Supporting Information

Pentacyclic Fused Diborepinium Ions with Ligand-Mediated Blue to Red Emission

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General Procedures: All air- and moisture-sensitive reactions were carried out under an inert atmosphere of argon using standard Schlenk techniques or in a MBRAUN LABmaster glovebox equipped with a -37 °C freezer. Reaction solvents including toluene and hexanes were purified by distillation over sodium (Na) metal. Diethyl ether and tetrahydrofuran (THF) were purified by distillation over Na/benzophenone. Dichloromethane (DCM), o-difluorobenzene (o-DFB), and chlorobenzene were purified via distillation over calcium hydride (CaH₂). Deuterated solvents were purchased from Cambridge Isotope Laboratories and distilled over Na/benzophenone (C_6D_6), Na/K alloy (tol-d₈) and CaH₂ (CD₂Cl₂). All reaction glassware was oven-dried overnight at 190°C. The NMR spectra were collected on Bruker Avance Neo 500mHz, Bruker Advance III 600mHz, Bruker Advance III 800mHz, Varian Inova 500mHz, or Varian 600mHz spectrometers. Proton and carbon signals are reported in ppm and referenced to residual solvent peaks in the deuterated solvent (¹H: C₆D₆ δ 7.16, CD₂Cl₂ δ 5.34 C₆D₅CD₃ δ 2.08 6.97 7.01 7.09; ¹³C: CD₂Cl₂ δ 53.84). All solution boron signals are reported in ppm and referenced to BF₃•Et₂O [¹¹B: $\delta = 0.0$] following the standards and procedures established by IUPAC¹ using the unified scale approach. In some cases, the borosilicate probe from the spectrometer can be observed from -20 to 40 ppm when the signal from the compound is too weak and broad to fully suppress the background signal due to similar frequencies. Phosphorus signals were referenced to H₃PO₄ [³¹P: $\delta = 0.0$] and fluorine signals and were referenced to CFCl₃ [¹⁹F: $\delta = 0.0$] using the same procedures stated above. All solid-state boron signals are reported in ppm and referenced to NaBF₄ [¹¹B: δ = -3.51]. All solid-state carbon signals are reported in ppm and referenced to adamantane. UV-vis data were collected on a Cary 60 UV-vis spectrometer coupled with a Unisoku CoolSpeK cryostat for variable temperature scans. Fluorescence data were collected on an Edinburgh Instruments FS5 spectrofluorometer equipped with a double monochromator for excitation and emission. Variable temperature

fluorescence spectra were collected on a Cary Eclipse fluorescence spectrometer coupled with a Unisoku CoolSpeK cryostat. Samples were prepared in 1 cm square quartz cuvettes. Absolute fluorescence quantum yields were determined using a Hamamatsu C11347-11 Quantaurus-QY Absolute PL Quantum Yield Spectrometer. Samples were prepared inside the glovebox in quartz Petri dishes (solid) or 1 cm square quartz cuvettes with Teflon screw caps (solutions). Solutions were prepared in o-DFB and data were collected with absorbance values below 0.1. Fluorescence lifetimes were recorded using a time-correlated single photon counting (TCSPC) method using an Edinburgh Instruments FS5 spectrofluorometer equipped with a double monochromator for excitation and emission. Measurements were made in the right-angle geometry mode, and the emission was collected through a polarizer set to the magic angle. The excitation source was a 337.5 nm excitation LED lamp. The instrument response function (IRF) was measured for solution samples using a Ludox[®] solution in deionized water. The quality of all decay fits was judged to be satisfactory, based on the calculated values of the reduced χ^2 (0.8-1.2) and Durbin Watson parameters and visual inspection of the weighted residuals. The following compounds were literature procedures: fused bis(stannacycle),² $1-Br^{3}_{,3}$ 2,6prepared according to (diisopropylphenyl)-4,4-diethyl-2,2-dimethyl-pyrrolidin-5-ylidene $[^{Et}CAAC],^4$ 1,3-bis-(2,6diisopropylphenyl)-imidazol-2-ylidene [IPr],⁵ 1,3-diisopropyl-4,5-dimethylimidazol-2-ylidene [I^{*i*}Pr₂],⁶ **2-Br**,³ **3-Br**,³ **4-Br**,³ bis(1-isopropyl-3-methyl-benzimidazol-2-ylidene)methane [CDC],⁷ [CDP].⁸⁻⁹ and hexaphenylcarbodiphosphorane Sodium tetrakis[3,5bis(trifluoromethyl)phenyl]borate (NaBArF₄) was purchased from Ambeed and dried under vacuum with P2O5 for one week. All other compounds were purchased from Sigma Aldrich and used as received.

Synthesis of 1-Cl



A solution of fused bis(stannacycle) (0.751 g, 1.30 mmol) in toluene (120 mL) was cooled to -78 °C before BCl₃ (1M in hexanes, 2.87 mL, 2.87 mmol) was added dropwise. The reaction was stirred at -78 °C for 3 hours before warming to room temperature for 30 minutes. The solvent was removed under vacuum and the crude pink solid was washed with hexanes (100 mL). **1-Cl** was isolated as an orange powder (432 mg, 1.16 mmol, 89.2% yield). ¹H NMR (600 MHz, CD₂Cl₂) δ = 9.17 (s, 2H), 8.88 (d, 2H), 7.80 (m, 4H), 7.65 (t, 2H), 7.51 (d, 2H), 7.35 (d, 2H). ¹¹B{¹H} NMR (192 MHz, C₆H₅Cl, 100 °C) δ = 58.5. Anal. Calcd. For C₂₂H₁₄B₂Cl₂: C, 71.25; H, 3.81. Found: C, 71.35; H, 3.98. *Due to poor solubility no sufficiently resolved ¹³C NMR could be obtained. Note: **1-Cl** is a strong Lewis acid. Recommended storage is inside the glovebox freezer in a taped vial to prevent potential coordination reactions initiated by solvent vapors in the glovebox atmosphere. **Synthesis of 2-Cl**



To a suspension of **1-Cl** (95.2 mg, 0.257 mmol) in toluene (4 mL), a solution of 2,6-(diisopropylphenyl)-4,4-diethyl-2,2-dimethyl-pyrrolidin-5-ylidene (^{Et}CAAC) (170 mg, 0.539 mmol) in toluene (2 mL) was added dropwise. The reaction was stirred at room temperature for 16 hours before the toluene was removed under vacuum. The crude solid was washed with hexanes

to give **2-Cl** as a light-yellow solid (228 mg, 0.227 mmol, 88.3 % yield). Crystals were grown from concentrated a concentrated THF solution at -37 °C. ¹H NMR (600 MHz, Tol-d₈, 20 °C) δ 8.78 (d, J = 8.5 Hz, 2H), 7.56 (s, 2H), 7.36 (t, J = 7.3 Hz, 4H), 7.26 – 7.21 (m, 2H), 6.86 (s, 4H), 6.73 (dd, J = 7.8, 1.6 Hz, 2H), 6.07 (d, J = 7.7 Hz, 2H), 5.84 – 5.75 (m, 2H), 3.34 (dt, J = 11.0, 5.8 Hz, 2H), 2.42 – 2.27 (m, 4H), 1.94 (dq, J = 15.3, 7.8 Hz, 2H), 1.87 (d, J = 6.2 Hz, 6H), 1.62 (dd, J = 14.2, 7.6 Hz, 2H), 1.46 (d, J = 7.9 Hz, 6H), 1.30 (s, 6H), 1.20 (d, J = 6.5 Hz, 6H), 0.95 (d, J = 6.5 Hz, 6H), 0.85 (s, 6H), 0.69 – 0.61 (m, 18H). Solid-state ¹³C NMR (CP/MAS, 20 kHz) δ 192.18, 144.01, 139.32, 137.76, 135.76, 133.37, 131.92, 129.49, 125.46, 84.73, 57.90, 40.76, 29.56, 28.12, 22.51, 20.64, 11.15. Solid-state ¹¹B NMR (MAS, 20 kHz) δ -0.8. Anal. Calcd. For C₆₆H₈₄B₂Cl₂N₂•THF: C, 78.57; H, 8.67; N, 2.62 %. Found: C, 78.62; H, 9.04; N, 2.47 %.

Synthesis of 3-Cl



To a suspension of **1-Cl** (36.8 mg, 0.099 mmol) in toluene (4 mL), a solution of 1,3-bis(2,6diisopropylphenyl)imidazol-2-ylidene (**IPr**) (70.10 mg, 0.180 mmol) in toluene (2 mL) was added dropwise. The reaction was stirred at room temperature for 16 hours before the toluene was removed under vacuum. The crude solid was washed with hexanes to give **3-Cl** as a white solid (65.8 mg, 0.087 mmol, 87.2% yield). ¹H NMR (600 MHz, tol-d₈, 100 °C) δ 8.13 (br s, 2H), 7.41 (br s, 2H), 7.04 (br s, 3H), 6.90 (br s, 4H), 6.70-6.65 (br m, 8H), 6.46-6.35 (br m, 7H), 6.31 (br s, 4H), 2.95 (br s, 8H, C*H*(CH₃)₂), 1.47 (br s, 12H, CH(CH₃)₂), 1.35 (br s, 12H, CH(CH₃)₂), 0.80 (br s, 12H, CH(CH₃)₂), 0.74 (br s, 12H, CH(CH₃)₂). *Compound **3-Cl** was not very soluble at room

temperature and the resolution on expected multiplicity was not able to be observed even at higher temperatures. Solid-state ¹³C NMR (CP/MAS, 20 kHz) δ 170.47, 146.17, 144.30, 140.27, 135.24, 132.93, 130.11, 127.38, 125.89, 124.56, 122.08, 29.41, 28.26, 26.54, 24.23, 23.23, 22.51, 21.36. Solid-state ¹¹B NMR (MAS, 20 kHz) δ -8.4. Anal. Calcd. For C₇₆H₈₆B₂Cl₂N₄: C, 79.51; H, 7.55; N, 4.88 %. Found: C, 79.16; H, 7.75; N, 4.73 %.

Synthesis of 4-Cl



To a suspension of **1-Cl** (22.8 mg, 0.062 mmol) in toluene (2 mL), a solution of 1,3-diisopropyl-4,5-dimethylimidazol-2-ylidene (**I**ⁱ**Pr**₂) (22.4 mg, 0.124 mmol) in toluene (2 mL) was added dropwise. The reaction stirred at room temperature overnight before the toluene was removed under vacuum. The crude solid was washed with hexanes to give **4-Cl** as a white solid (32.6 mg, 0.059 mmol, 96.2% yield). ¹H NMR (400 MHz, C₆D₆, 20 °C) δ 8.87 (d, *J* = 7.6 Hz, 2H), 8.75 (s, 2H), 7.50 (td, *J* = 7.4, 1.4 Hz, 2H), 7.28 (d, *J* = 6.3 Hz, 2H), 7.18 (d, *J* = 7.0 Hz, 2H), 7.15 (d, *J* = 5.1 Hz, 2H), 6.81 (d, *J* = 11.7 Hz, 2H), 4.69 (br s, 4H), 1.34 (s, 12H), 0.66 (d, *J* = 7.0 Hz, 24H). ¹³C NMR (126 MHz, C₆D₆, 20 °C) δ 137.77, 137.42, 134.01, 131.29, 130.75, 130.15, 128.35, 127.74, 127.38, 124.52, 49.58, 20.74, 10.01. *Due to coupling with quadrupolar nulcei, the carbon atoms adjacent to boron could not be resolved. ¹¹B NMR (192 MHz, C₆D₆, 20 °C) δ -2.5.

Synthesis of 5



To a suspension of **2-Cl** (77.8 mg, 0.0780 mmol) in Et₂O (3 mL), NaBAr^F₄ (145 mg, 0.164 mmoL) was added in one portion. A color change from white to clear red was observed. The reaction was stirred for 3 hours at room temperature before passing through a 0.45 µm PTFE syringe filter to remove fine white NaCl powder and dried. The sticky solid was triturated with hexanes (2 x 2 mL) to isolate 5 as a red powder (190 mg, 0.0716 mmol, 91.8 % yield). *The reaction also proceeds with 2-Br. Crystals were grown from a concentrated DCM solution at -37 °C. ¹H NMR (500 MHz, CD_2Cl_2 , 20 °C) δ 8.17 (br s, 1H), 8.01 (d, J = 7.9 Hz, 1H), 7.94 (t, J = 7.6 Hz, 1H), 7.88 (d, J = 7.0Hz, 1H), 7.84 – 7.68 (m, 21H), 7.63 (ddd, J = 8.1, 5.4, 2.9 Hz, 2H), 7.55 (s, 8H), 7.47 (d, J = 12.5 Hz, 1H), 7.41 (q, J = 7.8 Hz, 2H), 7.35 (d, J = 12.3 Hz, 1H), 7.21 (d, J = 7.5 Hz, 2H), 7.14 (d, J = 7.3 Hz, 1H), 7.06 (d, J = 7.6 Hz, 1H), 6.83 (s, 1H), 2.94 (s, 1H), 2.82 – 2.70 (m, 1H), 2.70 – 2.55 (m, 4H), 2.47 - 2.35 (m, 1H), 2.34 - 2.25 (m, 1H), 2.10 (h, J = 7.4 Hz, 1H), 1.99 - 1.85 (m, 1H),1.76 - 1.60 (m, 11H), 1.55 (s, 4H), 1.40 (d, J = 6.5 Hz, 4H), 1.29 (d, J = 6.5 Hz, 4H), 1.20 - 1.07(m, 10H), 0.87 (t, J = 7.3 Hz, 4H), 0.81 (q, J = 7.5 Hz, 6H), 0.67 (t, J = 7.4 Hz, 4H), 0.23 (s, 3H), -0.27 (d, J = 6.6 Hz, 3H), -0.36 (s, 1H). ¹³C NMR (126 MHz, CD₂Cl₂) δ 162.15 (dd, J = 99.5, 49.9 Hz, $BAr^{F_4}CF_3$), 145.36 (d, J = 24.8 Hz), 144.97, 144.91, 136.65, 136.39, 135.21, 134.58, 133.04, 132.69, 132.09, 131.14, 129.72 - 129.59 (m), 129.40 (dd, J = 5.8, 3.0 Hz), 129.15 (dd, J = 5.4, 2.6 Hz), 128.90 (dd, J = 5.7, 3.0 Hz), 128.65 (d, J = 15.2 Hz), 128.25, 127.93 (d, J = 18.8 Hz), 127.64, 127.44, 126.08, 123.91, 121.74, 117.89, 86.62, 86.13, 66.23, 66.19, 65.77, 31.06, 30.93, 30.69, 30.53, 30.44, 30.26, 30.19, 29.39, 27.38, 26.53, 25.86, 25.27, 24.98, 15.44, 10.38, 10.30. ¹¹B NMR (160 MHz, CD₂Cl₂) δ 59.7, -6.6. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) -62.8. Anal. Calcd. For C₁₃₀H₁₀₈B₄F₄₈N₂: C, 58.84; H, 4.10; N, 1.06 %. Found: C, 58.80; H, 4.04; N, 1.04 %.

Synthesis of 6



To a suspension of **3-Cl** (64.4 mg, 0.0561 mmol) in Et₂O (2 mL), NaBAr^F₄ (105 mg, 0.119 mmol) was added in one portion. A color change from white to an orange suspension was observed. The reaction was stirred for 3 hours at room temperature before passing through a 0.45 μ m PTFE syringe filter and removing the solvent. The sticky solid was triturated with hexanes (2 x 3 mL) to isolate **6** as a bright orange solid (125 mg, 0.0446 mmol, 79.5% yield). Crystals were grown from a concentrated DCM solution at -37 °C. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) δ 7.81 (td, *J* = 7.5, 1.5 Hz, 2H, FBP C*H*), 7.78 (s, 4H, IPr C*H*), 7.74 – 7.70 (m, 20H, BAr^F₄ C*H*/IPr C*H*), 7.55 (s, 8H, BAr^F₄ C*H*), 7.47 (t, *J* = 8.0 Hz, 6H), 7.40 (t, *J* = 7.5 Hz, 2H, FBP C*H*), 7.27 (d, *J* = 12.6 Hz, 2H, FBP C*H*=C*H*), 7.15 (d, *J* = 7.8 Hz, 8H, IPr C*H*), 6.86 (d, *J* = 12.4 Hz, 2H, FBP C*H*=C*H*), 2.52 (hept, *J* = 6.6 Hz, 8H, IPr C*H*(CH₃)₂), 1.09 (d, *J* = 6.7 Hz, 24H, IPr CH(CH₃)₂), 0.46 (d, *J* = 6.7 Hz, 24H, IPr CH(CH₃)₂). ¹³C NMR (101 MHz, CD₂Cl₂) δ 162.15 (dd, *J* = 99.9, 49.8 Hz, BAr^F₄ CF₃), 145.28, 145.17, 144.30, 140.44, 140.11, 138.58, 136.39, 135.94, 135.21, 133.52, 133.45,

133.24, 132.13, 131.51, 129.40, 129.06, 128.01, 126.35, 126.10, 125.70, 123.65, 117.88, 29.88 (IPr *C*H(CH₃)₂), 26.41 (IPr CH(*C*H₃)₂), 21.94 (IPr CH(*C*H₃)₂). ¹¹B{¹H} NMR (192 MHz, CD₂Cl₂, 20 °C) $\delta = 61.2$, -6.7. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) -62.8. Anal. Calcd. For C₁₄₀H₁₁₀B₄F₄₈N₄: C, 59.98; H, 3.95; N, 2.00 %. Found: C, 59.57; H, 3.82; N, 1.79 %.

Synthesis of 7



To a suspension of **4-Cl** (68.8 g, 0.0920 mmol) in Et₂O (3 mL), NaBAr^F₄ (171 mg, 0.193) was added in one portion. A color change from white to an orange suspension was observed. The reaction was stirred for 3 hours at room temperature before filtering and washing the solid with Et₂O (2 x 5 mL) and hexanes (2 x 5 mL). A bright orange solid was isolated (180 mg, 0.075 mmol, 82% yield). Crystals were grown from a concentrated DCM solution at -37 °C. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) δ 8.18 (s, 2H, FBP *CH*), 8.08 (td, *J* = 7.6, 1.4 Hz, 2H, FBP *CH*), 8.01 (dd, *J* = 8.0, 0.9 Hz, 2H, FBP *CH*), 7.75 (td, *J* = 7.7, 1.4 Hz, 2H, FBP *CH*), 7.72 – 7.69 (m, 16H, BAr^F₄ *CH*), 7.61 – 7.56 (m, 6H, FBP *CH*), 7.53 (s, 8H, BAr^F₄ *CH*), 4.21 (hept, *J* = 6.8 Hz, 4H, I⁴Pr₂ *CH*(CH₃)₂), 2.53 (s, 12H, *CH*₃), 1.28 (dd, *J* = 6.9, 4.7 Hz, 24H, CH(*CH*₃)₂). ¹³C NMR (126 MHz, CD₂Cl₂) δ 162.13 (dd, *J* = 100.0, 49.9 Hz, BAr^F₄ *C*F₃)., 147.39, 146.41, 142.84, 141.78, 138.14, 137.22, 135.65, 135.19, 134.12, 129.60, 129.39, 129.14, 128.22, 126.05, 123.89, 121.72, 119.23, 117.88, 66.17, 54.78 (I⁴Pr₂ *CH*(CH₃)₂), 21.99 (d, *J* = 13.3 Hz, I⁴Pr₂ CH(CH₃)₂), 10.69 (I⁴Pr₂ *CH*).

¹¹B NMR (161 MHz, CD₂Cl₂, 20 °C) δ 53.4, -6.9. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) δ -62.9. Anal. Calcd. For C₁₀₈H₇₈B₄F₄₈N₄•2CH₂Cl₂: C, 51.67; H, 3.23; N, 2.19 %. Found: C, 51.74; H, 3.06; N, 2.19 %.

Synthesis of 8



To a suspension of **1-Br** (60.1 mg, 0.131 mmol) in o-difluorobenzene, bis(1-isopropyl-3-methylbenzimidazol-2-ylidene)methane [CDC] (99 mg, 0.28 mmol) was added in one portion. The reaction immediately turned to a red suspension. After 5 minutes, NaBAr^F₄ (243 mg, 0.275 mmol) was added in one portion. The reaction was stirred for 17 hours before passing through a 0.45 μ m PTFE syringe filter and removing the solvent. The sticky solid was triturated with hexanes (3 x 3 mL) and **8** was isolated as a red solid (292 mg, 0.106 mmol, 81.1% yield). ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) δ 7.72 (t, *J* = 2.8 Hz, 16H, BAr^F₄ C*H*), 7.60 – 7.39 (m, 28H, BAr^F₄ C*H*/FBP C*H*/CDC C*H*), 7.39 – 7.29 (m, 4H, FBP C*H*), 7.09 (td, *J* = 7.4, 1.3 Hz, 2H, FBP C*H*), 6.87 (d, *J* = 12.5 Hz, 2H, FBP C*H*=C*H*), 6.53 (d, *J* = 13.1 Hz, 2H, FBP C*H*=C*H*), 4.30 (p, *J* = 7.0 Hz, 4H, CDC C*H*(CH₃)₂), 3.72 (br s, 12H, CDC C*H*₃), 1.05 (br s, 24H, CDC CH(C*H*₃)₂). ¹³C NMR (126 MHz, CD₂Cl₂) δ 162.14 (dd, *J* = 99.5, 49.9 Hz, BAr^F₄ CF₃), 157.52, 135.20, 133.91, 132.73, 131.90, 131.68, 130.49, 129.23, 128.40, 126.37, 126.06, 123.90, 121.73, 117.88, 117.84, 114.09, 112.04, 52.17 (CDC *C*H(CH₃)₂), 33.85 (CDC *C*H₃), 20.17 (CDC CH(*C*H₃)₂). ¹¹B NMR (161 MHz, CD₂Cl₂, 20 °C) δ 55.4, -6.6. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) δ -62.8. Anal. Calcd. for C₁₃₂H₉₄B₄F₄₈N₈: C, 57.71; H, 3.45; N, 4.08 %. Found: C, 57.52; H, 4.03; N, 4.00.

Synthesis of 9



To suspension (67.6 0.147 o-difluorobenzene, а of 1-Br mg, mmol) in hexaphenylcarbodiphosphorane [CDP] (166 mg, 0.309 mmol) was added in one portion. Reaction immediately turned cloudy yellow. After five minutes, NaBAr^F₄ (274 mg, 0.309 mmol) was added in one portion. Reaction was stirred for 17 hours before passing through a 0.45 µm PTFE syringe filter and removing the solvent. Sticky solid was triturated with hexanes (3 x 3 mL). Pale yellow solid isolated (407 mg, 0.131 mmol, 89.3% yield). Product can be further purified by suspending in diethyl ether and putting in freezer before filtering cold. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) δ 7.76 (t, J = 2.4 Hz, 16H, BAr^F₄ CH), 7.57 (s, 8H, BAr^F₄ CH), 7.22 (br s, 38H, PPh₃ CH)*, 7.11 (d, J = 7.4 Hz, 2H, FBP CH)*, 7.04 (br s, 22H, FBP CH)*, 6.89 (td, J = 7.4, 1.4 Hz, 2H, FBP CH), 6.84 (td, *J* = 7.4, 1.3 Hz, 2H, FBP C*H*), 6.75 (d, *J* = 7.6 Hz, 2H, FBP C*H*), 6.41 (s, 2H. FBP C*H*), 6.29 (d, J = 12.2 Hz, 2H, FBP CH=CH), 5.98 (d, J = 12.0 Hz, 2H, FBP CH=CH). *Peaks at 7.22, 7.11 and 7.04 overlap but total to 62 protons. ¹³C NMR (126 MHz, CD₂Cl₂, 20 °C) δ 162.19 (dd, $J = 99.7, 49.6 \text{ Hz}, \text{BAr}^{F_4} CF_3), 135.90, 135.23 (\text{BAr}^{F_4} CH), 134.23 - 133.83 (m, PPh_3 CH), 133.12,$ 133.01, 131.96 (FBP CH=CH), 130.46 (FBP CH=CH), 129.69 (dd, J = 5.5, 2.8 Hz), 129.44 (dd, J = 5.5, 2.6 Hz), 129.26 – 128.98 (m, PPh₃ C), 128.94 (dd, J = 6.1, 2.8 Hz), 128.27, 128.14, 127.94, 127.53, 127.10, 126.99, 126.10, 125.32, 123.94, 121.77, 117.91 (p, J = 4.1 Hz). ¹¹B NMR (161 MHz, CD₂Cl₂, 20 °C) δ 59.1, -6.6. ³¹P NMR (203 MHz, CD₂Cl₂, 20 °C) δ 24.1. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) δ -62.8. Anal. Calcd. for C₁₆₀H₉₈B₄F₄₈P₄: C, 62.00; H, 3.19 %. Found: C, 62.58; H, 3.21.

NMR data



Figure S1. ¹H NMR (600 MHz, CD₂Cl₂, 20 °C) spectrum of 1-Cl.



Figure S2. ¹¹B{¹H} NMR (192 MHz, C₆H₅Cl, 100 °C) spectrum of 1-Cl.



Figure S3. ¹H NMR (600 MHz, toluene-d₈, 20 °C) spectrum of 2-Cl.



Figure S4. ¹³C NMR (CP/MAS, 20 kHz) spectrum of 2-Cl.



Figure S5. Solid-state ¹¹B NMR (MAS, 20 kHz) spectrum of 2-Cl.



Figure S6. ¹H NMR (600 MHz, toluene-d₈, 100 °C) spectrum of **3-Cl**.



Figure S7. ¹³C NMR spectrum (CP/MAS, 20 kHz) of 3-Cl.



Figure S8. Solid-state ¹¹B NMR (MAS, 20 kHz) spectrum of 3-Cl.



Figure S9. ¹H NMR (400 MHz, C₆D₆, 20 °C) of **4-Cl**.



Figure S10. ¹³C NMR (126 MHz, C₆D₆, 20 °C) spectrum of 4-Cl.



Figure S11. ¹¹B NMR (160 MHz, CD₂Cl₂, 20 °C) spectrum of 4-Cl.



Figure S12. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of **5**. There is a signal from a protonated CAAC impurity at 8.19 ppm but overlaps with the signal at 8.17 ppm from **5** making the quantification of protonated CAAC a challenge. Other signals corresponding to protonated CAAC were not able to be identified due to the complex splitting from the compound signals in the aliphatic region. Although attempts were made to obtain NMR using other deuterated solvents, NMR signals were best resolved in CD₂Cl₂ and data was obtained of concentrated samples protected from light. Residual diethyl ether is present from the reaction and labeled in the spectrum.



Figure S13. Zoomed in ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of 5 from 6.4-8.7 ppm.



Figure S14. Zoomed in ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of 5 from -1.0-3.6 ppm.



Figure S15. ¹³C NMR (126 MHz, CD₂Cl₂, 20 °C) spectrum of 5.



Figure S16. ¹¹B{¹H} NMR (160 MHz, CD₂Cl₂, 20 °C) spectrum of **5**. Borosilicate probe could not be fully processed out due to weak and broad signal at 59.7 ppm having a similar frequency.



Figure S17. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) spectrum of 5.



Figure S18. ¹H-¹H correlated spectroscopy [COSY] (CD₂Cl₂, 20 °C) spectrum of 5.



Figure S19. Heteronuclear single quantum coherence spectroscopy [HSQC] (CD₂Cl₂, 20 $^{\circ}$ C)

spectrum of **5**.



Figure S20. Heteronuclear multiple bond correlation spectroscopy [HMBC] (CD₂Cl₂, 20 °C)

spectrum of **5**.



Figure S21. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of **6**. There is a signal from a protonated IPr impurity at 8.30 ppm that integrates to 0.17. Other signals corresponding to protonated IPr are labeled in grey. Although attempts were made to obtain NMR using other deuterated solvents, NMR signals were best resolved in CD_2Cl_2 and data was obtained of concentrated samples protected from light. Residual diethyl ether is present from the reaction and labeled in the spectrum.



Figure S22. Zoomed in ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of 6 from 6.5-8.5 ppm.



Figure S23. Zoomed in ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of 6 from 0.0-2.9 ppm.



Figure S24. ¹³C NMR (101 MHz, CD₂Cl₂) spectrum of 6.


Figure S25. ¹¹B $\{^{1}H\}$ NMR (161 MHz, CD₂Cl₂, 20 °C) spectrum of 6.



Figure S26. ¹⁹F NMR (471 MHz, CD_2Cl_2 , 20 °C) spectrum of 6.



Figure S27. Heteronuclear single quantum coherence spectroscopy [HSQC] (CD₂Cl₂, 20 °C)

spectrum of **6**.



Figure S28. Heteronuclear multiple bond correlation spectroscopy [HMBC] (CD₂Cl₂, 20 °C) spectrum of **6**.



Figure S29. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of **7**.



Figure S30. ¹³C NMR (126 MHz, CD₂Cl₂, 20 °C) spectrum of 7.



Figure S31. ¹¹B NMR (161 MHz, CD_2Cl_2 , 20 °C) spectrum of 7. The borosilicate probe could not be fully processed out without removing the weak and broad compound signal at 54.1 ppm due it having a similar frequency to the probe.



Figure S32. ¹⁹F NMR (376 MHz, CD₂Cl₂, 20 °C) spectrum of 7.



Figure S33. Heteronuclear single quantum coherence spectroscopy [HSQC] (CD₂Cl₂, 20 °C)

spectrum of 7.



Figure S34. Heteronuclear multiple bond correlation spectroscopy [HMBC] (CD₂Cl₂, 20 °C) spectrum of 7.



Figure S35. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of 8.



Figure S36. ¹³C NMR (126 MHz, CD₂Cl₂, 20 °C) spectrum of 8.



Figure S37. ¹¹B{¹H} NMR (161 MHz, CD₂Cl₂, 20 °C) spectrum of 8.



Figure S38. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) spectrum of 8.



Figure S39. Heteronuclear single quantum coherence spectroscopy [HSQC] (CD₂Cl₂, 20 °C)

spectrum of 8.



Figure S40. Heteronuclear multiple bond correlation spectroscopy [HMBC] (CD₂Cl₂) spectrum

for **8**.



Figure S41. ¹H NMR (500 MHz, CD₂Cl₂, 20 °C) spectrum of 9.



Figure S42. ¹³C NMR (126 MHz, CD₂Cl₂, 20 °C) spectrum of 9.



Figure S43. ¹¹B{¹H} NMR (161 MHz, CD₂Cl₂, 20 °C) spectrum of **9**. Borosilicate probe could not be fully processed out due to weak and broad signal at 59.1 ppm.



Figure S44. ³¹P NMR (203 MHz, CD₂Cl₂, 20 °C) spectrum of 9.



Figure S45. ¹⁹F NMR (471 MHz, CD₂Cl₂, 20 °C) spectrum of 9.



Figure S46. Heteronuclear single quantum coherence spectroscopy [HSQC] (CD_2Cl_2 , 20 °C) spectrum of 9.



Figure S47. Heteronuclear multiple bond correlation spectroscopy [HMBC] (CD₂Cl₂) spectrum

for **9**.

Photophysical Data



Figure S48. Normalized UV/vis (black trace) and fluorescence (red trace) spectra of **1-Br** (A) and **1-Cl** (B) in chlorobenzene. $\lambda_{ex} = 360$ nm.



Figure S49. Dilute absorbance and fluorescence spectrum of decomposed **5** in o-DFB ($\lambda_{ex} = 350$ nm, [0.007 mM]). Note: The concentrated sample of **5** in o-DFB is reported in Figure 5B (emission peak at 561 nm).



Figure S50. Dilute absorbance and fluorescence spectra of decomposed **6** in o-DFB ($\lambda_{ex} = 350$ nm, [0.005 mM]). Note: The concentrated sample of **6** in o-DFB is reported in Figure 5B (emission peak at 575 nm).



Figure S51. Dilute absorbance and fluorescence spectra of decomposed 7 in o-DFB ($\lambda_{ex} = 350$ nm, [0.001 mM]). A) Spectrum taken ten minutes after sample was prepared. B) Spectrum taken three hours after sample was prepared. Note: Compound 7 decomposes at lower concentrations and more slowly than 5 and 6. Compound 7 is fully decomposed after three hours and looks similar to 5 and 6.



Figure S52. CIE (1931) chromaticity diagram of VT fluorescence of **8** in DCM ($\lambda_{ex} = 480$ nm, [0.01 mM]).

Thermogravimetric Analysis (TGA) Data



Figure S53. TGA spectrum of 1-Br. *Small dip just above 100 °C is due to loss of toluene.



Figure S54. TGA spectrum of 1-Cl.



Figure S55. TGA spectrum of 5.



Figure S56. TGA spectrum of 6.



Figure S57. TGA spectrum of 7.



Figure S58. TGA spectrum of 8.



Figure S59. TGA spectrum of 9.

X-ray Crystallography Details

Low temperature single crystal X-ray diffraction data for 1-Cl, 3-Cl, 4-Cl, 5 and 6 were collected on a Bruker Kappa APEXII CCD system equipped with a fine-focus sealed tube (Mo K_{α}, $\lambda = 0.71073$ Å) and a graphite monochromator. Low temperature single crystal X-ray diffraction data for 2-Cl, 7, S5, S6, and S7 were collected on a Bruker D8 Venture PhotonIII Kappa fourcircle diffractometer system equipped with dual Incoatec IµS 3.0 micro-focus sealed X-ray tubes (Cu K α , $\lambda = 1.54178$ Å; Mo K α , $\lambda = 0.71073$ Å) and HELIOS double bounce multilayer mirror monochromators. Low-temperature diffraction data for 8 and 9 were collected on a Bruker-AXS Kappa Duo diffractometer equipped with *IµS* micro-sources, coupled to a Photon 3 CPAD detector, performing ϕ -and ω -scans, and using Mo K_{α} radiation ($\lambda = 0.71073$ Å). Data reduction was carried out with the program SAINT¹⁰ and semi-empirical absorption correction based on equivalents was performed with the program SADABS.¹¹ All structures were solved by dual-space methods using SHELXT¹² and refined against F^2 on all data by full-matrix least squares with SHELXL¹³ following established refinement strategies.¹⁴ Details about data quality and a summary of the residual values of the refinement are listed in Tables 1 and 2.

The structures 1-9 and S5-S7 were solved and refined using the Bruker SHELXTL Software Package¹² within OLEX2 1.5.¹⁵ The frames were integrated with the Bruker SAINT software package¹⁰ using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method (SADABS).¹¹ Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in geometrically calculated positions with $U_{iso} = 1.2U_{equiv}$ of the parent atom (1.5 U_{equiv} for methyl). The relative occupancies of each position of the disordered sites were freely refined, unless the disorder was symmetry related. In those cases, the occupancy was fixed at 50%. Constraints and restraints were used on the anisotropic displacement parameters and bond lengths of most of the disordered atoms.

Compound 8 crystallizes in the triclinic centrosymmetric space group P-1 with one half molecule of 8, one BAr^F₄ anion, and one molecule of diethyl ether in the asymmetric unit. The second half of 8 is generated by the crystallographic inversion center. The ether molecule was refined as completely disordered over two positions and six of the eight CF₃ groups on the BARF ion were also refined as disordered over two or, in one case, even three positions. All disorders were refined with the help of similarity restraints on 1-2 and 1-3 distances as well as similarity restraints on displacement parameters and advanced rigid-bond restraints.

Compound 9 crystallizes in the triclinic centrosymmetric space group P-1 with one half molecule of 9, one BAr^F₄ anion, and 1.5 molecules of dichloromethane in the asymmetric unit. The second half of 9 is generated by the crystallographic inversion center. The half occupied solvent molecule resides near an inversion center and is, therefore, disordered about that symmetry element. In addition, two independent positions could be established for that CH₂Cl₂ molecule, resulting in an affective four-component disorder (although only two of them are crystallographically unique). Furthermore, four of the eight CF₃ groups on the BAr^F₄ ion were refined as disordered over two positions. All disorders were refined with the help of similarity restraints on 1-2 and 1-3 distances as well as similarity restraints on displacement parameters and advanced rigid-bond restraints.

	1-Cl	2-Cl	3-Cl	4-Cl	5	6
CCDC	2344133	2344134	2344135	2344136	2344137	2344138
number						
Formula		C ₄₁ H ₅₈ BCl	C159H180B4Cl	$C_{44}H_{54}B_2Cl$	$C_{65}H_{54}B_2F_{24}$	$C_{142}H_{114}B_4Cl_4F$
	$C_{22}\Pi_1 4 \mathbf{D}_2 C \mathbf{I}_2$	NO ₂	4N8	₂ N ₄	Ν	$_{48}N_4$
FW (g/mol)	370.85	643.14	2388.14	731.43	1326.99	2973.88
Temp (K)	100.01	100.0	99.99	99.98	100.03	100(2)
λ (Å)	0.71073	0.71073	1.54178	0.71073	0.71073	0.71073
Size (mm)	0.373 ×	0.453 ×	0.145 ×	0.611 ×	0.2 × 0.28 ×	0.127 x 0.196 x
	0.053 ×	0.426 ×	0.076 ×	0.226 ×	0.3 ~ 0.28 ~	0.337
	0.052	0.202	0.046	0.198	0.12	
Crystal habit	orange	yellow	a larlage rad	colorless	orongo plato	red block
	needle	block	coloness rou	block	orange plate	
Crystal system	monoclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	C2/c	P-1	$P2_1/n$	P-1	P 2 ₁ /n
a (Å)	13.331(4)	24.7297(12)	10.1202(5)	11.2159(11)	12.5802(15)	13.601(3)
b(Å)	3.9432(11)	18.7599(8)	17.0454(8)	11.9173(12)	13.1420(16)	23.955(6)
c (Å)	16.631(5)	15.6595(7)	19.6957(11)	15.0102(16)	19.744(2)	21.060(4)
α (°)	90	90	95.587(4)	90	85.418(2)	90
β (°)	108.334(7)	97.779(2)	96.221(4)	90.326(3)	79.658(2)	96.006(6)
γ (°)	90	90	90.244(4)	90	73.127(2)	90
Volume (Å ³)	829.9(4)	7198.0(6)	3361.1(3)	2006.3(4)	3071.6(6)	6824.(2)
Ζ	2	8	1	2	2	2
Density (g/cm ³)	1.484	1.187	1.180	1.211	1.435	1.447
μ (mm ⁻¹)	0.393	0.142	1.218	0.198	0.134	0.205
F(000)	380.0	2792.0	1278.0	780.0	1354.0	3028
θ range (°)	1.609 to 25.357	1.972 to 33.788	2.267 to 68.602	2.182 to 31.015	1.62 to 33.751	1.70 to 25.39
Index ranges	-16 < h < 16	-38 < h < 38	-12 < h < 11	-16 < h < 16	-19 < h < 19	-16 < h < 16
C	$-4 \le k \le 4$	$-28 \le k \le 29$	$-20 \le k \le 20$	$-17 \le k \le 16$	$-20 \le k \le 20$	$-28 \le k \le 28$
	$-20 \le 1 \le 20$	$-21 \le 1 \le 24$	$-23 \le 1 \le 23$	$-21 \le 1 \le 21$	$-30 \le 1 \le 30$	$-25 \le 1 \le 25$
Reflns collected	8643	83023	49634	27359	119222	77462
Independent reflns	$1523 [R_{int} = 0.1091]$	14377 [$R_{int} = 0.0582$]	12273 [R _{int} = 0.1088]	6397 [R _{int} = 0.0350]	24545 [R _{int} = 0.0452]	12495 [R _{int} = 0.1018]
Data / restraints /parameters	1523/0/118	14377/0/44 4	12273/0/877	6397/0/241	24545/187/ 938	12495/75/985
GOF on F ²	1.018	1.050	1.008	1.028	1.021	1.008
$R_1 (I \ge 2\sigma(I))$	0.0501	0.0611	0.0561	0.0386	0.0516	0.0640
wR ₂ (all data)	0.1385	0.1918	0.1507	0.1038	0.1440	0.1430

Table S1: Crystallographic data for compounds 1-4 (Cl), 5-6

	7	8	9	S 5	S6	S7
CCDC	2344139	2344145	2344146	2344140	2344141	2344142
number						
Formula	$C_{110}H_{82}B_4Cl_4$	$C_{140}H_{114}B_4F_4$	$C_{166}H_{102}B_4Cl$	$C_{72}H_{88}B_2Cl_4$	$C_{84}H_{94}B_2Cl_8$	$C_{50}H_{58}B_2Cl_4$
	F ₄₈ N ₄	₈ N ₈ O ₂	$_{4}F_{48}P_{4}$	$F_{12}N_4O$	$F_{12}N_6O_8S_4$	$F_{12}N_8O_8S_4$
FW (g/mol)	2555.88	2895.63	3317.585	1657.12	1976.41	1418.70
Temp (K)	100.(2)	100(2)	100.15	100.00	100(2)	100.00
λ (Å)	0.71073	0.71073	0.71073	1.54178	0.71073	0.71073
Size (mm)	0.455 ×	0.320 x	0.665 ×	0.172×0.06	0.126 x	0.504 ×
	0.304 ×	0.100 x	0.445 ×	0.172×0.00	0.190 x	0.235×0.18
	0.283	0.065	0.195	~ 0.029	0.236	
Crystal habit	orange block	orange plate	colorless plate	pink needle	orange block	orange block
Crystal system	triclinic	triclinic	triclinic	monoclinic	monoclinic	triclinic
Space group	P-1	P-1	P-1	$P2_1/c$	P 2 ₁ /n	P-1
a (Å)	12.3947(8)	11.0428(5)	13.2079(5)	14.9640(6)	16.7454(5)	8.9168(4)
b(Å)	12.5964(8)	16.5514(8)	15.4895(6)	11.9337(5)	27.4896(9)	9.3168(4)
c (Å)	19.1553(12)	19.2623(8)	19.1541(6)	21.9364(9)	21.7003(6)	18.6398(7)
α (°)	79.135(2)	77.797(2)	80.403(1)	90	90	96.7530(10)
β (°)	72.923(2)	84.084(2)	84.517(1)	101.645(3)	112.1310(10)	92.3660(10)
γ (°)	89.308(2)	73.633(2)	72.088(1)	90	90	95.8310(10)
Volume (Å ³)	2804.6(3)	3298.1(3)	3672.4(2)	3836.7(3)	9253.2(5)	1527.60(11)
Ζ	1	1	1	2	4	1
Density (g/cm ³)	1.513	1.458	1.500	1.434	1.419	1.542
μ (mm ⁻¹)	0.235	0.133	0.240	3.157	0.414	0.425
F(000)	1290.0	1478	1680.5	1724.0	4087	728.0
θ range (°)	2.17 to 29.15	1.924 to 30.521	1.88 to 31.52	3.015 to 68.244	1.94 to 26.40	2.214 to 27.109
Index ranges	$-16 \le h \le 16$	$-15 \le h \le 15$	$-19 \le h \le 19$	$-18 \le h \le 18$,	$-20 \le h \le 20$,	$-11 \le h \le 11$,
	$-17 \le k \le 17$	$-23 \le k \le 23$	$-22 \le k \le 22$	$-14 \le k \le 13$,	$-34 \le k \le 34$,	$-11 \le k \le 11$,
	$-26 \le 1 \le 25$	$-22 \le 1 \le 27$	$-28 \le l \le 26$	$-23 \le l \le 26$	$-27 \le 1 \le 27$	$-23 \le 1 \le 22$
Reflns collected	85598	56332	222447	29511	155109	40018
Independent reflns	$15059 [R_{int} = 0.0394]$	19780 [R _{int} = 0.0627]	24400 [R _{int} = 0.0360]	6972 [R _{int} = 0.1116]	$18917 [R_{int} = 0.0899]$	6729 [R _{int} = 0.0315]
Data / restraints /parameters	15059/123/9 95	19780 / 3917 / 1180	24400/204/1 167	6972/0/486	18917 / 340 / 1426	6729/0/489
GOF on F ²	1.035	1.021	1.042	1.023	1.030	2.583
R_1 (I>2 σ (I))	0.0529	0.0636	0.0473	0.0625	0.0677	0.0809
wR ₂ (all data)	0.1492	0.1491	0.1342	0.1706	0.1908	0.2909

 Table S2: Crystallographic data for compounds 7-9, S5-S7



Figure S60. Side view of tetracoordinate FBP adducts **2-Cl** (A), **3-Cl** (B), and **4-Cl** (C), displaying distortion from planarity.



Figure S61. Molecular structures of **5** (A), **6** (B), and **7** (C) with their counteranions shown. Structures also shown in Figure 2. (Thermal ellipsoids are shown at 50% probability; H atoms and co-crystallized solvent were omitted for clarity.)



Figure S62. Molecular structures of 8 (A) and 9 (B) with their counteranions shown. Structures also shown in Figure 3. (Thermal ellipsoids are shown at 50% probability; H atoms and co-crystallized solvent were omitted for clarity.


Figure S63. Molecular structure of 5 depicting close contacts between H15C–B1.



Figure S64. Molecular structure of 7 depicting close contacts between H13–B1 and H22A–B1.



Figure S65. Molecular structure of 8 depicting close contacts between H14a–B1.



Figure S66. Molecular structure of **S5**. Isolated through the reaction of **2-Cl** with AgNTf₂ in Et₂O. Crystals grown from a DCM/Et₂O layer at room temperature. (Thermal ellipsoids at 50% probability; H atoms and co-crystallized DCM molecule omitted for clarity.) Selected bond lengths [Å]: B1–C1 1.555(5), B1–C12 1.611(6), B1–C11' 1.552(5), C12–N1 1.320(5), C4–C5 1.345(5), N1–C12–B1–C1 84.6(4).



Figure S67. Molecular structure of **S6**. Isolated through the reaction of **3-C1** with AgNTf₂ in Et₂O. Crystals grown from a DCM/Et₂O layer at room temperature. (Thermal ellipsoids at 50% probability; H atoms and co-crystallized DCM molecules omitted for clarity; only one of two crystallographically independent molecules shown.) Selected bond lengths [Å]: B1–C1 1.546(4), B1–C12 1.616(4), B1–C11' 1.539(4), C12–N1 1.362(4), C4–C5 1.338(4), N1–C12–B1–C1 106.1(4).



Figure S68. Molecular structure of **S7**. Isolated through the reaction of **4-Cl** with AgNTf₂ in Et₂O. Crystals grown from a DCM/Et₂O layer at room temperature. (Thermal ellipsoids at 50% probability; H atoms and co-crystallized DCM molecule omitted for clarity.) Selected bond lengths [Å]: B1–C1 1.545 (3), B1–C12 1.607(3), B1–C11' 1.531(4), C12–N1 1.341(3), C4–C5 1.366(4), N1–C12–B1–C1 87.3(3).

Theoretical Calculations

All calculations were performed using Orca 5.0.4, unless noted. Geometry optimizations employed the B3LYP density functional, Grimme's D3 dispersion correction with Becke-Johnson damping, and the def2-TZVP basis set, denoted as B3LYP-D3(BJ)/def2-TZVP.¹⁶⁻¹⁸ All optimizations were conducted in solvent via the conductor-like polarizable continuum model (CPCM) with parameters for either Et₂O or *o*-DFB.¹⁹ The resolution of identity approximation was applied to both Coulomb and Hartree-Fock exchange integrals with a 590-point integration grid. To ensure optimized geometries represented a minimum on the potential energy surface, analytical harmonic frequency calculations were performed. ADF 2024.1 was employed to perform the energy decomposition analysis (EDA) at the B3LYP-D3(BJ)/TZ2P level of theory.²⁰ NICS(1)_{ZZ} values were calculated at the B3LYP-D3(BJ)/6-311+G(d)/B3LYP-D3(BJ)/def2-TZVP level of theory. AICD plots were generated using AICD 3.0.4.²¹ Vertical excitations were calculated using TD-DFT at the CAM-B3LYP-D3(BJ)/def2-TZVP/B3LYP-D3(BJ)/def2-TZVP.²²



Figure S69. Frontier molecular orbitals of compound 5–9 at the B3LYP-D3(BJ)/def2-TZVP (CPCM, Et_2O)

	Compound 8	Compound 9
	$2[CDC]$ (Singlet) + $[FBP]^{2+}$	$2[CDP]$ (Singlet) + $[FBP]^{2+}$
	(Singlet)	(Singlet)
$\Delta E_{\rm int}$	-327.0	-401.1
$\Delta E_{ m Pauli}$	+539.5	+630.3
$\Delta E_{ m elstat}$	-347.4 (38%)	-403.4 (39%)
$\Delta E_{ m orb}$	-523.4 (57%)	-548.7 (53%)
$\Delta E_{ m disp}$	-40.8 (4%)	-79.4 (8%)
$\Delta E_{\text{orb}(1)}(+,-)$	-168.2 (32%)	-172.7 (31%)
$\Delta E_{\text{orb}(2)}(+,+)$	-173.2 (33%)	-175.1 (32%)
$\Delta E_{\text{orb}(3)}(+,-)$	-49.7 (9%)	-41.1 (7%)
$\Delta E_{\text{orb}(4)}(+,+)$	-43.4 (8%)	-38.8 (7%)
$\Delta F_{\text{out}}(\text{max})$	-88.8 (17%)	-1211(22%)

Table S3: EDA-NOCV Results for **8** and **9** at the B3LYP-D3(BJ)/TZ2P level of theory (kcal mol⁻¹)



Figure S70. Deformation densities $\Delta \rho_{(1)} - \Delta \rho_{(4)}$ associated with the pairwise orbital interactions $\Delta E_{(1)} - \Delta E_{(4)}$ for compound **8**. Eigenvalues v_i quantify the amount of transferred electron density (red – charge depletion; blue – charge accumulation).



Figure S71. Deformation densities $\Delta \rho_{(1)} - \Delta \rho_{(4)}$ associated with the pairwise orbital interactions $\Delta E_{(1)} - \Delta E_{(4)}$ for compound **9**. Eigenvalues v_i quantify the amount of transferred electron density (red – charge depletion; blue – charge accumulation).

Table S4: NICS(1)_{ZZ} results for carbene-stabilized mono- and diborepinium (B3LYP-D3(BJ)/6-311+G(d,p)).

	Outer annulated phenyl rings	Inner annulated phenyl rings	Borepinium
Monomeric ^{<i>i</i>Pr} NHC-borepinium	-27.6	NA	-9.2
5	-26.2	-27.9	-7.4
6	-26.4	-28.1	-7.5
7	-28.0	-28.5	-9.6



Figure S72. AICD isosurface (0.04) of the π system of 5 (A), 6 (B), 7 (C) at the B3LYP-D3(BJ)/6-311+G(d) level of theory.



Figure S73. Clar structures of 5, 6, and 7. Circles represent aromatic sextets according to Clar's rule.

Cartesian coordinates

Monomeric iPrNHC-borepinium

B	1 608539595602	2 534956142083	-0.043378323223
Č	-1.542485736096	2.419667370396	-0.016506380207
Č	6.277746259463	1.314514131442	-2.666402965623
č	0.711466476351	1.243827057216	-0.007410041005
Ĉ	-0.711466476351	1.222771394915	0.007410041076
Č	2.770981943625	1,737376376310	-2.203497942823
č	5.040009297396	0.650841516253	-2.064565145734
č	1 381107370418	-0.001293072938	-0.000000000281
č	0 440351315901	2 363304479154	-2 956681147470
c	-1 387546116253	-0.019044826210	-0.015818595439
c	0 703360824298	-1 219448379764	0.016303801030
c	-0.696922078462	-1 226812173219	-0.000575205381
c	5 148709456883	-0.870815360066	-1.941861780525
c	3 402660781887	0.536191650074	-4.018239765147
c	2 052012023565	0.00378310/100	4.175447800700
č	4.066520303505	0.186876240265	5 01/502176201
č	1 315738231/21	0.551205400658	5 307546236003
c	2 222762026020	0.551295400058	6 151410200000
C	1 000260025440	-0.337079203329	6 206416284765
C	2 915756962092	-0.1/80390000/2	-0.290410204703
C	2.013/30003902	2.492393392943	-0.984595529825
C	-1.239023813337	5./04959540900	0.309131330024
C	4.2058809/0413	4.584061040305	-4.141912484861
C	1.265334600780	3.80519129/426	0.824965466658
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6 B B C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.5784244443453
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442
6 B C C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.9848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.911455910943
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4 201359051946	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.9848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.02087239051946 -1.083065056055	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4.201359051946 -1.083065056055 -2.270580959768	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 8.119598907390
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.23161177820	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4.201359051946 -1.0830650556055 -2.270580959768 1.663716840197	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 4.504776727620
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4.201359051946 -1.083065056055 -2.270580959768 1.663716840197 0.45308221268	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4.201359051946 -1.083065056055 -2.270580959768 1.663716840197 0.452038221268	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.727514420000
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 - 0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4.201359051946 -1.083065056055 -2.270580959768 1.663716840197 0.452038221268 -0.243943741440 0.24162329(120)	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000
6 B B C C C C C C C C C C	0.707583968541 - 0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065056055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000 -7.903067298273 4.202115225401
6 B B C C C C C C C C C C	0.707583968541 - 0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065056055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000 -7.903067298273 4.303115325401
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 - 0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065055655 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000 -7.903067298273 4.303115325401 -4.676849690409
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 - 0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711 2.635274065797	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065056055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423 - 1.675511743188	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000 -7.903067298273 4.303115325401 -4.676849690409 -4.751314837941
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 - 0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711 2.635274065797 2.819199567251	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4.201359051946 -1.083065056055 -2.270580959768 1.663716840197 0.452038221268 -0.243943741440 0.241623226130 -0.730352076226 4.054057825423 -1.675511743188 2.768719842052	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000 -7.903067298273 4.303115325401 -4.676849690409 -4.751314837941 -5.097946550136
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711 2.635274065797 2.819199567251 2.642736889625	0.474712956502 -0.476730918657 -1.315740088057 3.417648374544 0.284632389535 -2.689422412700 -0.987532174700 -0.987532174700 -0.848186684176 -2.802180380836 2.481161233283 3.087583818912 1.769280900078 -2.510990401158 -1.020872396218 4.201359051946 -1.083065056055 -2.270580959768 1.663716840197 0.452038221268 -0.243943741440 0.241623226130 -0.730352076226 4.054057825423 -1.675511743188 2.768719842052 2.165920485793	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000 -7.903067298273 4.303115325401 -4.676849690409 -4.751314837941 -5.097946550136 1.757412367544
6 B B C C C C C C C C C C C C C C C C C	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.14808330178 2.451981841711 2.635274065797 2.819199567251 2.642736889625 2.792158778137	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065056055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423 - 1.675511743188 2.768719842052 2.165920485793 0.837167831462	-2.860742037043 2.862893215332 0.519690069393 -1.935488158550 -1.384771131502 0.897510366378 -0.822910569806 -3.760135683994 -4.871233114262 4.578424443453 -2.998490209442 -3.443995198902 5.914455910943 5.580682401145 -3.658111051721 -7.141193813484 -8.119598907390 -4.504776272620 3.547952759354 6.757514439000 -7.903067298273 4.303115325401 -4.676849690409 -4.751314837941 -5.097946550136 1.757412367544 2.483642971060
6 BBCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711 2.635274065797 2.819199567251 2.642736889625 2.792158778137 2.917025749213	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065056055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423 - 1.675511743188 2.768719842052 2.165920485793 0.837167831462 - 1.300867146513	$\begin{array}{l} -2.860742037043\\ 2.862893215332\\ 0.519690069393\\ -1.935488158550\\ -1.384771131502\\ 0.897510366378\\ -0.822910569806\\ -3.760135683994\\ -3.760135683994\\ -3.760135683994\\ -3.78424443453\\ -2.998490209442\\ -3.443995198902\\ 5.914455910943\\ 5.580682401145\\ -3.658111051721\\ -7.141193813484\\ -8.119598907390\\ -4.504776272620\\ 3.547952759354\\ 6.757514439000\\ -7.903067298273\\ 4.303115325401\\ -4.676849690409\\ -4.751314837941\\ -5.097946550136\\ 1.757412367544\\ 2.483642971060\\ -6.087453591499\end{array}$
6 B B C C C C C C C C C C	0.707583968541 - 0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711 2.635274065797 2.819199567251 2.642736889625 2.792158778137 2.917025749213 2.954249267730	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065056055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423 - 1.675511743188 2.768719842052 2.165920485793 0.837167831462 - 1.300867146513 2.068192228594	$\begin{array}{l} -2.860742037043\\ 2.862893215332\\ 0.519690069393\\ -1.935488158550\\ -1.384771131502\\ 0.897510366378\\ -0.822910569806\\ -3.760135683994\\ -4.871233114262\\ 4.578424443453\\ -2.998490209442\\ -3.443995198902\\ 5.914455910943\\ 5.580682401145\\ -3.658111051721\\ -7.141193813484\\ -8.119598907390\\ -4.504776272620\\ 3.547952759354\\ 6.757514439000\\ -7.903067298273\\ 4.303115325401\\ -4.676849690409\\ -4.751314837941\\ -5.097946550136\\ 1.757412367544\\ 2.483642971060\\ -6.087453591499\\ 0.257811725852\end{array}$
6 BBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.29226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.985683882515 2.148088330178 2.451981841711 2.635274065797 2.819199567251 2.642736889625 2.792158778137 2.917025749213 2.954249267730 3.330180941273	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.083065056055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423 - 1.675511743188 2.768719842052 2.165920485793 0.837167831462 - 1.300867146513 2.068192228594 - 2.454991011331	$\begin{array}{l} -2.860742037043\\ 2.862893215332\\ 0.519690069393\\ -1.935488158550\\ -1.384771131502\\ 0.897510366378\\ -0.822910569806\\ -3.760135683994\\ -4.871233114262\\ 4.578424443453\\ -2.998490209442\\ -3.443995198902\\ 5.914455910943\\ 5.580682401145\\ -3.658111051721\\ -7.141193813484\\ -8.119598907390\\ -4.504776272620\\ 3.547952759354\\ 6.757514439000\\ -7.903067298273\\ 4.303115325401\\ -4.676849690409\\ -4.751314837941\\ -5.097946550136\\ 1.757412367544\\ 2.483642971060\\ -6.087453591499\\ 0.257811725852\\ -2.406547089175\end{array}$
6 BBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711 2.635274065797 2.819199567251 2.642736889625 2.792158778137 2.917025749213 2.954249267730 3.330180941273 3.188159062130	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.0830650556055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423 - 1.675511743188 2.768719842052 2.165920485793 0.837167831462 - 1.300867146513 2.068192228594 - 2.454991011331 - 1.577850126590	$\begin{array}{l} -2.860742037043\\ 2.862893215332\\ 0.519690069393\\ -1.935488158550\\ -1.384771131502\\ 0.897510366378\\ -0.822910569806\\ -3.760135683994\\ -4.871233114262\\ 4.57842443453\\ -2.998490209442\\ -3.443995198902\\ 5.914455910943\\ 5.580682401145\\ -3.658111051721\\ -7.141193813484\\ -8.119598907390\\ -4.504776272620\\ 3.547952759354\\ 6.757514439000\\ -7.903067298273\\ 4.303115325401\\ -4.676849690409\\ -4.751314837941\\ -5.097946550136\\ 1.757412367544\\ 2.483642971060\\ -6.087453591499\\ 0.257811725852\\ -2.406547089175\\ 3.897944849102\end{array}$
6 BBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	0.707583968541 -0.709468797049 0.202053273562 0.015482830816 0.275871203938 0.453204119779 0.455196250059 0.464790455918 0.434922151060 0.853377434995 0.947580964653 1.292226631989 1.248717715118 1.364933192653 1.520061012739 1.834480120531 1.802947417612 2.223161177820 1.952562916958 1.985415092540 1.986083882515 2.148088330178 2.451981841711 2.635274065797 2.819199567251 2.642736889625 2.792158778137 2.917025749213 2.954249267730 3.330180941273 3.188159062130	0.474712956502 - 0.476730918657 - 1.315740088057 3.417648374544 0.284632389535 - 2.689422412700 - 0.987532174700 - 0.848186684176 - 2.802180380836 2.481161233283 3.087583818912 1.769280900078 - 2.510990401158 - 1.020872396218 4.201359051946 - 1.0830650556055 - 2.270580959768 1.663716840197 0.452038221268 - 0.243943741440 0.241623226130 - 0.730352076226 4.054057825423 - 1.675511743188 2.768719842052 2.165920485793 0.837167831462 - 1.300867146513 2.068192228594 - 2.454991011331 - 1.577850126590 - 1.962309480414	$\begin{array}{l} -2.860742037043\\ 2.862893215332\\ 0.519690069393\\ -1.935488158550\\ -1.384771131502\\ 0.897510366378\\ -0.822910569806\\ -3.760135683994\\ -4.871233114262\\ 4.57842443453\\ -2.998490209442\\ -3.443995198902\\ 5.914455910943\\ 5.580682401145\\ -3.658111051721\\ -7.141193813484\\ -8.119598907390\\ -4.504776272620\\ 3.547952759354\\ 6.757514439000\\ -7.903067298273\\ 4.303115325401\\ -4.676849690409\\ -4.751314837941\\ -5.097946550136\\ 1.757412367544\\ 2.48642971060\\ -6.087453591499\\ 0.257811725852\\ -2.406547089175\\ 3.897944849102\\ -3.809169978930\\ \end{array}$

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$ \begin{array}{c} \textbf{c} \begin{tabular}{ll} $$ 1.0013322.4483 + 0.4402165.569 \\ \hline begin{tabular}{ll} $$ 1.0013322.4483 + 0.4402165.569 \\ \hline begin{tabular}{ll} $$ 1.0013322.4483 + 0.4402165.569 \\ \hline begin{tabular}{ll} $$ 1.0013322.4483 + 0.1376216922 \\ \hline begin{tabular}{ll} $$ 1.0013322.4483 + 0.1376216922 \\ \hline begin{tabular}{ll} $$ 0.00234112 \\ \hline begin{tabular}{ll} $$ 0.002341112 \\ \hline begin{tabular}{ll} $$ 0.00234112 \\ \hline begin{tabular}{ll} $$ 0.00234112 \\ \hline begin{tabular}{ll} $$ 0.002341112 \\ \hline begin{tabular}{ll} $$ 0.0023411112 \\ \hline begin{tabular}{ll} $$ 0.0023411112 \\ \hline begin{tabular}{ll} $$ 0.00244111112 \\ $	C	4.00940394/302	-1.244525455499	2.821512251070	п	3.413420078440	-1./54606651650	-0.340003853855
$ \begin{array}{c} \textbf{L} 0.2000 \\ \textbf{L} 0.2$	C	4.265185501001	-1.165153227445	-6.440261565796	Н	3.648643432039	-4.56930/082313	-2.881/89525981
$ \begin{array}{c} c \\ c$	C	4.9/1065/10/52	-1.796835347529	-4.215271614829	Н	3.369/52246967	-2.504342895449	4.44288/21513/
$ \begin{array}{c} C & 0.203999394102 & 1.31(645109685 & 0.519393554761 & H & 3.342048255181 & 3.36871560600 & 0.077452065702 \\ C & 0.20234116406 & 2.66472030841 & 0.807745314022 & H & 4.0914146533 & 1.951937981040 & 0.077452065702 \\ C & 0.464434906 & 2.6647200841 & 0.807915357 & H & 4.925270425 & 0.2119475571 & 1.3135374615 \\ C & 0.46616530903 & 0.848877238146 & 3.758534920334 & H & 4.83846760734 & 1.04038905758 & 1.3330274675 \\ C & 0.46616530903 & 0.848877238146 & 3.758534920334 & H & 4.83846760734 & 1.04038905758 & 1.33302187884 \\ C & 0.4585571603511 & 2.474840188565 & 4.990181406796 & H & 5.06038766282 & 3.77801500293 & 2.5294756540 \\ C & 0.458477678 & 2.521307975 & 5.59165282484 & H & 5.37660571085 & 1.998332236488 & 2.504076973865 \\ C & 1.24355044788 & 2.521307975 & 5.5916282484 & H & 0.28149831503 & 4.47016304137 & 5.89872309811 \\ C & 1.32894169338 & 1.0201910607 & 5.5826558411 & H & 0.828149831563 & 4.47016304137 & 5.89872309811 \\ C & 1.328591669930 & 1.10241327182 & 7.14645366594 & H & 0.38101735108 & 0.61443023189 & 5.5846622019 & 1.4537497049601 \\ C & 1.324591649391 & 4.0201921353 & 8.1202649511 & H & 0.8484773 & 1.07326087348 & 6.3090414530 \\ C & -1.972448771 & 0.2752497345 & 5.5146472701 & 4.5292714980 \\ C & -1.972448771 & 0.2752497348 & 7.14645366594 & H & 0.548017073786 & 5.884562092 \\ C & -1.972448771 & 0.275249738 & 5.74447770 & H & -0.84844731 & 0.74724070 & 8.84445622092 \\ C & -1.972448771 & 0.275249738 & 5.74447770 & H & -0.84844771 & 0.72782087348 & 6.439094157 \\ C & -1.972448771 & 0.27514744779 & 0.2555845417 & 1.97871474789 & 2.55989070584 & 6.309907444570 & 8.444556992 \\ C & -1.972487219799 & 0.255573434 & -1.99701702 & H & -0.86443500143 & 3.097169245734 & -0.859875858 \\ C & -2.497763643537 & -0.3859837836 & -2.49469955106 & H & -0.7874720708 & 8.44856567921 \\ C & -2.4972484871 & 0.57577148 & H & -2.2376984872 & 0.4978731266 & -2.2378947744 & -2.2376989474 & -2.3775740584 & -2.2379744444 & -2.2376989474 & -2.3775740584 & -2.39797414644 & -2.23769894774 & -2.23769894974 & -2.377574918 & -2.37757497$	С	5.282001677089	-1.393972145155	-5.511837982308	Н	3.663668805868	-4.189379196743	-1.137764450862
$ \begin{array}{c} C & -0.22331 (67224 & -1.42128059945 & 1.936673324022 \\ \hline -0.282057940 & -0.2821029740 & -0.282102978104 & -0.0743059021 \\ \hline -0.4621513230 & -0.9807080173 & -0.2819052217 \\ \hline -0.4621513230 & -0.9807080173 & -0.2819052217 \\ \hline -0.4621513230 & -0.9807080173 & -0.2819052217 \\ \hline -0.4621513293 & -0.9807080173 & -0.2819052217 \\ \hline -0.4621513291 & -0.980708173 & -0.2819052217 \\ \hline -0.4621513291 & -0.980708173 & -0.2819052217 \\ \hline -0.4621513291 & -0.980708130 & -0.3807329102217 \\ \hline -0.4621513291 & -0.98081854 & -4.8618140400 \\ \hline -0.4555171091 & -0.98081854 & -4.8618140400 \\ \hline -0.4555171091 & -0.9808022 & -0.918140400 \\ \hline -0.4555171091 & -0.9808022 & -0.918140400 \\ \hline -0.3808123090775 & -5.91102262144 \\ \hline -1.25984200718 & -0.9831220484 \\ \hline -0.320812009918 & -0.0190070 & -5.82520584413 \\ \hline -0.320812009918 & -0.0190070 & -5.82520584413 \\ \hline -0.320812009918 & -0.0190070 & -5.82520584413 \\ \hline -0.28149493090 & -0.019077 & -5.8254536549 \\ \hline -1.859910007 & -5.82545365694 \\ \hline -0.8804215128 & -7.1049435366594 \\ \hline -0.88042574519 & -0.4481850933 & -3.55878417511 \\ \hline -0.86442574519 & -0.86442574519 & -5.834902234112 \\ \hline -0.942457970515 & -0.4481850933 & -3.55878417511 \\ \hline -0.94245797056 & -1.66301215 & 4.51999031044 \\ \hline -0.94042773 & 6.7694117302 \\ \hline -0.944359705151 & -0.44818569933 & -3.55878417511 \\ \hline -0.86442574519 & -0.86442574519 & -0.86445201 \\ \hline -0.942457970150 & -0.7951113 & 4.519904777 \\ \hline -1.9451457845 & -0.98701057 & -5.79511173 \\ \hline -0.94418720 & -0.86442574519 & -0.86442574519 \\ \hline -0.942152820 & -0.7686424 & -4.901175616 \\ \hline -0.9802214974480 & -0.8844560133 & -0.86442574519 \\ \hline -0.942152820 & -0.7686424 & -0.9801776 \\ \hline -0.942152820 & -0.7686424447700 \\ \hline -1.9429457571 & -0.948417710 \\ \hline -0.942152820 & -0.7678444441710 \\ \hline -0.94215299910290 & -0.2178791442477 \\ \hline -0.942152820 & -0.7685864 & -0.9801772 \\ \hline -0.942152820 & -0.7678485 & -0.9871714643 \\ \hline -0.930225991130 & -0.218797814 & -0.278177200 \\ \hline -2.94054383580 & -0.4625214648 & -0.981721700 \\ \hline -2.940542839970400 & -1.93178052 \\ \hline -2.9407439830 & -0.957814643 & -0.$	С	-0.209793934102	1.311645109658	-0.519393554761	Н	3.342048255181	3.368715606001	3.475266462712
C -0.258237594790 -0.258320549175 1.3854941323 II 4.40341446533 1.9519378104 007743200521 C -0.464345206016 2.64787950817 -0.87879871537 H 4.42523745423 0.1379494520 1.313052714679 C -0.4661453072927 2.80686552015 4.462280645510 II 4.46824057024 1.34104805578 -1.3230218784 C -0.46493872927 2.80686552015 1.24744801865 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.590114865 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.5901148656 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.590114865 -4.59011486 -4.5901 -4.59014868 -4.590114978361 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -4.5901498930 -5.584147310 -4.88014993158 -4.5901498930 -5.584494173302 -4.59054869 -5.584494173302 -4.59054869 -5.584494173 -4.90149149893 -5.585449417 -5.585686993 -5.58544158 -5.980149830 -2.62794484272959 -2.570548451 -5.9912381944 II -0.54201478736 -2.659787010577 -0.49811471362 -2.4394491893 -4.0375256343 -4.390017195616 H -0.98423348873 -1.07424692398 -4.553254515 -9.910238746 -4.300197195616 H -0.98423348873 -1.07424692398 -4.550556634 -4.300017195616 H -0.98423348873 -1.07424692398 -4.550545830 -4.2494177370 II +0.54304473730 -4.505550048 -4.825978100 -7.57147417632 -2.4394048939 -4.5057563043 -4.430017195616 H -0.9842344887 -5.0558656792 II -2.4394048938 -0.3425721380 -0.224552230 -7.676864878 -2.439177106 H -0.85823948917 -2.505593459 -4.571714821 -2.4393149838 -0.4327575614 H -0.425344484 -3.0918721606 -1.87833947312 -2.4393448873 -3.09176461378 H -2.52591810 -7.57174394 -2.591252344 -2.439157561 -4.8259714444 -2.591252404898	С	-0.023431167224	-3.421288059945	1.936873324022	Н	3.399309113973	4.208023659952	1.904740663705
C -0.462193293 0.95300537 0.25219305217 1 4.422249784238 0.21139494925 7.45931464515 -0.46616530993 0.84887739514 5.375335490234 H 4.83894760724 -1.30403805578 -2.2994255540 -0.43694372972 2.8068552015 4.65205015 -0.55505015 2.2994255540 -0.201972 -0.20197884 4.59014406515 -0.5950603706252 -0.373015060923 -0.213054756201 -0.225424520515 -0.55505401 -0.225424520515 -0.25505400 -0.25754560 -0.2575457252 -0.46481575660 -0.2575457540 -0.257547571 -0.257547571 -0.457457541730 -0.257545701057 -0.575571130 -0.481825741730 -0.2575475471 -0.2575900578 -0.441825491770 -0.257547464 +0.20771924773 -0.25759701057 -0.579571130 -0.257547464 +0.257547173 -0.2575568191 -0.2575474574 -0.2575568702 -0.25754574474 -0.25754744770 -0.8544550 -0.257547444 +0.2575474470 -0.8544550 -0.257547444 +0.25754744 +0.25754744 +0.257547444 +0.257547444 +0.25754744 +0.257547444 +0.257547444 +0.257547444 +0.257547444 +0.257547444 +0.257547444 +0.25754744 +0.257547444 +0.25754744 +0.25754744 +0.2595907056 +0.2571474270 -0.854455690 -0.25754944757 -0.2585907056 +0.24492708 +0.45754714021 -0.2595490756 +0.25754744 +0.2595490756 +0.25754744 +0.2595497510 +0.2595491754 +0.2595491754 +0.2595497545 +0.25754744 +0.2595491754 +0.2595497545 +0.25754444 +0.2575444	С	-0.282037594790	-0.288320549175	1.385449413243	Н	4.034141465353	1.951937981044	0.077432005021
C -0.4615132933 -0.87304873905 -0.87304873905 -0.8730487390578 -1.32081406155 C -0.4661530511 -2.4740818566 4.5022061057 -2.595060203 2.12994255440 C -0.85557106311 -2.4740818566 4.5022061072 2.95368021057 2.23904255440 C -0.8555710632 -1.7208420022 3.161026554411 1 5.77406571085 -9.97332122488 3.20047973865 C -1.23984203202 -1.7308450022 3.5102548411 1 -0.82021034566 -9.9832122488 3.50079775 5.91160445177 C -1.3598166014 1.101016607 5.2525584113 1 -0.28021034566 1.91855077 6.749511471302 C -1.359815659993 -1.5589850735 3.57879477101 1 -0.82021034566 1.5291427188 6.46300444320 C -1.9631579515 -0.4641271559 3.13897071072 1 -0.8430478773 6.263789700708 8.4445620902 C -2.43904498047 -0.7375206234 -3.09071797072 1 -1.1294314988 0.32497764444 8	С	-0.463442849605	2.684789506817	-0.897989715537	Н	4.492249784283	0.211394949520	1.313295274679
C -0.464105300993 0.44887229814 3.758354920324 H 4.838946700724 -1.30403009578 -1.32002187844 C -0.4504937272 2.6056550115 4.520181405796 H 4.605038766222 -3.773015006032 -2.90548720102 -2.230214468089 -2.22417306623 -2.231204146809 -2.22417306623 -2.231204146809 -2.22417306623 -3.773015006032 -1.908332242747313 -1.998332224173184 -3.504779735 -5.162534813 H -0.234414981310 -3.0271448501870 -5.60273708911 C -1.31652348131 -0.23414983150 1.224475447153 -3.546464015766 -3.546444175 -3.5414474744989 -3.5464464177 C -1.36145341114 2.29194145306 1.42653464544 H -0.3341071747 -6.567840454495 5.346464495 5.346464495 5.346464495 -5.3454471184320 C -1.3614537161 -0.44185534417711 H -0.84435404873 1.0742568744474 6.61600443200 C -1.3614597161 -0.43155977013 4.7397381477511 H -0.8453444773 1.07425678744771 -0.754755618444	С	-0.462159132933	0.983608203737	0.823193052217	Н	4.523284587935	-0.873048793005	-7.459814646515
C -0.430938729927 2.800865520157 4.8622866450 H -0.6062876628 -2.95360201257 2.95360201257 2.95360201258 2.95047582010 C -0.43557460738 -1.720842018856 4.5016208871 H 5.770415060923 2.1504758201 C -1.2389420382 -1.75084506229 3.5162368841 H 6.32638039938 -1.27144830150 -5.80872378911 C -1.3508456890 1.1012171285 7.1445336594 H 0.33141735509 0.60143022813 -5.54549061576 C -1.8259416890 1.1012171285 7.14453365914 H 0.82414735108 0.66143022813 5.354741711 C -1.95443875515 0.44818556933 3.555878417511 H -0.864423745159 0.65798701077 6.73598701077 6.73598701077 6.7362807446 0.8325447768 6.4004943520 C -1.974428717 -0.35545670921 H 0.35080717018 H 0.83776481 6.3024997434 6.055568670921 C -1.974428717 0.3508074170 7.30539997101072 H 1.1294344873 <td>С</td> <td>-0.466165369093</td> <td>0.848877298345</td> <td>3.758354920324</td> <td>Н</td> <td>4.838946760724</td> <td>-1.304038095578</td> <td>-1.323002187884</td>	С	-0.466165369093	0.848877298345	3.758354920324	Н	4.838946760724	-1.304038095578	-1.323002187884
C -247340188563 -4590181406796 H 5.06603876622 -377301500023 -215954782010 C -0344411773 -3.098561195 3.0582805371 H 8.1297466731 -92211446889 -25220186828 -3.5047673855 C -124555046758 -252139933 3.67162028248 H 6.363693938 -1271485501870 -5.80273708911 C -1350534819 -0.2314193505 8.126204584 H -0.236309398 -0.66180120157 -19485474747049691 C -136163248819 -0.23141931530 8.12620495017 H -0.8644107376 2.657840154495 5.3546496015766 C -19631575015 -0.4481559933 -555878417511 H -0.826443060143 0.0716924672 -5555687092 C -19631557280 -0.222845116 -0.1013727048 H -0.85443064473 0.0716924672 -555687092 C -2.4396491890 -0.355206329 -7576667822 -17791317048 H -23555889177 -505595070508 -55756670921 C -2.4396491820 -0.2555849177 </td <td>С</td> <td>-0.436938729927</td> <td>2.806865520157</td> <td>4 862280645510</td> <td>н</td> <td>4.604220501057</td> <td>2,953680201526</td> <td>2,299342565440</td>	С	-0.436938729927	2.806865520157	4 862280645510	н	4.604220501057	2,953680201526	2,299342565440
C -0.94441177933 -3.098351618109 3.0042380571 H 4.812974667913 -1.9220143889 -2.52240780023 C -1.238453046758 -2.521380790775 -5.911622062484 H 5.736657105 -9.9833322488 -5.0007907865 C -1.3583660994 1.0201790607 -5.855584113 H -0.24149831505 -4.70163048127 -9.983332488 C -1.8250460950 1.1021171282 7.14645366594 H -0.38140755078 -6.661430228139 -5.54649061576 C -1.8250460950 1.10241271282 7.14645366594 H -0.38140753078 -6.661430228139 -5.54649061576 C -1.97244827299 0.2559547012715 7.1909331944 H -0.864435049177 -0.74234087348 -6.3409418500 C -1.9724484717 0.55558670921 1.0172423087348 6.4090418520 -2.3479764446 8.25797610377 -5.05556870921 C -2.41797464877464 N.0552228211 4.0701770148 H -2.85197617070 -3.25490770444 N.057247008 N.879703461 C	č	-0.855571603511	-2 474840188565	-4 590181406796	н	5 066038766282	-3 773015060923	-2 150547582010
C -128984203382 -17054986292 1.451620628474 H 6.35268059108 -12953235488 -350407973865 C -1235591691894 1.00199106607 -5.58265584113 H -0.25414981505 4.2704580127 -193160144517 C -135085691984 1.00199106607 -5.58265584113 H -0.25414981505 4.2704580127 -193160144517 C -1352591698950 1.102413271825 7.14645536594 H -0.33410735078 0.6613928139 -5.45696015766 C -183084201314 2.2919912350 8.125204965017 H -0.84423745159 0.66139738 0.66139211471302 C -193259716511 -0.4481556993 -3.55878417511 H -0.82971924971 -233958591641 -0.182544171683 C -1974348727959 0.25953492738 -6.76440347701 H -0.8493348473 1.07423097348 6.64390044350 C -243964198028 -0.05282831 -4.07013278198 H -0.8443360134 3.097169246724 -5.05556867021 C -243964198028 -0.05282831 -4.0701327048 H -0.9802704488 0.218074464 8.62371166523 C -243964198028 -0.25887824 5115 7.91013381964 H -0.9802704488 0.218074464 8.62371166523 C -243964198208 -0.05288782 5.117959113048 H -1.3781379483 -0.342697348 6.6439004350 C -240762399061 -216584738164 -1.770523573488 H -1.788179442777 -2.27016630798 4.383947312 C -230504419 -2.06987825 5.117959113048 H -1.37813794647 8.263799707444 8.82271166523 C -2305044419 -2.069877384 6.0707172784 H -1.913937396160 H -0.4770170661 3.8704 -4.3879473456 C -2305053057 -0.8359787858 -244659955100 H -1.67470170661 -0.187064138704 -3.249814791492 C -239006135057 -0.83571557 -0.90351592833 H -1.60165214645 -2.491817492 C -239006143507 -0.325927314 -0.2707714464 H H -1.913937391616 -0.87064138704 -3.27981474782 C -23900612464597 -0.07351255 -2.40633860096 H -2.407470170611 -0.187064138704 -2.4781479475 C -2390204449 -2.00897583024 -4.82787940948 -2.49124842452 C -3309244494 -2.40984978148 -3.49181742277 B -2.4005365280624 -2.8289211745 C -3392374444 -2.4048595510 H -2.4782195974 -2.4405648378 -4.35061498709 C -3392374449 -2.40494594505 -1.91778079007 H -2.74822197974 -2.4405683063 -7.728120281848 C -33072452445345 -0.01797714565 H -2.4491771900 H -2.6427371496 -2.34981248454 C -3.40427854949 -0.0767444574 -3.24918185657	c	-0.948441177933	-3 080536181105	3 005428305371	н	4 812974267913	-1 922014468899	2.130347382010
$ \begin{array}{c} C & 1 = 2 + 3 + 5 + 3 + 5 + 3 + 1 + 1 + 2 + 3 + 5 + 3 + 1 + 2 + 3 + 5 + 3 + 5 + 3 + 3 + 5 + 3 + 3 + 3$	č	1 2808/2303382	1 7705/0806202	3 451632068874	и П	5 774660571085	1 008337376488	3 50/076073865
$ \begin{array}{c} c & 1.2588.50 + 1.2518.500.907.0 \\ c & 1.2508.500.993.0 \\ c & 1.2201.994.1235.0 \\ c & 1.2201.993.1131.4 \\ c & 1.292.994.1235.0 \\ c & 1.2201.993.1131.4 \\ c & 1.924.393.0 \\ c & 1.924$	c	1 242550446759	-1.770349800292	5.011602602404	11	6 226280200208	1.271449501970	5 909722709011
$ \begin{array}{c} c & -3.538.50091984 \\ c & -1.5016238811 \\ c & -3.538.500919845 \\ c & -1.516238811 \\ c & -2.5209169850 \\ c & -1.520210343861 \\ c & -2.5209169850 \\ c & -1.520210343861 \\ c & -2.5209169850 \\ c & -1.5018432111 \\ c & -2.91114 \\ c & -2.911144 \\ c & -2.9111444 \\ c & -2.911144 \\ c & -2.911144 \\ c & -2.911144 \\ c & -2.91114$	C	-1.245550440758	2.321380/90/73	-5.911092082484	п	0.320360399396	-1.2/14463016/0	-3.808/23/08911
C -1.81209169890 1.102432171823 3.06/10/94137449 H +0.820/24054499 1.9482.06/2039 1.43/49/049691 C -1.82080169890 1.102413271825 7.14645356594 H -0.8442374519 3.65748045449 5.383492234112 C -1.934389705151 -0.44818556933 -3.55587817511 H -0.824127713 2.2557987010577 -6.7495111471302 C -1.934389705151 -0.44818556933 -3.55587817511 H -0.84933488737 1.07425067373 6.6633904443520 C -2.41797480417 0.7357506324 -3.030017195616 H -0.98022704480 2.180746747 -5.055568670921 C -2.43954918208 +0.0526228211 4.677013727048 H +1.22536884917 -5.25559870508 3.35080151377 C -2.4517951827 1.6739077013 -7.70533571488 H +1.27330584963 0.41225591810 -7.6747551166321 C -2.46376239006 -2.6589473816 -1.775239771072 H +1.27831744477 -2.97016630708 -4.858794703461 C -2.46475239006 -2.6589473816 -0.20751458 H +1.37730634963 0.41225591810 -7.67475261398 C -2.94107484597 1.30705214757 6.300511557 6.300511578 H -1.674701706013 3.25306390707 0.597147478392 C -2.99105444497 -1.3075014757 6.3005315592833 H +1.617401760613 3.25308290760 -5.877147478392 C -3.910054920960 -1.58153372157 -3.905407897878 H -2.25602210648 2.49181727106 -1.875833947512 C -3.910054920960 -1.58153372157 -3.90540789787 H -2.25602210648 2.4981872106 -1.87583947512 C -3.94023828111 -9.48779440 8.3102577765 H -2.240333860054 -0.82678949475 -5.571714748213 C -3.542942854110 -0.325349273065 H -2.4442650548 -2.49818727106 -1.87583337551 C -3.54297284548 0.047771393 -7.217693097 H -2.8733104553 -4.977051864912 -4.8778131375 C -3.54292745100 -3.25324877 2.12778079097 H -2.8733104553 -4.9879811754 5.173757912021 C -3.44192578310 -0.427213282 -2.832108985170 H -2.244225614413 -2.2988911754 5.173757912021 C -3.44195785334 -1.24527213022 -1.4795350966 H -2.4442563053 -4.98267841474 -0.198182897 C -3.98812444857 1.034394269015 1.35534125785 H -2.240234858 -4.79839117545 5.173757912021 C -3.44195785334 -4.247034818652 H -3.3005429644 +1.2222648147 C -3.981044874 -1.249548787 2.44764958787 1.941898498 C -4.977144852489 -1.97771498 -4.849471892 C -3.988124484877 1.249548787 1.44954877	C	-1.359836691984	1.030199106607	-5.582655844113	Н	-0.284149831505	4.4/016304812/	-1.9316034451//
C -1.820901098950 1.10241327182 7.149453566594 H -0.324107353078 0.661492819 -5.456499015766 C -1.80484071314 2.29199412530 8.125624965017 H -0.84642374159 3.65784054495 5.383492214112 C -1.95435976151 -0.4481556993 3.55587817511 H -0.8201292471 3.23590857161 -0.18254117683 C -1.974248272595 0.255953492738 -6.764403477701 H -0.84642376143 3.09716924671 -0.82564724 C -2.43964189208 -4.0552822821 4.23907371072 H -0.86443250043 3.09716924671 -0.855670921 C -2.4396419208 -0.5558407318 - 4.709013727048 H -1.223565849480 - 5.83597764472070 8.844456269902 C -2.4396419208 -4.05566087822 5.119759113048 H -1.788179442777 - 2.97054637008 -4.838794703461 C -2.26530435057 0.8359873887856 - 2.4465995106 H -1.67470176061 3.250369270508 -4.838794703461 C -2.29596133057 0.8359873887856 - 2.4465995106 H -1.67470176061 3.2503692770540 + 7.59714778292 C -2.991004846597 1.307052014757 6.09351592833 H -1.601652514645 -2.491864747 -2.51775568473146 -1.77052373458 H -1.67470176061 -1.08706413870 + 7.5571477829 C -2.991004846597 1.307052014757 6.09351592833 H -1.601652514645 -2.49878949475 - 6.57171402213 C -3.91004846597 1.307052014757 6.09351592833 H -1.601652514645 -2.49878949475 - 6.571771402213 C -3.91004846597 1.307052014757 6.09351492785 H -2.20805260449 2.582229811 2.336010321446 C -3.462283811 1.948787794408 3.81302577655 H -2.949503581 -0.677061689412 4.87783133765 C -3.9927641192 -0.39534122284 C -3.99276411284 3.9022448587 - 2.417593530966 H -2.4245630643 -1.22226461473 1.919180497862 C -3.98276411284 3.9022448587 -2.417593530966 H -2.42452464374 1.919180497862 C -3.98276411284 3.9022448587 -2.417593530966 H -2.42452464372 -2.919263889381 -0.67161689412 4.87781337651 C -3.9427641284 -1.425272138928 -2.821108958170 H -2.643544441360 -2.9869244643 -3.906489484 -3.8106257192021 C -3.98276411284 3.90244575 -1.437306146127 H -3.424921442350 -4.928971484441360 -2.98697204437 H 0.85222507961 -2.64437649115 6.75644607312 H -3.4269891424 -3.306168622 C -3.927374126430 -1.76759845 -3.4473705104 H -3.426973528	C	-1.516253488319	-4.2023/2139533	3.6/0/9413/449	Н	-0.820230534569	1./91856262059	1.45/49/049691
C -1.804840131314 2.29199412350 8.122624965017 H -0.8430147573 2.65798701657 -6.749511471302 C -2.21207945365 -1.65601291155 4.519990331944 H -0.84301487571 2.256798701657 -6.749511471302 C -1.95435976515 -0.44818556933 -3.55587817017 H -0.84933484737 1.074236087347 6.749511471202 C -1.954359755154 -0.42224265115 -7.91023351964 H -0.84933484737 1.074236087348 6.643090443520 C -2.44976480417 0.7357506324 -3.0901719561 H -0.98022704482 0.21807464720 8.84445629002 C -2.439649189208 +0.0562225211 4.697013727048 H +1.225365884917 -5.20559070508 3.35080151377 G -2.950751827 1.673909077013 4.73999701702 H -1.2943314983 -0.32459776444 8.62371166521 C -2.6407629906 1.2.6584738164 - 1.770323571348 H -1.377306384963 0.41928591810 -7.675475261398 C -2.9616434597 1.3075201457 6.0951559383 H -1.6774170150613 3.225092070 7.597147478392 C -2.99106444597 1.3075201457 6.0951559383 H -1.67701760163 3.2508920760 7.597147478392 C -2.95092364419 -2.06989277381 -0.27077144643 H -1.931937396166 -1.087064138704 -7.23212023208 C -3.341902795263 2.43417528215 2.4063350006 H -2.2650220644 -2.265177149631 2.236010521445 C -3.466253400 3.94924906 1.51534121258 2.4063380096 H -2.4942630643 -2.2981151 2.316010521445 C -3.45462883811 1.94878779408 3.81302577655 H -2.49053835881 -0.67701688412 4.87781337651 C -3.359494961 1.91853421225 2.417693530906 H -2.47331048526 2.9512628397 -6.21829710688 C -3.257812288794 1.94878794408 3.81302577655 H -2.49353835881 -0.67701688412 4.87781337651 C -3.358494961106 -3.23505383213 -2.417693530966 H -2.4426306434 -2.222106168941 2.487781337651 C -3.358494961156 -3.23505439213 -2.417693530966 H -2.4426306434 -2.2987983166 -2.9405998579 C -3.388161284548 0.04372751307 -2.149547772900 H -2.482731448540 -2.989787316 -0.246472885 C -4.27741264 3.8022744873 1.3376514 -4.347304583 -4.935981755 -4.2189797192021 C -3.388161284548 0.04372751307 -2.149547772900 H -3.2452444432 -0.938236565 3.95596565427 C -3.27812288791 1.38249771393 5.524159353652 H -3.30296127041 -2.9897831366 5.3566967563 C -4.25741646314 1.166220324	С	-1.825091698950	1.102413271825	7.146455366594	Н	-0.334107353078	0.661430228139	-5.456496015766
$ \begin{array}{c} C & -2.212104953656 & -1.663601291155 & 4.519909331944 & H & -0.543014787736 & 2.657987010577 & -6.749511471302 \\ C & -1.954128727595 & 0.255953492738 & -6.764403477701 & H & -0.82071294773 & 2.35796859164 & -0.182541171683 \\ C & -1.974248272858 & 0.2528240 & -1.2558578471511 & H & -0.84643360043 & 3.09716924672 & -0.856567021 \\ C & -2.4396419208 & 4.0562228281 & 4.07013727048 & H & -1.2253658494076472070 & 8.844456209902 \\ C & -2.4396419208 & 4.05566087822 & 1.19759113048 & H & -1.22356858406 & 0.41928591810 & -7.657457361398 \\ C & -2.6350405290 & -2.7656640782 & -1.07052373458 & H & -1.788179442777 & -2.970166307098 & 4.83794703461 \\ C & -2.97056435057 & -0.8397878563 & -2.94459955106 & H & -1.64740176061 & 3.2503662970 & 7.59714478292 \\ C & -2.99100446597 & 1.307052014757 & 6.09351592833 & H & -1.67470176061 & -1.08706113877 & 7.59714747292 \\ C & -2.9906435057 & -0.839778164 & -1.77052377458 & H & -2.9875658064 & -0.870641377 & 7.597147478292 \\ C & -3.900544499 & -0.989277381 & -0.270774146433 & H & -1.60162514645 & -2.948949475 & -6.571771405213 \\ C & -3.64026838111 & -9.87371498 & -9.9540497978 & H & -2.90575658064 & -0.827061689412 & 4.87783133765 \\ C & -3.75827453040 & 1.349426015 & 1.36534121228 & H & -2.9053825881 & -0.6701689412 & 4.8778133765 \\ C & -3.75827453040 & -3.93054394778 & -2.147593530966 & H & -2.4492639643 & -2.9225641475 & 0.195180497862 \\ C & -3.92674112864 & 3.08222448857 & 2.14778079007 & H & -2.63731448563 & -4.9797381165 & -2.14959777085 \\ C & -3.75827453104 & -1.44749248505 & -1.44759774 & 2.34676611078 & 8.65927700483 \\ C & -3.75827453104 & -1.4475971397 & -2.149594777200 & H & -2.64324414160 & -2.99778134656 & -2.94063908859 \\ C & -4.9774521897 & -1.247597144 & -1.425361284441450 & -2.99778134650 & -2.95921864888 & 4.8710361862 \\ C & -3.7582747112864 & -0.42727183987 & -1.43730616417 & H & -3.0703232137 & -0.40837770689 \\ C & -3.7582747128457 & -1.2475718198 & +3.22926127009 & -2.929218648383 & -9.5983750666 \\ T & -2.748524497177 & -2.447594777199 & -1.45730614447 & -3.249$	С	-1.804840131314	2.291994125350	8.122624965017	Н	-0.864425745159	3.657840454495	5.383492234112
C -1.943459765151 -0.44818556933 -3.555878417511 H -0.882071924971 3.235968591641 -0.182544171683 C -1.942145228820 -0.222842651156 7.910233851964 H -0.864433600343 3.007169246724 -5.055568670921 C -2.2147974680417 0.7357206234 -3.030017195616 H -0.98022704880 2.18074647207 8.844456269902 C -2.439649189208 -4.05362228211 4.07301727048 H -1.12243149838 -0.324507705464 8.623711666321 C -2.636710571827 1.673900777013 + 4.753997071072 H -1.12943149838 -0.324507705464 8.623711666321 C -2.636710571827 1.673900777013 +75399701702 H -1.27343684963 0.3245070598 -4.8879403461 C -2.647476239961 -2.165894738164 -1.77052357488 H -1.788179449777 -2.970166031098 -4.8879403461 C -2.9590544419 -2.066982773814 -0.270774146443 H -1.93193736106 -1.087064138704 7.25212025208 C -3.3190549060 1.5815371576 -0.93515592833 H -1.60162514645 -2.491817271696 -1.875833947512 C -3.390249060 1.5815371575 -3.9054097878 H -2.2602216455 -2.491812721606 -1.875833947512 C -3.3054092060 1.5815371576 -3.90540479878 H -2.2602216455 -2.491812721666 -1.875833947512 C -3.549493611060 -3.25505898213 -2.47603330966 H -2.44054503 -4.257824097 -6.571771140213 C -3.549493611060 -3.25505898213 -2.471693330966 H -2.440550529 C -2.91510263807 -6.2182770088 C -3.598476411284 -3.8022446557 2.12778079007 H -2.45321448503 -4.925892830 -6.2182770088 C -4.257412643304 1.166220324192 -6.45113481550 H -2.84931445503 -4.935983115 -2.346101321446 C -3.4622848545 1.7738675040 4.24240245250 H -3.282226461754 0.195180497862 C -4.97322846571 -1.3583712176 -3.14954777200 H -2.4543214553 -4.92589263836 -6.591257104437 C -4.2473716463014 1.166220324192 -6.45113481550 H -2.849891241595 -0.298728648548 &8.457103618662 C -4.97322848545 1.7738675404 4.24240245250 H -3.2672953007 H -2.248765013156 -2.4069633565 5.056652753307 H 0.8329424591 -1.95708900463 -1.457306164127 H -3.46539713245 -4.36064332455 5.925420481647 H -2.560312424907936 -4.4449558057 -1.5937458314 -4.5937357148 H -3.3005404244 -0.21387134222 -1.328124212878 H 0.58227905660 1.1357716 -5.347337818 H -3.8457714974 +3.	С	-2.212104953656	-1.663601291155	4.519909331944	Н	-0.543014787736	2.657987010577	-6.749511471302
C 1.974248272959 0.255953492738 6.76440347701 H 0.489324848773 1.074236087348 6.643090443520 C 1.92611558280 0.2284265116 7.910233851994 H 0.880227044880 1.91723666724 5.05586670921 C 2.43974680417 0.735752065243 4.40970137207018 H 1.22336848917 5.20559700508 3.5800151373 C 2.635103751827 1.673900777013 4.75397071072 H 1.122433149838 0.419285591810 7.675475261398 C 2.247956444557 1.0705214757 6.039315592433 H -1.7371046453 2.4916172106 1.8783947512 C 2.931005444657 1.0705214757 6.033155924833 H -1.0871046613 3.23058777106 1.8733947512 C 3.341592775263 2.441752815881 H -2.0876568024 -0.8276894475 5.57171146213 C 3.341592777055 H -2.20035652961 -0.8276894475 5.517711405213 C 3.34527775755 H -2.409358378149 -2.5297004837 7.21780704747	С	-1.954359765151	-0.448185569933	-3.555878417511	Н	-1.082071924971	3.235968591641	-0.182544171683
C -1.962115528820 -0.222842651156 7.910233851964 H -0.864433000343 3.007169246724 -5.055566670921 C -2.439649189208 -4.05352206323 -4.05362228811 4.697013727048 H -1.223365884917 -5.205595070508 3.358001513773 C -2.635103751827 1.673090777013 4.753997071072 H -1.12433149838 -0.324507764464 8.623711666321 C -2.203040462520 -2.767668087822 5.119759113048 H -1.788179442777 -2.91106434507 -4.838794703461 C -2.205904345057 0.4359878863 -2.906824419 -0.06982771814 -0.207714144433 H -1.01162514645 -2.91817271696 -1.875833947512 C -3.91004846597 1.30705201477 6.93515592833 H -2.400378658062 0.826789494755 -6.5717714478292 C -3.4917528404 1.34978779408 3.81025777655 H -2.40035885881 0.677061689412 4.877813137551 C -3.594943611060 -3.235058398213 -2.1779309807 H -2.441266306843 -1.222	С	-1.974248272959	0.255953492738	-6.764403477701	Н	-0.849334848773	1.074236087348	6.643090443520
C -2.147974680417 0.73572065243 4.300017195616 H -0.980227044880 2.180746472070 8.8444562690902 C -2.43504018908 4.057013720048 H -1.22363584917 -5.20559070508 3.53008113173 C -2.635103751827 1.673900777013 4.75397071072 H -1.129433149838 -0.24507764464 8.623711666211 C -2.64776239061 -1.65894738164 -1.770523573458 H -1.674701760613 3.250089207109 -8.533947512 C -2.9910236444597 -3.0052014757 6.0335155928333 H -1.60165216445 -2.49181752015 -3.2310054920960 T.23210232208 C -3.34162251263 -2.4053380096 H -2.005365024 -0.8276894475 6.5717146213 C -3.34162283111 -1.94847794408 S.13025777655 H -2.4003365296 -2.9110248842 H.73717146213 C -3.54949711060 -3.3508398213 -3.241709330966 H -2.4426464843 -1.22226461474 0.1918137313765 C -3.5494974510606 -3.345427717464	С	-1.962115528820	-0.222842651156	7.910233851964	Н	-0.864433600343	3.097169246724	-5.055568670921
$ \begin{array}{c} C = 2.439649189208 & -4.0354622282811 & 4.697013727048 & H = 1.22356588497 & 5.20559507059 & 3.350801513773 \\ C = 2.635103751827 & 1.673900777013 & 4.753997071072 & H = 1.12433149818 & -0.324507764464 & 8.623711666321 \\ C = 2.60300462592 & -2.76766807822 & 5.119759113048 & H = 1.373106384963 & 0.419285591810 & -7.675475261398 \\ C = 2.67806435057 & -0.85393785866 & -2.494659955106 & H = 1.674710760613 & 3.2505920700 & 7.5797147478292 \\ C = 2.991004846597 & 1.307052014757 & 6.093315592833 & H = 1.60165214645 & -2491817271696 & -1.875833947512 \\ C = 2.3900244419 & -2.00892773814 & -0.27077446443 & H & -1.33137396106 & -1.087064138704 & 7.3212120232208 \\ C = 3.341592795263 & 2.434175282155 & 2.406333860096 & H & 2.20875558062 & -0.826789494755 & -6.571771405213 \\ C = 3.0920492060 & 1.58133721576 & -3.905404978978 & H & -2.2500210648 & 2.58225981151 & 2.336010321446 \\ C = 3.64262883811 & 1.948787794408 & 3.81302577655 & H & 2.249035883584 & -0.677061689412 & 4.877831337651 \\ C = 3.982764112864 & 3.802224668577 & 2.12778079007 & H & -2.873310485503 & -0.677061689412 & 4.877831337651 \\ C = 3.98276412864 & 3.802224668577 & 2.12778079007 & H & -2.873310485503 & -0.677081689412 & 4.8770913207088 \\ C = 4.257416463014 & 1.16622032419 & -2.419247772900 & H & -2.873310485503 & -0.298778331636 & 0.24063098859 \\ C = 4.257416463014 & 1.16220324192 & -2.832108958170 & H & -2.63454441360 & -2.98778331636 & 0.24063098859 \\ C = 4.257416463014 & 1.0520324192 & -2.832108958170 & H & -2.63454441360 & -2.98778331636 & 0.24063098859 \\ C = 4.257416463014 & 1.16220324192 & -2.832108958170 & H & -2.63454441360 & -2.98778331636 & 0.24063098859 \\ C = 4.257416463014 & 1.16220324192 & -2.419547772900 & H & -2.6345744413856 & -2.98778331636 & 0.24065098859 \\ C = 4.257416480314 & 1.16520324192 & -2.149547772900 & H & -2.6345744413850 & -2.987678331656 & 2.987576654327 \\ C = 5.27821228791 & 1.38267791852 & H & -3.002961270019 & -2.53925640848 & 8.48770341866 & 2.987783314607 & H & -2.5976389215 & -0.595876654327 \\ H & 0.552225970961 & -2.$	С	-2.147974680417	0.735752063243	-4.309017195616	н	-0.980227044880	2.180746472070	8 844456269902
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Č	-2 439649189208	-4 053622282811	4 697013727048	Н	-1 225365884917	-5 205595070508	3 350801513773
C 2.80300462592 2.2767686087822 4.519759113048 H 1.5773066384963 0.412285591810 -7.675475261398 C 2.2647762399061 2.165894738164 -1.070322373458 H -1.1781179442777 2.970166307088 4.838794703461 C 2.296644419 -2.069892773814 H -0.27077446443 H -1.875833947512 C -3.905029060 1.58153721576 -0.90540477655 H -2.490135885381 -0.8767061689412 4.877831337651 C -3.690520560 1.58153721576 -9.90540477855 H -2.21003586528062 -0.8767849494755 -6.71771045213 C -3.642628388111 1.94878779400 3.813025777655 H -2.40035865280643 -1.221707061689412 4.877831337651 C -3.3548245410 0.34272513076 -2.446630484 -2.21205270706 -2.18277700889 C -3.8381761160 -3.3520558398213 -2.447671386630843 -2.21095744 -2.386161327 C -3.8381761166 -2.149547771900 H -2.6345414463164 -2.688712477974 <td< td=""><td>c</td><td>-2 635103751827</td><td>1 673900777013</td><td>4 753997071072</td><td>н</td><td>-1 120433140838</td><td>-0 324507764464</td><td>8 623711666321</td></td<>	c	-2 635103751827	1 673900777013	4 753997071072	н	-1 120433140838	-0 324507764464	8 623711666321
$ \begin{array}{c} -2.84300.040.522 - 2.0100.00081622 - 2.0100.00081622 - 0.1197.95113046 \\ -2.6477.65299661 - 2.0100.65894738164 - 0.170025373458 \\ -2.796563435057 - 0.83593878866 - 2.49465995106 \\ +1 -1.67470170601 - 3.25036207706 \\ -2.911004846597 - 1.307052014757 \\ -2.95902364419 - 2.006982773814 - 0.270774146443 \\ +1 -1.931937396106 - 1.087064138704 - 7.23212032208 \\ -3.3452795253 - 2.44317528215 - 2.40633360096 \\ +2.008756580624 - 0.827689497357 - 6.57177140213 \\ -3.49756588024 - 0.82768949755 - 6.57177140213 \\ -3.4987879448 & 3.813025777655 \\ +2.290025883811 - 1.948787794408 \\ -3.831612834548 & 0.043727513076 - 2.149547772900 \\ -3.348297411264 & 3.2402388213 - 2.417693530966 \\ +2.271045883548 & -0.043727513076 - 2.149547772900 \\ -4.014575853354 - 1.24527213828 - 2.83210898170 \\ -4.014575853354 - 1.24527213828 - 2.83210898170 \\ -4.201457853354 & -1.24527213828 - 2.83210898170 \\ -4.201457853354 & -1.24527213828 - 2.83210898170 \\ -4.201457853354 & -1.24527213828 - 2.83210898170 \\ -4.201457853354 & -1.24527213828 - 2.83210898170 \\ -4.2744221697974 & 2.346766110378 \\ 8.689272004437 \\ -4.2734521935 & -4.47449545875 \\ -4.97328483454 & 1.166220324192 \\ -4.97328483454 & -1.793788076404 \\ -1.26280124182 & -4.37845794001 \\ +2.36867933232 & -0.66884848 \\ -8.87103618662 \\ -2.378212288791 & 1.38249771393 \\ -5.278212288791 & 1.38249771393 \\ -5.278212288791 & 1.38249771393 \\ -5.278212288791 & 1.38249771393 \\ -5.278212288791 & 1.38249771393 \\ -5.278212288791 & 1.38249771393 \\ -5.278212288791 & 1.38249771393 \\ -5.278212288791 & 1.38249771393 \\ -5.27821288874 & -1.07618484441350 \\ -2.98912414520 & -2.9978331636 \\ -2.34324824643 & -3.93794594001 \\ +2.342892184432 & 1.70158360095 \\ -2.69720037325794 \\ +0.8522397970 & -3.6544454534 \\ -0.201873782214221828 \\ +0.8567332322 & -1.601845544 \\ +3.60053701244 & -3.0278528268081 \\ -3.32087318266 & -3.248326996559 \\ +2.348326492696 & -3.44376491150 & -7.644376491150 & -7.678448267557149 \\ -3.3200572822 & -2.872118248789 \\ +2.6920219510676 & -2.24993683148 \\ +2.4974503992124 & -2.47455481556 \\ -2$	c	2.033103731827	2 767686087822	4./JJJJJJ/0/10/2	11	1 277206284062	0.410285501810	7.675475261209
$ \begin{array}{c} -2.087/0.2399.06 & -2.0383947.0364 & -2.0405395106 & -1.070253/5436 & H & -1.681/9442/11/-2.9700301095 & -2.0383747.0360 & -2.0581747.0361 & -2.05050200760 & -2.0581747.0362 & -2.491817271666 & -1.878833947512 & -2.95052024441 & -2.00698277381 & -0.27074146443 & H & -1.931937396106 & -1.08706413870 & -7.32312032208 & -2.319094920960 & 1.5815372157 & -3.90540479878 & H & -2.2602201648 & -2.852225981151 & -2.36005201464 & -2.491817271666 & -2.8777171405213 & -2.37001232146 & -2.3691292060 & -1.878531372157 & -3.90540479878 & H & -2.2602201648 & 2.582225981151 & -2.36005321446 & -2.4918172710869 & -2.35049391106 & -3.23503839214 & -2.41709353066 & H & -2.444266306843 & -1.22226461473 & -2.19817717200 & -2.1494777200 & H & -2.7331048503 & -4.93599311754 & 5.173757912021 & -3.836154164301 & 1.16622032419 & -2.41959351066 & -1.878533164 & -2.49877831636 & -2.40639098859 & -2.42574112864 & 3.802224044532 & -2.14954777200 & H & -2.6454444166-306843 & -1.22226461473 & 5.80227004437 & -2.14954777200 & H & -2.452474164301 & H & -0.62033419 & -2.14954777200 & H & -2.6454444166-306843 & -1.26203419 & 5.173757912021 & -2.42574164301 & H & -0.62034219 & -2.452415593 & -0.2688364884 & 8.487103618662 & -2.495771393 & 5.241559350525 & H & -3.609812415953 & -0.2688364884 & 8.487103618662 & -2.497322848545 & 1.77836750440 & 4.224024542250 & H & -3.002961270019 & 0.599280250583 & -6.58576654327 & 0.3308737582 & -0.61145527018 & -4.457571439 & 4.53026529132 & 2.50903732529 & -0.6314552708 & -1.93775826 & -0.6314552708 & -1.3527795641412 & H & -3.42692184424 & -2.0183186655 & 5.2692767583071 & H & -3.6679333228 & 4.160352605601 & -2.6983454848 & -3.4961158557 & H & -3.050634444 & -2.0746500955 & -1.920736527830 & H & -3.0456137372 & -0.5214527079 & -3.4534384575 & -1.78077346 & -3.439759186374 & H & -3.3661485744 & -3.3661485449 & -3.49761450575 & -1.292736527830 & H & -3.46567313224 & -0.213871342322 & -1.328124212878 & H & -0.053201376 & -0.04834798658 & H & -4.50063404244 & -0.213871342322 & -1.328124212878 & H & -0.237375$	c	-2.803004023920	-2.707080087822	1 770522572459	П 11	1 70017044203	0.419265591610	4 929704702461
$ \begin{array}{c} \begin{tabular}{l l l l l l l l l l l l l l l l l l l $	C	-2.04//02399001	-2.103694/36104	-1.//05255/5456	п	-1./001/9442///	-2.9/010030/098	-4.838/94/03401
$ \begin{array}{c} C = 2.911004846039' 1.307052014/57 & 0.093515592833 & H & -1.60165214643 & -2.4918172/1090 & -1.87383394/512 \\ C = 2.950023644419 & -2.006982773814 & -0.270774146443 & H & -1.931937396106 & -1.08706413870 & 7.23212032208 \\ C = 3.341592795263 & 2.434175282155 & 2.406333860096 & H & -2.008756530624 & -0.826789494755 & -6.5711714052113 \\ C = 3.642628838111 & -1.948787794408 & 3.813025777655 & H & -2.490358835881 & -0.677061689412 & 4.877831337651 \\ C = 3.55827453040 & 1.394394269015 & 1.355341212288 & H & -2.210035365296 & 2.951262883907 & -6.2182977100889 \\ C = -3.534930611060 & -3.23505839821 & -2.417093530966 & H & -2.444266306843 & -1.22226641274 & 0.195180497862 \\ C = -3.982764112864 & 3.802224468577 & 2.127780790907 & H & -2.873310485503 & -4.935939117545 & 5.173757912021 \\ C = -3.834164234548 & 0.04372751307 & -2.149547772900 & H & -2.748221975974 & 2.346766110378 & 8.689272004437 \\ C = -4.014575853354 & 1.245272138928 & -2.832108958170 & H & -2.634544441360 & -2.987978331636 & 0.240639098859 \\ C = 4.257416463014 & 1.16620324192 & 6.451134815505 & H & -3.802961270019 & 0.5992802556563427 \\ C = -3.7324212288791 & 1.38249771393 & 5.24155936525 & H & -3.527295063091 & -2.630042318266 & 5.925420481647 \\ H & 0.273745210935 & -4.7449548075 & 1.93122014619 & H & -3.317035213375 & 0.408313865655 & 1.566927653077 \\ H & 0.33298737826 & -0.61415527081 & 5.457945594001 & H & -3.64275571449 & 4.550265629132 & 2.87043602569 \\ H & 0.8622917702 & -3.65237383447 & -5.397395186374 & H & -3.370673283123 & 2.100332205797 & -4.448957557 \\ H & 0.8571322499 & 1.045199946571 & -6.63333606659 & H & -3.46937802244 & -4.207465090556 & -1.920736527830 \\ H & 0.864826164363 & -3.088943294521 & 5.061912634337 & H & -3.370673283123 & 2.10033220671574 \\ H & 0.864826164363 & -3.088943294521 & 5.061912634337 & H & -3.08674733224 & -3.287648214212878 \\ H & 1.5335001340 & 0.354807757346 & +8.614807580251 & H & -4.609357016200 & -2.1371434247237 & -4.348967557 \\ H & 1.956506132505 & 2.491647119588 & 1.862259228040 & H & -5.77920212490 &$	C	-2./9050545505/	-0.833938/83803	-2.494659955106	Н	-1.0/4/01/00013	3.250369290760	1.075022047512
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	C	-2.91100484659/	1.30/052014/5/	6.093515592833	Н	-1.601652514645	-2.49181/2/1696	-1.8/583394/512
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	С	-2.959023644419	-2.069892773814	-0.2/0//4146443	Н	-1.931937396106	-1.08/064138/04	7.232120232208
$ \begin{array}{c} C & -3.190054920960 & 1.581533721576 & -3.905404978978 & H & -2.2560216948 & 2.582225981151 & 2.336010321446 \\ C & -3.64262883111 & 1.94787794048 & 3.81302577655 & H & -2.490358835881 & 0.677061698412 & 4.877831337651 \\ C & -3.755827453040 & 1.394394269015 & 1.355341212288 & H & -2.210035365296 & 2.951262883907 & -6.218297700889 \\ C & -3.98276411266 & 3.80222446857 & 2.127780790907 & H & -2.473310485503 & -4.93599311754 & 5.17375712021 \\ C & -3.831612834548 & 0.04372751307 & -2.149547772900 & H & -2.748221795974 & 2.346766110378 & 8.689272004437 \\ C & -4.014575853354 & 1.245272138928 & -2.832108958170 & H & -2.63454441360 & -2.98797831636 & 0.240639098859 \\ C & -4.257416463014 & 1.166220324192 & 6.451134815505 & H & -3.02961270019 & 0.59928025088 & -6.958576654327 \\ C & -5.278212288791 & 1.38249777139 & 5.52415936525 & H & -3.022961270019 & 0.59928025088 & -6.958576654327 \\ H & 0.273745210935 & -4.47495458075 & 1.931226014619 & H & -3.317035213375 & 0.408313856555 & 1.566927653077 \\ H & 0.81293424591 & -1.795708900463 & -1.457306164127 & H & -3.4289214432 & 2.500037325794 & -4.48950715746 \\ H & 0.52225070961 & -2.64437649115 & 6.756146077302 & H & -3.664275571439 & 4.55026509132 & 2.870436029569 \\ H & 0.852293197720 & -3.652373838474 & -5.393759186374 & H & -3.3706332123 & 2.509037325794 & -4.48950715746 \\ H & 0.55225070961 & -2.64437649115 & 6.756146077302 & H & -3.685679333228 & 4.160035260560 & 1.128767794743 \\ H & 0.85871322499 & -1.045199946571 & -6.638336906859 & H & -3.40058292444 & -4.207465090556 & -1.920736527830 \\ H & 0.858671322499 & -1.04519946571 & -6.638336906859 & H & -3.40508292444 & -4.207465090556 & -1.920736527830 \\ H & 0.856471322490 & -2.49406872144 & -8.842229368653 & H & -4.500634042449 & -0.213871342322 & -1.328124212878 \\ H & 1.535301340 & 0.354507757346 & -8.6148075802 & H & -4.500634042449 & -0.213871423728706 \\ H & 0.980441681097 & -2.149406872144 & -8.8422929368653 & H & -4.500634012449 & -0.213871342322 & -1.328124212878 \\ H & 1.595506132502 & 2.49114835037 & -2.5643501781$	С	-3.341592795263	2.434175282155	2.406333860096	Н	-2.008756580624	-0.826789494755	-6.571771405213
$ \begin{array}{c} C & -3.64262883811 & 1.94878779408 & 3.813025777655 & H & -2.49053835881 & -0.677061689412 & 4.877831337651 \\ c & -3.5827453040 & 1.394394260051 & 1.355341212288 & H & -2.210035365290 & 2.95126288907 & -6.218297700889 \\ C & -3.58161284548 & 0.043727513076 & -2.147547772900 & H & -2.87310485503 & -4.935993117545 & 5.173757912021 \\ c & -3.83161284548 & 0.043727513076 & -2.149547772900 & H & -2.63454441360 & -2.987978331636 & 0.24063908859 \\ C & -4.973228485845 & 1.778386750440 & 4.224024542250 & H & -3.002961270019 & 0.599280250583 & -6.958576654327 \\ c & -4.973228485845 & 1.778386750440 & 4.224024542250 & H & -3.002961270019 & 0.599280250583 & -6.958576654327 \\ C & -4.973228485845 & 1.778386750440 & 4.224024542250 & H & -3.002961270019 & 0.599280250583 & -6.958576654327 \\ c & -3.75122288791 & 1.382497771393 & 5.524155936625 & H & -3.527295630091 & -2.63042318266 & 5.925420481647 \\ H & 0.273745210935 & -4.474495458075 & 1.931220114619 & H & -3.317035213375 & 0.408313860555 & 1.566927653077 \\ H & 0.813293424591 & -1.795708900463 & -1.457306164127 & H & -3.428992184432 & 1.701358360095 & 0.350483253750 \\ H & 0.36223197720 & -3.652373838474 & -5.393759186374 & H & -3.370673283123 & 2.509037325794 & -4.448950715746 \\ H & 0.552225070961 & -2.644376491150 & 6.756146077302 & H & -3.6867373228 & 4.160035260560 & 1.128767797444 \\ H & 0.85871322499 & -1.045199946571 & -6.638336906859 & H & -3.4050871429 & -3.3661485349 & -3.4014497557 \\ H & 0.86426164363 & -3.088943294521 & 5.061912634337 & H & -4.609357016200 & -2.95221808666 & -2.014576757574 \\ H & 0.85871322499 & -1.045199946571 & -6.638336906859 & H & -3.405080292444 & -4.207465090556 & -1.920736527830 \\ H & 0.86426164363 & -3.088943294521 & 5.061912634337 & H & -4.609357016200 & -2.952211080666 & -2.3143548488.331401724451 \\ H & 1.92637948003 & -0.404387782651 & H & -4.500634024494 & -0.21387134222 & -1.328124212878 \\ H & 1.5353001340 & 0.35450775374 & -8.614807580251 & H & -4.600357016200 & -2.952211080666 & -2.3143548488333 \\ H & 1.78550753922 & 2.9793033101$	С	-3.190054920960	1.581533721576	-3.905404978978	Н	-2.256022016948	2.582225981151	2.336010321446
C -3.755827453040 1.394394269015 1.355341212288 H -2.21033365296 2.95126288307 -6.218297700889 C -3.389493611060 -3.230508398213 -2.41769330966 H -2.444266306843 -1.22226614754 0.195180497862 C -3.831612834548 0.043727513076 -2.149547772900 H -2.873310485503 -4.935993117545 5.173757912021 C -4.014575833354 1.1245272138928 -2.83108958170 H -2.63454441360 -2.89779331636 0.240639098859 C -4.274716463014 1.166220324192 6.451134815505 H -2.809216170019 0.599282648848 8.487103618662 C -5.278212288791 1.382497771393 5.524155936525 H -3.02961270019 -0.59928260555 1.566927653077 H 0.81393424591 -1.795708900463 -1.45736164127 H -3.34299218421 1.701358360095 0.530482353750 H 0.33087375826 -0.651415527081 5.457945594001 H -3.664275571439 4.55026562132 2.870430029669 H 0.862293197720 -3.652373838474 -3.3305146176274 -3.366148554349 <	С	-3.642628838111	1.948787794408	3.813025777655	Н	-2.490358835881	-0.677061689412	4.877831337651
C -3.349493611060 -3.235058398213 -2.417693530966 H -2.44266306843 -1.222264614754 0.1951180497862 C -3.831612834548 0.043727513076 -2.149547772900 H -2.748221975974 2.346766110378 8.689272004437 C -4.01457853354 1.245272138928 -2.832108958170 H -2.6344441360 -2.987978331636 0.24063098859 C -4.257416463014 1.166220324192 6.4511138415505 H -2.898912415953 -0.29828648848 8.487103618662 C -4.973228485845 1.778386750440 4.224024542250 H -3.002961270019 0.59928025083 -6.958576654327 C -5.278212288791 1.382497771393 5.524155936525 H -3.31703521375 -0.4081385655 1.566927650377 H 0.033987375826 -0.651415527081 5.45794594001 H -3.467275571439 4.550265629132 2.87043602569 H 0.825225070961 -2.644376491150 6.756146077302 H -3.665657318264 -3.261748634349 -3.4901449575573 H 0.85642614363 -3.088482164363 -3.0884821643633 -0.418350551	С	-3.755827453040	1.394394269015	1.355341212288	Н	-2.210035365296	2.951262883907	-6.218297700889
C -3.982764112844 3.802224468577 2.127780790907 H -2.873310485503 -4.935993117545 5.173757912021 C -3.831612834548 0.043727513076 -2.149547772900 H -2.748221975974 2.346766110378 8.689272004437 C -4.014578853354 1.245272138928 -2.832108958170 H -2.63454441360 -2.987978331636 0.240639098859 C -4.257416463014 1.166220324192 6.451134815505 H -2.808912415953 -0.269828648848 8.487103618662 C -5.278212288791 1.38249777139 5.5221455936525 H -3.827295630091 -2.630042318266 5.925240481647 H 0.813293424591 -1.79570890463 -1.457306164127 H -3.4289218432 1.70135836095 0.350483253750 H 0.86293197720 -3.652373838474 -5.393759186374 H -3.370673283123 2.509037325794 -4.448950715746 H 0.862293197720 -3.6423754244 -3.490144957557 H -3.86567333228 4.16035266569112 2.870436029569 H	С	-3.549493611060	-3.235058398213	-2.417693530966	Н	-2.444266306843	-1.222264614754	0.195180497862
C -3.831612834548 0.043777513076 -2.149547772900 H -2.748221975974 2.346766110378 8.689272004437 C -4.014575853354 1.245272138928 -2.832108958170 H -2.634544441360 -2.987978331636 0.240639098859 C -4.25741645014 1.166220324192 6.451134815505 H -3.02961270019 0.599280250583 -0.598576654327 C -5.278212288791 1.382497771393 5.524155936525 H -3.527295630091 -2.630042318265 5.526562763077 H 0.813293424591 -1.75708900463 -1.457306164127 H -3.3627328123 2.509037325794 -4.44895071576 H 0.352293197720 -3.652373838474 -5.393759186374 H -3.370673283123 2.509037325794 -4.448950715746 H 0.55225070961 -2.644376491150 6.756146077302 H -3.366507333228 4.160035206560 1.128767794743 H 1.067614365246 -3.24231282166 0.179767297044 H -3.346563718264 -3.366148654349 -3.9014957557 H 0.864826164133 -0.389839294521 5.061912634337 H -4.500530	С	-3.982764112864	3.802224468577	2.127780790907	Н	-2.873310485503	-4.935993117545	5.173757912021
C -4.014575853354 1.245272138928 -2.832108958170 H -2.634544441360 -2.987978331636 0.240639098859 C -4.257416463014 1.166220324192 6.451134815505 H -2.898912415933 -0.26982648848 8.487103618662 C -4.257228485845 1.77838670440 4.224024542250 H -3.002961270019 0.59928025058 -6.958576654327 C -5.278212288791 1.382497771393 5.524155936525 H -3.527295630091 -2.630042318266 5.925420481647 H 0.2339087375826 -0.651415527081 5.457945594001 H -3.32067281123 2.509037325794 -4.448950715746 H 0.862293197720 -3.652373838474 -5.393759186374 H -3.366673783228 -1.6003550506 1.128767794743 H 1.067614365246 -3.242312821506 0.179767297044 H -3.46563718264 -3.366148654349 -3.490144957557 H 0.88842164363 -3.08847394521 5.061912634337 H -4.0387120876 -1.92736527830 H 0.86482164363 -3.24231282150 0.11797024875 H -4.20746509658 -1.9207365278	С	-3.831612834548	0.043727513076	-2.149547772900	Н	-2.748221975974	2.346766110378	8.689272004437
C -4.257416463014 1.166220324192 6.451134815505 H -2.898912415953 -0.269828648848 8.487103618662 C -4.973228485845 1.778386750440 4.224024542250 H -3.002961270019 0.599280250583 -6.958576654327 C -5.278212288791 1.382497771393 5.524155936525 H -3.527295630091 -2.60042318266 5.925420481647 H 0.813293424591 -1.795708900463 -1.457306164127 H -3.3428992184432 1.701358360095 0.30483235750 H 0.830987375826 -0.651415527081 5.457945594001 H -3.664275571439 4.550265629132 2.870436029569 H 0.652293197720 -3.652373838474 -5.393759186374 H -3.340653783228 4.160035260560 1.128767794743 H 0.658225070961 -2.644376491150 6.756146077302 H -3.46567833228 4.207465090556 -9.20736527830 H 0.864826164363 -3.08943294521 5.061912634337 H -4.308771208676 -1.952852680812 -0.090023645230 H 0.864826164363 -3.089493294521 5.061912634337 H -4.510	С	-4.014575853354	1.245272138928	-2.832108958170	Н	-2.634544441360	-2.987978331636	0.240639098859
C -4.973228485845 1.778386750440 4.224024542250 H -3.002961270019 0.599280250583 -6.958576654327 C -5.278212288791 1.382497771393 5.524155936525 H -3.527295630091 -2.630042318266 5.925420481647 H 0.273745210935 -4.474495458075 1.931226014619 H -3.317035213375 0.408313856555 1.566927653077 H 0.339087375826 -0.651415527081 5.457945594001 H -3.664275571439 4.550265629132 2.870436029569 H 0.862293197720 -3.652373838474 -5.393759186374 H -3.370732284 4.160035260560 1.128767794743 H 1.067614365246 -3.242312821506 0.179767297044 H -3.465637138264 -3.366148654349 -3.490144957557 H 0.858713224999 -1.045199946571 -6.638336906859 H -4.308771208676 -1.922852680812 -0.090023645230 H 0.980441681097 -2.149406872144 -8.842229368653 H -4.500634042449 -0.213871342322 -1.328124212878 H 1.226260301374 5.204118350351 -3.39314617664 H -4.	С	-4.257416463014	1.166220324192	6.451134815505	Н	-2.898912415953	-0.269828648848	8.487103618662
C -5.278212288791 1.382497771393 5.524155936525 H -3.527295630091 -2.63042218266 5.925420481647 H 0.273745210935 -4.474495458075 1.931226014619 H -3.317035213375 0.408313856555 1.566927653077 H 0.813293424591 -1.795708900463 -1.457306164127 H -3.428992184432 1.701358360095 0.350483253750 H 0.862293197720 -3.652373838474 -5.393759186374 H -3.367673283123 2.509037325794 -4.448950715746 H 0.552225070961 -2.644376491150 6.756146007302 H -3.365653718264 -3.360148654349 -3.40014957577 H 0.858713224999 -1.045199946571 -6.638336906859 H -3.405680292444 -2.07465090556 -1.920736527830 H 0.86426164363 -3.088943294521 5.061912634337 H -4.038771208676 -2.952852680812 -0.9009023645230 H 1.226260301374 -2.149406875144 -8.8142229368653 H -4.500830922444 -2.207465093957 -1.920736527830 H 1.23626301340 0.354507757346 -8.61480780251 H	С	-4 973228485845	1.778386750440	4 224024542250	н	-3.002961270019	0.599280250583	-6.958576654327
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	č	-5 278212288791	1 382497771393	5 524155936525	н	-3 527295630091	-2 630042318266	5 925420481647
$\begin{array}{llllllllllllllllllllllllllllllllllll$	н	0.273745210935	-4 474495458075	1 931226014619	н	-3 317035213375	0.408313856555	1 566927653077
$\begin{array}{llllllllllllllllllllllllllllllllllll$	н	0.813203424501	-1 795708900463	-1 457306164127	н	-3 428002184432	1 701358360095	0.350483253750
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	и П	0.220097275926	-1.755708500405	5 457045504001	11 11	2 664275571420	4 550265620122	2 870426020560
$\begin{array}{llllllllllllllllllllllllllllllllllll$	11	0.559087575820	-0.031413327081	5 202750196274	П 11	-3.0042/33/1439	4.550205029152	4 448050715746
$\begin{array}{llllllllllllllllllllllllllllllllllll$	п	0.802295197720	-5.0525/56564/4	-3.393/391803/4	п	-3.5/00/5265125	2.309037323794	-4.446950/15/40
$\begin{array}{llllllllllllllllllllllllllllllllllll$	п	0.552225070961	-2.0443/0491150	0./501400//502	Н	-3.0850/9555228	4.160035260560	1.128/6//94/43
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H	1.06/014365246	-5.242512821506	0.1/9/6/29/044	H	-3.340303/18264	-3.300148654349	-3.49014495/55/
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	0.858/13224999	-1.045199946571	-6.638336906859	Н	-3.405080292444	-4.207465090556	-1.920/3652/830
$\begin{array}{llllllllllllllllllllllllllllllllllll$	н	0.864826164363	-3.088943294521	5.061912634337	Н	-4.038//12086/6	-1.952852680812	-0.090023645230
H1.2262603013745.204118350351-3.339314617664H-4.5108339122490.8797636963397.473483900868H1.1533530013400.354507757346-8.614807580251H-4.8507169375891.2730949021541.334107124451H1.392637948003-0.4043847086097.671797024875H-4.609357016200-2.952211080606-2.314354843833H1.7855905399222.9793035310154.822784218539H-5.0824742718203.7455438155622.150013502839H1.662450440665-3.228688422880-7.596435017818H-4.8197148028551.921439256877-2.534615979042H1.9676750609121.10508848019-7.223609449409H-5.7799202120951.9704612769013.513723169079H2.0198039581180.8382484296916.561738316502N0.8161764705171.2775861400873.897215747920H2.243803418966-2.600117729685-2.341324086533N1.236399320419-1.779197286531-4.381620284438H2.5047262498960.677648154674-4.861443752370N-0.817930853487-1.273804882599-3.904578914929H2.2430351932174.937075658864-5.148724153140-2.333665039138-8.6850430146467H2.6292015927672.985423807311-0.254737560854B-0.4128764029388.3295703892150.519115121236H2.9221951067680.278139843812-8.481777424297B-1.6362412038372.4855107142470.018815234177	Н	0.980441681097	-2.149406872144	-8.842229368653	Н	-4.500634042449	-0.213871342322	-1.328124212878
H1.1533530013400.354507757346-8.614807580251H-4.8507169375891.2730949021541.334107124451H1.392637948003-0.4043847086097.671797024875H-4.609357016200-2.952211080606-2.314354843833H1.7855905399222.9793035310154.822784218539H-5.0824742718203.7455438155622.150013502839H1.662450440665-3.22868422880-7.596435017818H-4.8197148028551.921439256877-2.534615979042H1.5965061325052.4916471195881.862259228040H-5.7799202120951.9704612769013.513723169079H1.9676750609121.105088848019-7.223609449409H-6.3210072499081.2560446651575.824928790660H2.0198039581180.8382484296916.561738316502N0.8161764705171.2775861400873.897215747920H2.243803418966-2.600117729685-2.341324086533N1.236399320419-1.779197286531-4.381620284438H2.5047262498960.677648154674-4.861443752370N-0.817930853487-1.273804882599-3.904578914929H2.243803418966-2.333665039138-8.6850430146467H2.6292015927672.985423807311-0.254737560854B-0.4128764029388.3295703892150.519115121236H2.9221951067680.278139843812-8.481777424297B-1.6362412038372.4855107142470.018815234177	Н	1.226260301374	5.204118350351	-3.339314617664	Н	-4.510833912249	0.879763696339	7.473483900868
H1.392637948003-0.4043847086097.671797024875H-4.609357016200-2.952211080606-2.314354843833H1.7855905399222.9793035310154.822784218539H-5.0824742718203.7455438155622.150013502839H1.662450440665-3.228688422880-7.596435017818H-4.8197148028551.921439256877-2.534615979042H1.965061325052.4916471195881.862259228040H-5.7799202120951.9704612769013.513723169079H1.9676750609121.105088848019-7.223609449409H-6.3210072499081.2560446651575.824928790660H2.0198039581180.8382484296916.561738316502N0.8161764705171.2775861400873.897215747920H2.243803418966-2.600117729685-2.341324086533N0.2817930853487-1.273804882599-3.904578914929H2.216224490444-2.9409962386146.217662525759N-1.2378608184761.7804775361404.378852147211H2.8896311932174.937075658864-5.1487241531407H2.6292015927672.985423807311-0.254737560854B-0.4128764029388.3295703892150.519115121236H2.9221951067680.278139843812-8.481777424297B-1.6362412038372.4855107142470.018815234177	Н	1.153353001340	0.354507757346	-8.614807580251	Н	-4.850716937589	1.273094902154	1.334107124451
H1.7855905399222.9793035310154.822784218539H-5.0824742718203.7455438155622.150013502839H1.662450440665-3.228688422880-7.596435017818H-4.8197148028551.921439256877-2.534615979042H1.5965061325052.4916471195881.862259228040H-5.7799202120951.9704612769013.513723169079H1.9676750609121.105088848019-7.223609449409H-6.3210072499081.2560446651575.824928790660H2.0198039581180.8382484296916.561738316502N0.8161764705171.2775861400873.897215747920H2.243803418966-2.600117729685-2.341324086533N1.236399320419-1.779197286531-4.381620284438H2.5047262498960.677648154674-4.861443752370N-0.811730853487-1.273804882599-3.904578914929H2.216224490444-2.9409962386146.217662525759N-1.2378608184761.7804775361404.378852147211H2.4403655835311.219578410753-0.2073572271034.378852147211H2.6292015927672.985423807311-0.254737560854B-0.4128764029388.3295703892150.519115121236H2.9221951067680.278139843812-8.481777424297B-1.6362412038372.4855107142470.018815234177	Η	1.392637948003	-0.404384708609	7.671797024875	Н	-4.609357016200	-2.952211080606	-2.314354843833
H1.662450440665 1.596506132505-3.228688422880 2.491647119588-7.596435017818 1.862259228040H-4.8197148028551.921439256877 1.970461276901-2.534615979042 3.513723169079H1.9676750609121.105088848019 1.05088848019-7.223609449409 6.561738316502H-5.7799202120951.970461276901 1.2560446651573.513723169079 5.824928790660H2.0198039581180.8382484296916.561738316502 -2.600117729685N0.816176470517 1.2775861400871.277586140087 3.897215747920H2.243803418966-2.600117729685 -2.60117729685-2.341324086533 -4.861443752370N1.236399320419 -1.779197286531-4.381620284438H2.5047262498960.677648154674 -4.861443752370-4.861443752370 NN-0.817930853487 -1.237860818476-1.273804882599 -3.904578914929H2.216224490444 -2.940996238614-2.070357227103 -0.207357227103N-0.817930853487 -1.2378608184761.780477536140 4.378852147211H2.489631193217 -2.333665039138-8.685043014646 -8.6850430146467H2.629201592767 -2.985423807311 H-0.254737560854 -8.481777424297B-0.412876402938 -1.6362412038378.329570389215 2.4855107142470.519115121236 0.018815234177	Н	1.785590539922	2.979303531015	4.822784218539	Н	-5.082474271820	3.745543815562	2.150013502839
H1.5965061325052.4916471195881.862259228040H-5.7799202120951.9704612769013.513723169079H1.9676750609121.105088848019-7.223609449409H-6.3210072499081.2560446651575.824928790660H2.0198039581180.8382484296916.561738316502N0.8161764705171.2775861400873.897215747920H2.243803418966-2.600117729685-2.341324086533N1.236399320419-1.779197286531-4.381620284438H2.5047262498960.677648154674-4.861443752370N-0.817930853487-1.273804882599-3.904578914929H2.216224490444-2.9409962386146.217662525759N-1.2378608184761.7804775361404.378852147211H2.4403655835311.219578410753-0.207357227103H2.6292015927672.985423807311-0.254737560854B-0.4128764029388.3295703892150.519115121236H2.9221951067680.278139843812-8.481777424297B-1.6362412038372.4855107142470.018815234177	Н	1.662450440665	-3.228688422880	-7.596435017818	Н	-4.819714802855	1.921439256877	-2.534615979042
H1.9676750609121.105088848019-7.223609449409H-6.3210072499081.2560446651575.824928790660H2.0198039581180.8382484296916.561738316502N0.8161764705171.2775861400873.897215747920H2.243803418966-2.600117729685-2.341324086533N1.236399320419-1.779197286531-4.381620284438H2.5047262498960.677648154674-4.861443752370N-0.817930853487-1.273804882599-3.904578914929H2.216224490444-2.9409962386146.217662525759N-1.2378608184761.7804775361404.378852147211H2.4403655835311.219578410753-0.207357227103N-1.2378608184761.7804775361404.378852147211H2.746542407936-2.333665039138-8.6850430146467H2.6292015927672.985423807311-0.254737560854B-0.4128764029388.3295703892150.519115121236H2.9221951067680.278139843812-8.481777424297B-1.6362412038372.4855107142470.018815234177	Н	1.596506132505	2.491647119588	1.862259228040	Н	-5.779920212095	1.970461276901	3.513723169079
H 2.019803958118 0.838248429691 6.561738316502 N 0.816176470517 1.277586140087 3.897215747920 H 2.243803418966 -2.600117729685 -2.341324086533 N 1.236399320419 -1.779197286531 -4.381620284438 H 2.504726249896 0.677648154674 -4.861443752370 N -0.817930853487 -1.273804882599 -3.904578914929 H 2.216224490444 -2.940996238614 6.217662525759 N -1.237860818476 1.780477536140 4.378852147211 H 2.440365583531 1.219578410753 -0.207357227103 N -1.237860818476 1.780477536140 4.378852147211 H 2.629201592767 2.985423807311 -0.254737560854 B -0.412876402938 8.329570389215 0.519115121236 H 2.922195106768 0.278139843812 -8.481777424297 B -1.636241203837 2.485510714247 0.018815234177	Н	1.967675060912	1.105088848019	-7.223609449409	Н	-6.321007249908	1.256044665157	5.824928790660
H 2.243803418966 -2.600117729685 -2.341324086533 N 1.236399320419 -1.779197286531 -4.381620284438 H 2.504726249896 0.677648154674 -4.861443752370 N 1.236399320419 -1.779197286531 -4.381620284438 H 2.216224490444 -2.940996238614 6.217662525759 N -0.817930853487 -1.273804882599 -3.904578914929 H 2.440365583531 1.219578410753 -0.207357227103 N -1.237860818476 1.780477536140 4.378852147211 H 2.889631193217 4.937075658864 -5.148724153140 -2.333665039138 -8.685043014646 7 H 2.629201592767 2.985423807311 -0.254737560854 B -0.412876402938 8.329570389215 0.519115121236 H 2.922195106768 0.278139843812 -8.481777424297 B -1.636241203837 2.485510714247 0.018815234177	Н	2.019803958118	0.838248429691	6.561738316502	N	0.816176470517	1.277586140087	3.897215747920
H 2.504726249896 0.677648154674 -4.861443752370 N -0.817930853487 -1.273804882599 -3.904578914929 H 2.216224490444 -2.940996238614 6.217662525759 N -0.817930853487 -1.273804882599 -3.904578914929 H 2.440365583531 1.219578410753 -0.207357227103 N -1.237860818476 1.780477536140 4.378852147211 H 2.889631193217 4.937075658864 -5.148724153140 -2.333665039138 -8.685043014646 7 H 2.629201592767 2.985423807311 -0.254737560854 B -0.412876402938 8.329570389215 0.519115121236 H 2.922195106768 0.278139843812 -8.481777424297 B -1.636241203837 2.485510714247 0.018815234177	Н	2.243803418966	-2.600117729685	-2.341324086533	N	1.236399320419	-1.779197286531	-4.381620284438
H 2.007/202490044 -2.940996238614 6.217662525759 N -1.237860818476 1.780477536140 4.378852147211 H 2.440365583531 1.219578410753 -0.207357227103 N -1.237860818476 1.780477536140 4.378852147211 H 2.746542407936 -2.333665039138 -8.685043014646 7 H 2.629201592767 2.985423807311 -0.254737560854 B -0.412876402938 8.329570389215 0.519115121236 H 2.922195106768 0.278139843812 -8.481777424297 B -1.636241203837 2.485510714247 0.018815234177	н	2 504726240806	0.677648154674	-4 861443752370	N	-0.817930853487	-1 273804882500	-3 904578014020
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ц	2.304720249090	_2 040006238614	6 217662525750	IN NI	-1 237860818476	1 780477526140	4 378852147211
H 2.74550535351 1.21557610755 -0.207537227105 H 2.889631193217 4.937075658864 -5.148724153140 H 2.746542407936 -2.333665039138 -8.685043014646 H 2.629201592767 2.985423807311 -0.254737560854 H 2.922195106768 0.278139843812 -8.481777424297	ц	2.210224490444	1 210578/10752	-0.207357227102	18	1.23/0000104/0	1.700777550140	7.3/003217/211
II 2.887031173217 4.937073038004 -3.148724133140 II 2.746542407936 -2.333665039138 -8.685043014646 7 II 2.629201592767 2.985423807311 -0.254737560854 B -0.412876402938 8.329570389215 0.519115121236 II 2.922195106768 0.278139843812 -8.481777424297 B -1.636241203837 2.485510714247 0.018815234177	п п	2.770303363331	1.2175/0410/33	-0.20/33/22/103				
In 2./4034240/930 -2.333003039138 -8.063043014040 / H 2.629201592767 2.985423807311 -0.254737560854 B -0.412876402938 8.329570389215 0.519115121236 H 2.922195106768 0.278139843812 -8.481777424297 B -1.636241203837 2.485510714247 0.018815234177	H	2.009031193217	4.95/0/2028804	-3.140/24133140	7			
H 2.029201592/07 2.98542380/311 -0.254/3/500854 B -0.4128/6402938 8.329570389215 0.519115121236 H 2.922195106768 0.278139843812 -8.481777424297 B -1.636241203837 2.485510714247 0.018815234177	H	2.740542407936	-2.333003039138	-0.000043014046	1	0.410076400000	0.2205502215	0.510115101007
н 2.922195106768 0.278139843812 -8.481777424297 В -1.636241203837 2.485510714247 0.018815234177	H	2.629201592767	2.98542380/311	-0.254/5/560854	В	-0.4128/6402938	8.329570389215	0.519115121236
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