.3, 123.2, 126.3, 128.3, 128.5, 130.0, 130.1, 130.6, 134.4, 136.1, 143.6, 152.0, 154.6. MS(ESI) observed *m/z* 1229.42 ([M+Na]⁺), calcd for C₆₉H₅₁B₃F₆N₆NaO₆ *m/z* 1229.40. Anal. Calcd for C₆₉H₅₁B₃F₆N₆O₆•1.5H₂O•1/4C₆H₁₄: C, 67.46; H, 4.62; N, 6.70. Found: C, 67.58; H, 4.70; N, 6.32.

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Figure S1. Absorption spectral changes of **1** (4.0 μ M) upon addition of (a) KTFPB (0–0.8 mM) and (b) RbTFPB (0–0.4 mM) in CHCl₃-CH₃OH (10:1). Inset shows the binding isotherm at 552 nm analyzed by a nonlinear least-square regression (calculated lines are shown in solid lines).

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Figure S2. Absorption spectral changes of **2** upon (a) K^+ , (b) Rb^+ , and (c) Cs^+ in CHCl₃-CH₃OH (10:1). Inset shows the binding isotherm at 364 nm analyzed by a nonlinear least-square regression (calculated lines are shown in solid lines).





Figure S3. Absorption spectral changes of **2** upon **3** in CHCl₃-CH₃OH (10:1). Inset shows the binding isotherm at 531 nm analyzed by a nonlinear least-square regression (calculated lines are shown in solid lines).

6. ¹H NMR spectral changes of 2 upon addition of Cs⁺.



Figure S4. ¹H NMR spectral changes of **2** (1 mM) upon addition of CsTFPB in CDCl₃-CD₃OD (10:1).

7. ¹⁹F NMR spectral change of 1 upon addition of Cs⁺.



Figure S5. ¹⁹F NMR spectra of **1** (0.5 mM) in the (a) absence and (b) presence of CsTFPB (2.5 mM) in CDCl₃-CD₃OD (10:1).

8. ¹¹B NMR spectral change of 1 upon addition of Cs⁺.



Figure S6. ¹¹B NMR spectra of **1** (0.5 mM) in the (a) absence and (b) presence of CsTFPB (2.5 mM) in CDCl₃-CD₃OD (10:1).





Figure S7. ¹H NMR spectral changes of **2** (1.0 mM) upon addition of **3** in CDCl₃-CD₃OD (10:1). Asterisk denotes the residual solvent peaks. Phenylene protons are indicated with filled circles.

10. ¹H NMR spectra of 2+3 at low temperature



Figure S8. ¹H NMR spectra of **2** in the presence of (a), (b) 1 equiv or (c), (d) 2 equiv of **3** in CDCl₃ recorded at (a), (c) 298 K and (b), (d) 218 K. Filled circles in (d) denotes the free **3**. Asterisks denotes the solvent peaks and residual H_2O .

11. Fluorescence spectral changes of 2 upon addition of 3



Figure S9. Fluorescence spectra of 2 in CHCl₃-CH₃OH (10:1).

12. Geometry optimized structures of 1 and 2



Figure S10. Geometry optimized structure of (a) **1** and (b) **2** by DFT calculation at the B3LYP/6-31G* level. Hydrogen atoms were omitted for clarity.

1 C1 1.41714661 -5.208704801 -0.135657823 2 C2 1.632210412 -6.616194667 -0.174692851 3 H3 0.963939507 -7.274868222 -0.2409068 4 C4 2.979109892 -6.79809148 -0.100374277 5 H5 3.199187095 -5.54800465 -0.05082301 7 C7 4.939726378 -5.24800413 0.002713716 8 C8 5.381604093 -3.33297732 0.065631904 9 C9 6.693593418 -3.39068831 0.228161821 10 H10 7.505410245 -3.889543029 0.22997455 12 H12 7.22531537 -1.451958163 0.50667755 13 C13 5.20866374 -1.699313222 0.25507969 14 N14 2.61137251 -4.55491544 -0.0732752 15 N15 4.4780473 -2.84234863 0.995811549 16 2.947755462 -3.05755127 -0.12887905 17 </th <th></th> <th></th> <th></th> <th></th> <th></th>					
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16 B16 2.947559462 -3.05755127 -0.12887905 17 F17 2.32288432 -2.342348463 0.905821549 18 F18 2.510961221 -2.57358284 -1.352938138 19 C19 5.967996547 -6.33324955 -0.03330363 20 C20 6.256452082 -7.056301603 1.119549529 21 C21 7.164239746 -8.105645933 1.034103849 22 H22 7.36981024 -8.607834543 1.813611861 23 C23 7.78072978 -8.430792194 -0.180214295 24 C24 7.477866339 -7.704338797 -1.29121217 25 H25 7.89519152 -7.93085761 -2.114397169 26 C26 6.579246835 -6.644373788 -1.261816129 27 C27 5.632667262 -6.738642442 2.427019079 28 H28 4.67386304 -6.93781607 2.38889639 29 H29 5.760473143 -5.789042305 2.6627108821 30 H30 6.051440694 -7.281774771 <	15	N15	4.4780473	-2.842301507	0.042935113
17 F17 2.32288432 -2.342348463 0.905821549 18 F18 2.510961221 -2.573588284 -1.352938138 19 C19 5.967996547 -6.333234955 -0.03330363 20 C20 6.256452082 -7.056301603 1.119549529 21 C21 7.164239746 -8.607834543 1.813611861 22 H22 7.36981024 -8.607834543 1.813611861 23 C23 7.780725978 -8.40792194 -0.180214295 24 C24 7.477866339 -7.704338797 -1.29121217 25 H25 7.89519152 -7.930385761 -2.114397169 26 C26 6.579246835 -6.644373788 -1.261816129 27 C27 5.632667262 -6.738462442 2.427019079 28 H28 4.67386304 -6.939781607 2.3889639 29 H29 5.760473143 -5.789042305 2.627108821 30 H30 6.051440694 -7.281774771 3.128374574 31 C31 8.764691315 -9.9506089316	16	B16	2.947559462	-3.057555127	-0.12887905
18 F18 2.510961221 -2.573588284 -1.352938138 19 C19 5.967996547 -6.33234955 -0.03330363 20 C20 6.256452082 -7.056301603 1.119549529 21 C21 7.164239746 -8.105645933 1.034103849 22 H22 7.369981024 -8.607834543 1.813611861 23 C23 7.780725978 -8.430792194 -0.180214295 24 C24 7.477866339 -7.704338797 -1.29121217 25 H25 7.89519152 -7.393085761 -2.114397169 26 C26 6.579246835 -6.644373788 -1.261816129 27 C27 5.632667262 -6.738642442 2.427019079 28 H28 4.67386304 -6.939781607 2.38889639 29 H29 5.760473143 -5.789042305 2.67108821 31 C31 8.764691315 -9.5900194504 -2.503934468 32 H32 8.462926249 -10.21549133 <t< td=""><td>17</td><td>F17</td><td>2.322888432</td><td>-2.342348463</td><td>0.905821549</td></t<>	17	F17	2.322888432	-2.342348463	0.905821549
19 C19 5.967996547 -6.33234955 -0.0330363 20 C20 6.256452082 -7.056301603 1.119549529 21 C21 7.164239746 -8.105645933 1.034103849 22 H22 7.369981024 -8.607834543 1.813611861 23 C23 7.780725978 -8.40792194 -0.180214295 24 C24 7.477866339 -7.704338797 -1.291212217 25 H25 7.89519152 -7.930385761 -2.114397169 26 C26 6.579246835 -6.644373788 -1.261816129 27 C27 5.632667262 -6.738642442 2.427019079 28 H28 4.67386304 -6.939781607 2.38889639 29 H29 5.760473143 -5.789042305 2.627108821 30 H30 6.051440694 -7.28174771 3.128374574 31 C31 8.764691315 -9.956089316 -0.28162939 31 H33 8.03401955 -10.06405702 0.5	18	F18	2.510961221	-2.573588284	-1.352938138
20 C20 6.256452082 -7.056301603 1.119549529 21 C21 7.164239746 -8.105645933 1.034103849 21 L22 7.369981024 -8.607834543 1.813611861 23 C23 7.780725978 -8.430792194 -0.180214295 24 C24 7.477866339 -7.704338797 -1.29121217 25 H25 7.89519152 -7.930385761 -2.114397169 26 C26 6.579246835 -6.644373788 -1.261816129 27 C27 5.632667262 -6.738642442 2.427019079 28 4.67386304 -6.939781607 2.3889639 29 H29 5.760473143 -5.789042305 2.627108821 30 H30 6.051440694 -7.281774771 3.128374574 31 C31 8.764691315 -9.596089316 -0.28162393 32 H32 8.462926249 -10.21549133 -0.51702523 34 H34 9.65348624 -9.252797103 -0.5102924 </td <td>19</td> <td>C19</td> <td>5.967996547</td> <td>-6.333234955</td> <td>-0.03330363</td>	19	C19	5.967996547	-6.333234955	-0.03330363
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	C20	6.256452082	-7.056301603	1.119549529
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	21	C21	7.164239746	-8.105645933	1.034103849
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22	H22	7.369981024	-8.607834543	1.813611861
24C247.477866339-7.704338797-1.2912121725H257.89519152-7.930385761-2.11439716926C266.579246835-6.644373788-1.26181612927C275.632667262-6.7386424422.42701907928H284.67386304-6.9397816072.3888963929H295.760473143-5.7890423052.62710882130H306.05140694-7.2817747713.12837457431C318.764691315-9.596089316-0.2816293932H328.462926249-10.21549133-0.97880402733H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.510292435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.4245235338H385.258998916-5.914252649-0.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.99077187941H413.0653744-0.438551174-0.910705522423.2816114021.490136366-0.3384027743H432.5247202551.80302543-0.82071756144C4243.29466662.3996684090.39070996245C455.1054643341.919322821.1289152246<	23	C23	7.780725978	-8.430792194	-0.180214295
25H257.89519152-7.930385761-2.11439716926C266.579246835-6.644373788-1.26181612927C275.632667262-6.7386424422.42701907928H284.67386304-6.9397816072.3888963929H295.760473143-5.7890423052.62710882130H306.051440694-7.2817747713.12837457431C318.764691315-9.590689316-0.2816293932H328.462926249-10.21549133-0.97880402733H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.5102929435C356.23051539-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.4245235338H385.258989816-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.9077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.1289152246H465.6192432442.5204145641.657623988 </td <td>24</td> <td>C24</td> <td>7.477866339</td> <td>-7.704338797</td> <td>-1.291212217</td>	24	C24	7.477866339	-7.704338797	-1.291212217
26C266.579246835-6.644373788-1.26181612927C275.632667262-6.7386424422.42701907928H284.67386304-6.9397816072.3888963929H295.760473143-5.7890423052.62710882130H306.051440694-7.2817747713.12837457431C318.764691315-9.596089316-0.2816293932H328.462926249-10.21549133-0.97880402733H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.5102929435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.42452353338H385.258998916-5.914252649-0.33189539990C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10421976	25	H25	7.89519152	-7.930385761	-2.114397169
27 $C27$ 5.632667262 -6.738642442 2.427019079 28H28 4.67386304 -6.939781607 2.38889639 29H29 5.760473143 -5.789042305 2.627108821 30H30 6.051440694 -7.281774771 3.128374574 31C31 8.764691315 -9.596089316 -0.28162939 32H32 8.462926249 -10.21549133 -0.978804027 33H33 8.803401955 -10.06405702 0.576700523 34H34 9.654348624 -9.252797103 -0.51029294 35C35 6.230515599 -5.900194504 -2.503934468 36H36 6.668205133 -6.324402687 -3.27195768 37H37 6.536473299 -4.972223438 -2.424523533 38H38 5.258998916 -5.914252649 -2.630731619 39C39 4.699862241 -0.331895399 0.33200569 40C40 3.592892518 0.156085571 -0.390771879 41H41 3.06553744 -0.438551174 -0.910705522 42C42 3.281611402 1.490133666 -0.338460277 43H43 2.524720255 1.80302543 -0.820717561 44 4.029546066 2.399668409 0.390709962 45C45 5.105463343 1.919322982 1.128991522 46H46 5.619243244 2.520414564 1.657623998 47C47 5.434608154 0.581844535 <td>26</td> <td>C26</td> <td>6.579246835</td> <td>-6.644373788</td> <td>-1.261816129</td>	26	C26	6.579246835	-6.644373788	-1.261816129
28H284.67386304-6.9397816072.3888963929H295.760473143-5.7890423052.62710882130H306.051440694-7.2817747713.12837457431C318.766691315-9.596089316-0.2816293932H328.462926249-10.21549133-0.97880402733H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.5102929435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.97223438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33763985 <td>27</td> <td>C27</td> <td>5.632667262</td> <td>-6.738642442</td> <td>2.427019079</td>	27	C27	5.632667262	-6.738642442	2.427019079
29H295.760473143-5.7890423052.62710882130H306.051440694-7.2817747713.12837457431C318.764691315-9.596089316-0.2816293932H328.462926249-10.21549133-0.97880402733H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.5102929435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.9077187941H413.06553744-0.438551174-0.9107052242C423.2816114021.490136366-0.33846027744C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33366343550C504.9307022264.757963120.336634345	28	H28	4.67386304	-6.939781607	2.38889639
30H306.051440694-7.2817747713.12837457431C318.764691315-9.596089316-0.2816293932H328.462926249-10.21549133-0.97880402733H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.5102929435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.318953990.33200056940C403.5928925180.156085571-0.9007187941H413.06553744-0.438551174-0.91070522242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.913229821.12899152246H465.6192432442.5204145641.6576239847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	29	H29	5.760473143	-5.789042305	2.627108821
31C318.764691315-9.596089316-0.2816293932H328.462926249-10.21549133-0.97880402733H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.5102929435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.97222438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.99077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	30	H30	6.051440694	-7.281774771	3.128374574
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	31	C31	8.764691315	-9.596089316	-0.28162939
33H338.803401955-10.064057020.57670052334H349.654348624-9.252797103-0.5102929435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.4245253338H385.258998916-5.914252649-2.63073161939C394.699862241-0.318953990.3200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	32	H32	8.462926249	-10.21549133	-0.978804027
34H349.654348624-9.252797103-0.5102929435C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	33	H33	8.803401955	-10.06405702	0.576700523
35C356.230515599-5.900194504-2.50393446836H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	34	H34	9.654348624	-9.252797103	-0.51029294
36H366.668205133-6.324402687-3.2719576837H376.536473299-4.972223438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.8207156144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	35	C35	6.230515599	-5.900194504	-2.503934468
37H376.536473299-4.972223438-2.42452353338H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.8207156144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	36	H36	6.668205133	-6.324402687	-3.27195768
38H385.258998916-5.914252649-2.63073161939C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	37	H37	6.536473299	-4.972223438	-2.424523533
39C394.699862241-0.3318953990.33200056940C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.1289152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	38	H38	5.258998916	-5.914252649	-2.630731619
40C403.5928925180.156085571-0.39077187941H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	39	C39	4.699862241	-0.331895399	0.332000569
41H413.06553744-0.438551174-0.91070552242C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	40	C40	3.592892518	0.156085571	-0.390771879
42C423.2816114021.490136366-0.33846027743H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	41	H41	3.06553744	-0.438551174	-0.910705522
43H432.5247202551.80302543-0.82071756144C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	42	C42	3.281611402	1.490136366	-0.338460277
44C444.0295460662.3996684090.39070996245C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	43	H43	2.524720255	1.80302543	-0.820717561
45C455.1054633431.9193229821.12899152246H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	44	C44	4.029546066	2.399668409	0.390709962
46H465.6192432442.5204145641.65762399847C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	45	C45	5.105463343	1.919322982	1.128991522
47C475.4346081540.5818445351.10424197648H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	46	H46	5.619243244	2.520414564	1.657623998
48H486.1711558660.2713553681.61739918149C493.8450862723.8636641520.33376398550C504.9307022264.757963120.336634345	47	C47	5.434608154	0.581844535	1.104241976
49 C49 3.845086272 3.863664152 0.333763985 50 C50 4.930702226 4.75796312 0.336634345	48	H48	6.171155866	0.271355368	1.617399181
50 C50 4.930702226 4.75796312 0.336634345	49	C49	3.845086272	3.863664152	0.333763985
	50	C50	4.930702226	4.75796312	0.336634345

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51	1151		5 040700076	4 500750079	0 200697060
51	HOI		5.848/898/0	4.522/520/8	0.39908/009
52	C52		4 426099824	6 032553/3	0 227098722
52	052		4.420077024	0.05255545	0.227090722
53	H53		4.929132227	6.83856773	0.210398706
C 4	054		2.022022(0/	6 012112721	0 1 40 2 1 40 5 2
54	C54		3.023023686	5.913112/31	0.148214052
55	C55		2 079397415	6 926644888	0.09231966
	000		2.077577115	0.920011000	0.07251700
56	C56		0.711624052	6.58237056	0.129773528
57	C57		0.404002461	7 11696271	0.024291521
57	C3/	-	0.404003461	/.440803/4	0.034381531
58	H58		0.384080071	8 305787757	0.018878103
50	1150	-	0.504700071	0.575702752	-0.010070175
59	C59	-	1.520392068	6.651164832	0.034674478
(0	11(0		2 424245241	(044021951	0.025142529
60	H00	-	2.424545241	0.944931851	-0.025142538
61	C61	_	1.077532145	5 311639063	0 14029041
01	001		1.077552145	5.511057005	0.14027041
62	N62		2.698817563	4.546485758	0.203479235
62	NI62		0.270025007	5 205102605	0 222007722
05	1005		0.2/095599/	5.295102095	0.232007722
64	B64		1 224751309	4 058752222	0 220540042
	501		1.221731309	1.030732222	0.220310012
65	F65		0.940375811	3.331988793	-0.937319634
66	E66		1.042450064	2 270705574	1 227750594
00	F00		1.045459904	5.270705574	1.557759584
67	C67		2.522895415	8.321641355	-0.110562275
60	0(0		2 5220 52024	0.040400101	0.000000000
68	C68		2.533853924	9.243429131	0.929238082
60	C60		2 082462711	10 52925129	0.678025685
09	009		2.902402/11	10.52625126	0.078925085
70	H70		3.006825588	11.14993444	1.395806581
71	071		2 401022250	10.04025	0.579(214(2
/1	C/I		5.401022258	10.94235	-0.5/8031402
72	C72		3 344893911	10 01579804	-1 616385135
72	072		5.511095911	10.01579001	1.010505155
73	H73		3.610132708	10.28359319	-2.489446664
74	C74		2 007022254	0 716020272	1 412546054
/4	U/4		2.90/853354	0./109383/2	-1.413340934
75	C75		2.098636548	8.88000842	2.348327051
76	1176		2.1201(0201	0.6700026002	2.01/102/22
/6	п/б		2.132168381	9.6/8036893	2.915103473
77	H77		2 702366612	8 1965/1092	2 700526645
//	11//		2.702500012	0.170541072	2.707520045
78	H78		1.182955038	8.529344666	2.329377908
70	C70		2 0020//07/	10.24/20/14	0.7750001(0
/9	C/9		5.895000070	12.34030014	-0.//3992102
80	H80		3 943695073	12 54395451	-1 735070078
00	1100		5.5 15055075	12.0 1000 101	1.755070070
81	H81		4.78220733	12.44100292	-0.3/5132233
82	H82		3 273820064	12 97311603	-0 346368893
02	1102		5.275627704	12.97511005	-0.5+0508075
83	C83		2.907634776	7.766186132	-2.596312534
0.4	1104		2 521200(05	7.00245406	2 419 49 70 52
64	п 84		5.521599095	1.02545420	-2.41848/032
85	H85		3 197599589	8 245546746	-3 400303215
00	1100		2 00172762	5.212210070	2 72 410 5022
86	H86		2.001/2/63	/.41/3138/8	-2./34105833
87	C87	-	2 005073601	4 152736919	0.080226625
07	207		2.005075001	4.152750515	0.000220023
88	C88	-	1.91/580/16	3.009619889	0.869/964/6
80	1100		1 1720/002	2 800222581	1 449652705
0)	1107	-	1.17504005	2.077552501	1.440033703
90	C90	-	2.894612286	2.030822284	0.829331257
01	1101		2 201171112	1 248420702	1 259642002
91	П91	-	2.8011/1115	1.246450/02	1.558045095
92	C92	-	4 011059153	2 186400911	0 023483779
~~	<i>C</i> /2		1.001000100	2.100 1009 11	0.020100779
93	C93	-	4.091303156	3.3104/246/	-0.822345295
04	H04		4 821870072	3 /11/08/308	1 /1032360/
24	1194	-	4.0210/09/2	5.411098598	-1.419525004
95	C95	-	3.095692983	4.252162888	-0.769524478
06	1106		2 157722015	5 009604071	1 242264122
90	1190	-	5.157752615	5.0080949/1	-1.342204123
97	C97	-	5 187458469	1 337891612	0.04619664
20	600		6.50.500.50	1.00000012	0.01019001
98	C98	-	6.505332729	1.842936312	-0.0522518/2
00	100		6 740300042	2 760678745	0 1/18830283
33	1199	-	0.740390042	2.700078745	-0.148839283
100	C100	-	7.390045813	0.803070721	0.014163368
101	11101		9 227600795	0.962992074	0.009409249
101	птот	-	8.55/000/85	0.802883074	-0.008408248
102	C102	-	6 628173883	-0 372917592	0 119684316
102	0102		= 022002 102	1.0000001.00	0.1002/1721
103	C103	-	7.033983409	-1.68/82/168	0.100361524
104	C104	-	6 109912204	-2 723867/00	0.050537516
107	C107	_	6.107712204	4.1005000	0.0000007010
105	C105	-	6.307233105	-4.109799958	-0.114116127
106	H106		7 1/2525522	_1 557202002	_0 158807276
100	11100	-	/.143333333	-4.33/303803	-0.1300923/0
107	C107	-	5.081467363	-4.681808953	-0.195956758
100	11100		4.010050205	C (00505000	0.0074(0770
108	H108	-	4.910059305	-5.609525283	-0.30/4627/8
100	C109	_	1 006500645	-3 6628/7605	-0.087270101
107	2107	-		-5.002077005	0.00/2/9191
110	N110	-	5.27049935	-0.013791942	0.137945262
111	N111		4 720402224	1 1702777	0.052791720
111	11111	-	4./39402324	-2.4//833//3	0.052/81/39
112	B112	-	4 123418658	-1.065928503	0.316498128
112	E112		1.125 113050	0.502526505	0.501/01/20
113	F113	-	3.113534803	-0.792724113	-0.59467507
114	F114	-	3 670110001	-0 003080361	1 625677471
114	-	-	5.070110091	-0.222000301	1.023077471
115	C115	-	8.510535933	-1.974847913	-0.004018633
114	C114		0.0552005((2.07950(10	1 20046214
110	C110	-	9.20002900	-2.07850619	1.20040314
117	C117	-1	0 635316073	-2 298704006	1.080913025
110	U1110	1	1 1 50 1 50 1 0 1	2.290701000	1.070/05/20
118	H118	-1	1.150173194	-2.383363737	1.8/3605662
110	C119	_1	1 27022222	-7 307/35781	-0 120767070
119	0119	-1	1.2/022/833	-2.37/433/81	-0.120/0/9/9
120	C120	-1	0.503684885	-2.2804714	-1.266127811
101	LIIOI	1	0.020440564	1 222020705	0 110514(00
121	п121	- 1	0.930448564	-2.333032/95	-2.112514629
122	C122	-	9 12003479	-2 086910459	-1.219776993
122	C122		0.50101777	1.005050555	1.217770775
123	C123	-	8.594346623	-1.925053311	2.53266339
124	H124		7 0020170	2 602172571	2 627607506
124	11124	-	1.07571/9	-2.0024/23/1	2.02/09/390
125	H125	-	9.260102049	-2.042849176	3.242412382
120	L1120		9 100225205	1.021700572	2 (01102(1
126	H126	-	8.199335205	-1.031/985/2	2.60110361
127	C127	-1	2 75122523	-2.620427651	-0 203165443
100	11100	:	2.75122525	2.02012/001	0.200100 (45
128	H128	-1	2.937025557	-3.58208804	-0.183046026

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129	H129	-1	3.095024479	-2.238040265	-1.038144297
130	H130	-1	3.189579346	-2.186661727	0.558680512
131	C131	-	8.367182318	-1.966360077	-2.545501026
132	H132	-	7.850465172	-1.133819488	-2.553233265
133	H133	-	9.007401609	-1.959873647	-3.285825663
134	H134	-	7.757685357	-2.727619613	-2.645749179
135	C135	-	2.638831049	-3.878490224	-0.165218741
136	C136	-	1.690387722	-3.167537389	0.570360434
137	H137	-	1.963769627	-2.427807187	1.100340971
138	C138	-	0.372216896	-3.523530503	0.538875263
139	H139		0.257277342	-3.023879472	1.045265256
140	C140		0.070473304	-4.609222871	-0.221896652
141	C141	-	0.874573481	-5.280459663	-0.990974804
142	H142	-	0.591442875	-5.999571835	-1.543932805
143	C143	-	2.216041613	-4.932045131	-0.972214021
144	H144	-	2.84203234	-5.407174181	-1.506257686

Geometries (Z matrices) of **2**

UU				
1	B1	2.611648729	3.304987706	0.053345381
2	F2	2.203923037	2.867334673	1.314176154
3	F3	2.085270388	2.527098257	-0.965329287
4	B4	-4.125596609	0.556383895	0.385864703
5	F5	-3.599283938	0.482025742	-0.902663194
6	F6	-3.144042914	0.420879974	1.356812897
7	B7	1.666694344	-3.867393212	-0.00780843
8	F8	1 364507924	-3 231320394	1 193888295
9	F9	1 402729797	-3.065483731	-1 109308083
10	N10	4 183773693	3 285756197	0.038934251
11	N11	2 170124819	4 793604095	-0.191513866
12	N12	4 866260886	1 028222206	0.55780/166
12	N12	5 211052727	0.56068521	0.557894100
13	N13	-3.211032/2/	-0.30008331	0.303/1042/
14	N14 N15	0.641320699	-3.194302777	-0.10412/4/3
15	N15	3.181009201	-4.270394391	0.041040103
16	C16	4.9/6355/42	2.227820035	0.351/54906
17		6.304/11352	2.683012693	0.555644264
18	HI8	7.136657343	2.04538764	0.816041153
19	C19	6.31207575	4.048813132	0.352476862
20	H20	7.153287947	4.722335118	0.430675305
21	C21	4.982323641	4.429643562	0.03467046
22	C22	4.439015922	5.704012165	-0.186175952
23	C23	3.053276517	5.86342192	-0.338087957
24	C24	2.310916012	7.006087787	-0.734678178
25	H25	2.72678251	7.982933394	-0.935359612
26	C26	0.990635801	6.617185555	-0.833461765
27	H27	0.140788282	7.219371889	-1.11772676
28	C28	0.920651508	5.241532158	-0.485977741
29	C29	-0.333419822	4.47749307	-0.380892132
30	C30	-1.324059169	4.650549083	-1.373720367
31	031	-1.05343276	5.335168546	-2.534234579
32	C32	-0 207079184	4 63802177	-3 456314918
33	H33	0.686647957	4 237533632	-2 96505525
3/	H3/	0.08/259319	5 366507625	-4 216355703
35	H35	-0.751/3298	3 811517783	-3 93156857
36	C36	2 623245855	4 167414081	1 171064227
27	027	2 501222418	4.107414081	2 112020017
20	C28	-5.391522418	4.425141555	-2.112029017
20		-3.644932679	5.542154241	-5.01//14555
39	П39 Ц40	-3.938/84//8	2.391910703	-2.483004873
40	H40	-3.03056/098	3.249334902	-3.748262928
41	H41	-4.//1021202	3.592052893	-3.540/20661
42	C42	-2.944916519	3.462018864	0.004402223
43	C43	-1.926693081	3.190925879	0.930591728
44	H44	-2.156623609	2.609206578	1.814998845
45	C45	-0.645518574	3.69893654	0.746489409
46	H46	0.118091298	3.520689724	1.492338831
47	C47	-4.360120659	3.156609016	0.291677335
48	C48	-5.394943322	4.120964934	0.388224885
49	H49	-5.263467973	5.17914891	0.213922342
50	C50	-6.552963206	3.452325612	0.736516222
51	H51	-7.537276823	3.87231768	0.886420583
52	C52	-6.225356181	2.074101419	0.835028976
53	C53	-7.061552257	0.962554283	1.023554103
54	C54	-6.551989626	-0.336970759	0.880325575
55	C55	-7.20624306	-1.595389278	0.948217238
56	H56	-8 2453211	-1 74803594	1 201872888
57	C57	-6 266674797	-2 558481893	0.633287018
58	H58	-6 40425108	-3 628686812	0 573016986
50	C59	-5 033765675	-1 89/115/030	0.415/155/187
57	037	-5.055/05025	-1.074113037	0.41343340/

		- j (-)	, , ,	
60	C60	-3 75101232	-2 570144107	0.131906204
60	200	2 (12227(01	2.3/014410/	1.02(400555
61	C61	-3.64222/604	-3.362583596	-1.026499555
62	062	-4.661344241	-3.372484233	-1.947463701
(2	002	4.59(11902)	2 221045222	2 029709
63	663	-4.586118926	-2.331045323	-2.928/98
64	H64	-4.405937227	-1.355921393	-2.462889719
65	1165	5 549792421	2 227069975	2 115220508
65	П03	-3.348/82431	-2.52/0088/5	-3.443239308
66	H66	-3.788395552	-2.53725581	-3.65351368
67	C67	-2 517738/139	-1 17/969088	-1 223798278
07	01	-2.517738439	-4.174909088	-1.223798278
68	068	-2.446573764	-4.935052842	-2.36645716
69	C69	-1 450148607	-4 513168913	-3 306157928
70	1170	0.47(00(170	4.2(22(0220	2.92(052299
/0	H/0	-0.4/69961/9	-4.302209329	-2.820955588
71	H71	-1.75184792	-3.577930059	-3.795445883
72	H72	-1 377727295	-5 3076787	-4.052177587
72	11/2 272	-1.577727275	-5.5070787	-4.032177387
73	C/3	-1.505128986	-4.241997663	-0.241112885
74	C74	-1 588580569	-3 38645133	0 868855293
75	1175	0.707424282	2 200011256	1 (0(20050
/5	H/3	-0.797424283	-3.399811330	1.00030039
76	C76	-2.689653441	-2.555983966	1.047416123
77	H77	2 740266818	1 016504005	1 010687350
//	11//	-2.749200818	-1.910504095	1.919087559
78	C78	-0.499369677	-5.315544652	-0.338970572
79	C79	-0.81803197	-6 681160408	-0 563913554
,,,	1100	1.01750.4207	0.001100400	0.505715554
80	H80	-1.81/58429/	-/.056/39286	-0.72568508
81	C81	0.358981664	-7.399250475	-0.504514759
01	1192	0 494717092	9 469071542	0 601257152
82	1102	0.484/1/983	-8.4080/1343	-0.00125/152
83	C83	1.404637163	-6.466348467	-0.280605841
81	C84	2 7878/0801	-6 672020605	-0 182812026
04	005	2.70/042001	-0.072727073	-0.102012020
85	085	3.655636579	-5.586959747	-0.003279733
86	C86	5 062772674	-5 55816585	0 183137947
00	1107	5.002772074	< 100010000 < 10000110000	0.167706047
87	H8/	5./133/0131	-6.420804425	0.16//9604/
88	C88	5,417188441	-4.238341473	0.382045685
80	1100	(402427495	2 924500925	0.5(457520)
89	H89	6.402437485	-3.834509835	0.5645/5396
90	C90	4.236029076	-3.458480469	0.277869467
01	C01	4 104014404	1 09662254	0 264420270
91	C91	4.194914404	-1.98002334	0.304439279
92	C92	4.788300789	-1.361264387	1.481282471
03	093	5 23471604	-2 11001/33/	2 542362103
,,	0))	5.25471004	-2.110014554	2.542502105
94	C94	4.20359968	-2.575351315	3.422//816/
95	H95	3 358246196	-2 994697893	2 866559588
00	1100	2.040771(4	1.757529(2)(1.050102521
96	H96	3.840//164	-1./5/538636	4.059193521
97	H97	4.658611941	-3.346115343	4.048862187
08	C08	4 067540178	0.027442066	1 502224299
90	0.98	4.907349178	0.02/445000	1.505554588
99	099	5.582972663	0.601710339	2.587950649
100	C100	4 701366956	1 298133571	3 479298451
100	11101	4.010004212	1.0(155(40)	2.027252025
101	HI0I	4.018904313	1.961556426	2.937252025
102	H102	5.339168754	1.883169437	4.145672103
102	11102	4 112050007	0.596607262	4.072192504
105	H103	4.112039097	0.38000/303	4.072182394
104	C104	4.559632559	0.816311562	0.406048995
105	C105	3 888/03130	0 194075876	-0.658441077
105	0105	5.000475157	0.194073870	-0.030441077
106	H106	3.535789578	0.796405194	-1.485632571
107	C107	3 708749228	-1 184683949	-0 679139994
107	11100	3.21706749226	1.(50054514	1.52252(200
108	H108	3.21/068/05	-1.652854514	-1.522526209
109	C109	5.332849004	6.886287088	-0.264162301
110	C110	5 102282272	0.011715170	0 545276527
110	0110	3.102383372	0.011/131/2	0.5455/055/
111	H111	4.270761661	8.001972124	1.243419897
112	C112	5 946987488	9 118806109	0 476531614
112	11112	5.240207400	0.02(0.02520	1 117000075
113	n113	5.762352712	9.9/620/5/8	1.11/900065
114	C114	7.02739531	9.124271291	-0.407866559
115	H115	7 683112024	9 989038374	-0 462747189
115	0110	7.003112324	0.01.10.100-	-0.402/4/107
116	C116	7.261332132	8.014494092	-1.222063107
117	H117	8 095150827	8 014989402	-1.918922645
110	C119	C 404C20051	(001041027	1 140055755
118	U110	0.424030851	0.90194183/	-1.148833/33
119	H119	6.600426625	6.045515272	-1.792687684
120	C120	_8 /08559012	1 172106047	1 321211215
120	0120	-0.470330012	1.1/210004/	1.554244545
121	C121	-9.501898242	0.611025336	0.526298118
122	H122	-9 220162021	0.031604316	-0 347601144
122	6122	-9.220103031	0.031034310	-0.54/071144
123	C123	-10.84830964	0.819062965	0.822364236
124	H124	-11.61197809	0.387773497	0.180953081
127	C125	11 0100007	1 500045015	1.0207004
125	0125	-11.2138885	1.582245515	1.932/094
126	H126	-12.26361268	1.740503635	2.164417169
107	C127	10 22492054	2 142544047	2 742020057
127	0127	-10.22482034	2.14554404/	2.142030931
128	H128	-10.5013105	2.734544108	3.611755582
120	C129	-8 877111561	1 0/15680106	2 411178616
129	0127	-0.0//444304	1.74,007100	2.7444/0040
130	H130	-8.109424583	2.372901318	3.082197469
131	C131	3 337218872	-8 052689982	-0 264979668
1.51	C101	0.1.1.1.0.5.10.1	0.032007702	1 410 50 15 ((
132	C132	3.146105434	-8.830650024	-1.418524566
133	H133	2 604965012	-8 411421769	-2.26151681
124	C124	2.001200012	10 10107000	1 404750050
134	U134	3.66/509512	-10.1218/238	-1.494/58969
135	H135	3.521117616	-10.70773795	-2.39820053
120	C126	A 2775(1(AE	10 6501046	0.41009(222
130	0150	4.377301043	-10.0381840	-0.419080223
137	H137	4.77994773	-11.66574432	-0.479280583

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	, , ,		
138 C138	4.567814217	-9.894770307	0.734044224
139 H139	5.112753389	-10.30756562	1.578671836
140 C140	4.055706509	-8.599876093	0.810383616
141 H141	4.193597229	-8.011828257	1.712944097

13. Electrostatic potential surface of 1, 2, and tetramethyl-BODIPY



Figure S11. Electrostatic potential surfaces of (a) **1**, (b) **2** and (c) tetramethyl-BODIPY by DFT calculation at the B3LYP/6-31G* level.





¹³C NMR spectrum of **1**



¹H NMR spectrum of **2**



¹³C NMR spectrum of **2**



Reference

1 Spartan08 for Windows; Wavefunction, Inc.: Irvine, CA.